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Argonne National Laboratory

COLLECTED ALGORITHMS 1960-1963

from the

Communications of the Association
for Computing Machinery

by

R. E. Grench and H. C. Thacher, Jr.

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COLLECTED ALGORITHMS 1960-1963
from the
Communications of the Association
for Computing Machinery

Compiled and Edited by

R. E. Grench
Reactor Engineering Division
and
H. C. Thacher, Jr.
Reactor Physics Division

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COLLECTED ALGORITHMS 1960-1963

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R. E. Grench and H. C. Thacher, Jr.

I. INTRODUCTION

An algorithm may be defined* as "any method of computation consisting of a comparatively small number of steps; the steps to be taken in a preassigned order and usually involving iteration, which are specifically adapted to the solution of a problem of some particular type." Much of the effort of the casual computer user is devoted to developing and programming algorithms for relatively standard tasks, such as the evaluation of special functions, the solution of systems of linear equations, the estimation of definite integrals, sorting of data, and so forth. Even if he succeeds in finding a description of a suitable procedure, he must often spend considerable effort in translating the rather vague prescriptions of a prose description into a more or less complete computer subroutine.

Normal English prose and conventional mathematical notation are not only unacceptable for input to a computer, but also inconvenient for communicating the dynamic processes of computation from one individual to another. The international ALGOL language can satisfy both these needs. Although its use as a machine input language has grown rather slowly, at least in this country, it is the internationally accepted method of describing numerical calculations in most journals devoted to computation. Many papers describing original research on numerical methods now include an ALGOL program to specify the calculation which was performed. In addition, several journals now include columns of algorithms for common tasks, along with comments on previously published methods.

Among the journals in which algorithms appear more or less regularly are: Communications of the Association for Computing Machinery, BIT (Nordisk Tidskrift for Informations Behandling), Computer Bulletin, and Numerische Mathematik. The algorithms in Numerische Mathematik are outstanding from the standpoints of quality and careful editing. However, they are rather few in number. By far the widest variety of algorithms have been published in the Communications of the Association for Computing Machinery.

*The International Dictionary of Applied Mathematics, D. Van Nostrand Co., Inc., Princeton, 1960, p. 32.

In this report, we have collected and reprinted the first 220 algorithms published in this journal, between February 1960 and December 1963, with remarks and certifications pertaining to them which were published through 1964. These algorithms are those which were published while J. H. Wegstein was editor of the Algorithms column. For the benefit of readers who are unfamiliar with the ALGOL language, we have also reprinted a tutorial description of the language by H. R. Schwarz, originally published in the Communications of the Association for Computing Machinery. We wish to express our gratitude to the Association for Computing Machinery and to Dr. Schwarz for permission to reprint this copyrighted material.

II. SUGGESTIONS TO THE USER

The following suggestions are intended to aid the casual computer user who desires a guide in writing a subroutine for a particular task.

This volume includes two indexes: one by general subject, and one by author. In the first, prepared by G. E. Forsythe, the algorithms are arranged according to a modification of the SHARE classification. Having determined the classification which includes the task to be accomplished, a reference to this index will give the numbers and descriptive titles of algorithms in this area. The comments for each algorithm include a statement of what the algorithm accomplishes and a general description of the method used, often with a reference to a more extended discussion. The Certifications (results of tests of the algorithm) and Remarks which follow each algorithm, often contain very helpful information.

If several algorithms appear equally applicable, the user must make a choice. Although there is no substitute for a thorough knowledge of computing methods, or the advice of a qualified consultant, the following criteria may be helpful. (1) More recent algorithms are apt to represent improvements on earlier ones. (2) Wherever possible, use algorithms for which a certification appears. Many of the algorithms in this group were not certified before publication and contain more or less serious errors. The certifications also include numerical results which will be useful in testing your own program. (3) Certain algorithms are written recursively, i.e., call upon themselves. This type of programming is usually inefficient. Many ALGOL translators do not provide for this feature, and hand translation into other languages is usually quite difficult. Thus, recursive algorithms should be avoided if there is any other alternative.

Having selected an algorithm, the task remains of adapting it to the computing system available. If an ALGOL translator is included in your system, this may be fairly trivial. If only a less sophisticated language is provided, the task may be somewhat more tedious, because of the limitations of the target language. Thus, for example, the limitation of Fortran to positive integer subscripts frequently makes the resulting program appear clumsy. The article by Dr. Schwarz will provide more than sufficient instruction in the meaning of the ALGOL, and the ease of translation will depend principally upon the user's familiarity with the language which he is translating.

When the adaptation has been completed, the user should test his program as thoroughly as possible. Tests against the values given in Certifications and problem collections will not only insure against errors in transcription, but will also give an intuitive feeling for the behavior of the method which is often more useful than a rigorous mathematical treatment.

Testing is, of course, absolutely necessary for uncertified algorithms, where the user may have to contend with minor or major errors in the original program. If errors are discovered, their prompt dissemination by publication in the Communications of the Association for Computing Machinery is highly recommended.

An Introduction to ALGOL

H. R. SCHWARZ

Swiss Federal Institute of Technology, Zurich, Switzerland

1. Programming Languages in General

To solve a numerical problem with the use of a computer, the solution must be described in terms of the computer, i.e. in computer notation, before it can be given to the machine. Unfortunately, however, the computer notations are not only much different from classical mathematical notation but also different among themselves, and many of the difficulties of programming may be attributed to these variations.

Frequent attempts have been made to bridge the gap between computer and classical mathematical notation by devising notations somewhere between the two extremes in order to combine the advantages of both:

Such algorithmic notations, as we shall call them, have the appearance of classical mathematical notation but include certain dynamic elements which remind one of ordinary programming. Before explaining the technical details, however, let us review the historical facts. (More information may be found in [1, 2, 3].)

In 1951 Rutishauser worked out a notation for numerical processes which could have been translated into machine notation by the machine itself. Unfortunately this translation could not be done by the small relay computer Z4, which was then in operation in the Swiss Federal Institute. Moreover, the notation was somewhat clumsy and not very efficient, and therefore it was never used in practise. On the other hand, it did prove for the first time that programming could be made fully automatic.

*Comm. ACM 5 (Feb 1962), 82-95.

However, this early work [1] on automatic programming did not receive much attention until the FORTRAN system was announced. Shortly after that (more exactly, after the Darmstadt meeting on computing machines in 1955), a European group for automatic programming was formed that subsequently worked out an algorithmic notation which was ready for publication at the end of 1957. However, it was decided to hold back the publication and to try to discuss the subject with the ACM. In a joint conference of the ACM group with the GAMM group (GAMM was the official name of the European group mentioned above) which took place in May 1958 at Zurich, the two groups combined their proposals for algorithmic notations into one and thus ALGOL was born [4].

After the preliminary publication, much interest in the subject developed and the final result of further discussions and publications was the January 1960 Conference in Paris. At this conference a completely new version of ALGOL was created and its concept was published in [5].

Prior to the Paris Conference, Rutishauser held some lectures on the first version of ALGOL at the Summer Conference in Chapel Hill, N.C. from August 17 to 28, 1959. These lectures have been published [6], and the present paper represents an adaptation of them to ALGOL 60 in accordance with a suggestion at the Matrix Symposium held by SIAM in Gatlinburg, April 24-29, 1961.

I wish to acknowledge my indebtedness to Prof. H. Rutishauser for his generous support at that time, thus enabling me to write the present paper.

2. A First Look at ALGOL

By definition, ALGOL is a means of describing numerical processes in an easily readable form that is ready for automatic translation into a machine program. The description of a numerical method in terms of ALGOL is called the ALGOL program for the method. Such an ALGOL program consists of statements like the following:

$$x := 2 \times p \times q ; \quad y := 2 \times q \times q - p \times p$$

which mean that the variables on the left side of the symbol $:=$ should be given the values which result from the expressions on the right side. Further features allow one to describe repeated execution of a statement for several values of a subscript (subscripts are always written in square brackets):

$$h := 0 ;$$

$$\text{for } k := 1 \text{ step } 1 \text{ until } n \text{ do } h := h + a[k] \times b[k]$$

Here h obtains the value zero at the beginning; then for every k the product $a[k] \times b[k]$ is added to h ; thus at the end h is the inner product of the two vectors a and b . This example shows already that the for statement corresponds to a loop in ordinary programming. The treatment of nested loops is described later.

In computations, frequently operations must be carried out only if a certain condition is fulfilled; an example may illustrate the treatment of such cases in ALGOL:

```
if z < 0 then z := 0
```

Here z is unchanged if $z \geq 0$, because then the statement $z := 0$ is skipped. But if z is negative, z is replaced by zero; thus in the whole, the statement replaces z by $\text{Max}(0, z)$.

An additional feature is the label, which allows one to mark any statement of an ALGOL program. This may be used for referring to statements in explanations, but more important is the possibility to jump to such labeled statements. *Example:*

```

:
a33: x := p×x+q×y ;
:
go to a33
:
```

Here **a33** is a label and **go to a33** means an unconditional jump to the statement carrying that label; i.e. **go to** corresponds to the unconditional jump order in ordinary programming. Conditional jumps can be treated by combination of **if** and **go to** statements:

```
if x ≠ 0 then go to a33
```

Except for such **go to** statements (and conditional statements, which are explained later), the statements of an ALGOL program are carried out in sequence.

3. Variables and Expressions

In §2 we have given a preliminary description of some features of ALGOL. In order to enable the reader to make full use of ALGOL, exact definitions are given in the ALGOL report [5]. It is the purpose of this paper to give further explanations and examples in order to make the ALGOL report more familiar.

(a) The *basic symbols* from which ALGOL is built up are listed in (AR2).¹ The meanings of the operators need no further explanations, except $\neg$ and $\equiv$, which are the symbols for logical negation and equivalence.

(b) For another class of delimiters no symbols were available; therefore words had to be used in place of them. These words, which in handwriting and typewriting are always underlined and in printing are always set in boldface type, are called *word delimiters*; they have, like $\times$ and $+$, fixed meanings and should not be translated into other languages.

¹ In this way we shall cite sections of the ALGOL Report [5]: (AR2) refers to section 2.

(c) An important notion is the identifier **I**. An *identifier* is a string of letters and digits *that begins with a letter*. Thus **xe7c**, **p**, **a**, **p123** are identifiers, but **17** and **7ae** are not.

In ALGOL, identifiers are used as names of variables and other entities occurring in computations. They may be chosen quite freely. Thus a variable may be given a name like **vcrit** or **z2asymm**, and greek letters may be transcribed into "alpha" or "omega". However, no delimiters may be used within an identifier, e.g. **v-crit** is not allowed as an identifier, because it could not be distinguished from the difference of the variables **v** and **crit**.

Moreover, it should be kept in mind that some few combinations (see AR3.2.4) are already reserved as names of the elementary functions of analysis and should therefore not be used. But besides these exceptions, identifiers have no fixed meanings like the word delimiters, from which they are distinguished by the boldface type used for the latter.

(d) In (AR3 to 5), the rules are given for *building up* expressions, statements and declarations from the basic symbols. To understand these rules, let us consider an example:

(subscripted variable) ::= (array identifier) [(subscript list)]

(See AR3.1.1.) By applying the recursive syntactic definition, this example has the following meaning: A subscripted variable (collective abbreviation **V**) consists of an array identifier **I**, followed by a sequence of arithmetic expressions **E** in square brackets and separated by commas.

Examples:

a[**k**+1,**k**-**i**] ; **b**[0.5×(**i**+**k**)+0.5×**abs**(**i**-**k**)] ; **c**[**i**,3,**k**]

As the definition of **V** occurs in (AR3.1.1), expressions (which are admitted as subscripts) are not yet defined, but it is to be understood that anything is admitted as **E** that fits the definition of arithmetic expressions given later in (AR3.3) [see also below under (e)]. Since according to this definition arithmetic expressions may themselves contain subscripted variables, the following construction is allowed:

a[**u**[**k**],**v**[**k**],**w**[**u**[**j**],**v**[**j**]]]

In most cases, however, the subscript positions of subscripted variables will be occupied just by simple variables and integers (these are special cases of expressions).

(e) (AR3.3) shows the rules for the construction of *arithmetic expressions*, which are the backbone of ALGOL:

First, the syntactic rules in (AR3.3.1) define numbers, variables (simple or subscripted), and functions (to be defined later) as expressions. Thus, **17** and **a**[**k**] are expressions.

Second, any connection of expressions according to the rules of arithmetic (including exponentiation) is again an expression. Finally, an arbitrary expression, if enclosed in parentheses, is again an expression, i.e. one may write additional parentheses at will.

Third, in ALGOL even conditional arithmetic expressions are admitted, which means that according to a condition

one of two alternative expressions is chosen. An example may illustrate this feature:

(if $m < n$ then m else n)

Here the resulting value of that conditional expression is taken as m if m is less than n and as n in the opposite case. Thus the expression has the meaning of $\text{Min}(n, m)$.

The operational meaning of an expression is partially given by the composition rules; it is always the number which results if the expression is evaluated with the actual values of the occurring variables along the rules of ordinary arithmetic. There are, however, a few cases like $a/b/c$ where² the operational meaning must be defined by additional rules (so-called precedence rules). The precedence rules of ALGOL are given in (AR3.3.5.1).

(f) The definition of *Boolean expressions* (AR3.4) is quite analogous to the definition of arithmetic expressions, and the operational meaning can also be defined analogously. But, in addition, Boolean expressions are generated by arithmetic relations (equations and inequalities) of the general form: $E_1 \rho E_2$, where E_1 and E_2 are arithmetic expressions and ρ is any of the six relational operators. Thus,

$(a \vee b) \wedge (c \vee d)$
 $(u \neq 0) \wedge (v > w) \wedge (z = p)$ (the parentheses may
 $(a-b/2+p > 0) = g$ even be omitted)

are Boolean expressions. The operational meaning of $E_1 \rho E_2$ is

true, if the relation holds with the actual values of the variables occurring in E_1 and E_2 ;
false, if the relation does not hold.

A Boolean variable or expression cannot take values other than **true** or **false**.

(g) Since the general form of a function already uses the notion of parameter, general functions are therefore explained under procedures. *Functions* have the form $I_f(E, E, \dots, E)$, i.e. a function name I_f (an identifier) followed by a list of expressions in parentheses. The operational meaning is a single number (the value of the function). How this value is computed from the actual values of the expressions E must be defined by a corresponding procedure declaration (see §8.a).

(h) A *label* must be either an identifier or an integer; thus 17 and Ab7 are labels. Labels may be used to mark certain statements in an ALGOL program.

A *simple designational expression* may be either a label as defined above, or (formally) a variable with one single subscript position (a switch variable), i.e. L or $I[E]$. The operational meaning is in either case a label, namely L if the expression is already a label L , but if it is a switch

² Such situations should be avoided by writing a sufficient number of parentheses, but notwithstanding an operational meaning must be defined also for such expressions as long as they obey the composition rules formally.

variable $I[E]$ the operational meaning must be defined by a switch declaration for the identifier I (see §5.c).

As in the case of arithmetic expressions, *conditional designational expressions* are also admitted. *Example*:

if $k > n$ then 130 else $s[k]$

4. Statements

Expressions may be interpreted as orders to compute something according to given rules, but otherwise they have no independent dynamic meaning. Only the statements of ALGOL are essentially dynamic; they are the sentences of the language.

For statements we introduce the collective abbreviation S , which means that in all following composition rules any statement is admissible for an S , provided this is not explicitly forbidden.

(a) COMPOUND STATEMENTS AND BLOCKS (AR4.1)

Before defining the various kinds of statements, we refer to the possibility that any sequence of statements can be grouped together into one statement (which is then called a *compound statement*) just by enclosing them between the word delimiters **begin** and **end**:

begin S ; S ; ... ; S **end**

Such a compound statement³ S_c may be used in place of any S occurring in definitions of elements of ALGOL. It may be used also in the above definition; therefore some of the statements in a compound statement may already be compound, e.g.:

begin S ; S ; **begin** S ; S ; S ; S ; S **end end**

On the other hand, there is one restriction: Only statements and declarations (see below) may be enclosed between **begin** and **end**; therefore it is not permissible to group a sequence like

S ; S ; **begin** S ; S ; S

together into one compound statement, since **begin** is not a statement or declaration. In other words, if a statement S is at the same time part of two different statements S_c and S_{cc} , then either $S_c \subset S_{cc}$ or $S_{cc} \subset S_c$.

If a sequence of statements is preceded by some declarations D (see §5) and enclosed between **begin** and **end**, this combination is called a *block*. It is of the general form

begin D ; D ; ... ; D ; S ; S ; ... ; S ; S **end**

Such a block introduces a new level of nomenclature, which means that all declarations in the head of the block are only valid inside the block. Outside the block the declared quantities have no existence; thus they are said to be local quantities to the block.

On the other hand, each of the statements S above may again be a compound statement or a block. Thus the

³ Note that the statements are separated from each other by semicolons, but no semicolon is needed after **begin** or before **end**.

notion of *nonlocal entities* is introduced: An entity occurring in a block but not being declared inside this block is called nonlocal and represents the same quantity inside the block and at least in the level immediately outside it.

(b) ASSIGNMENT STATEMENT (AR4.2)

An assignment statement, $V := E$ for example, assigns a new value, namely the value of the expression E at the moment, to the variable V on the left side of the assignment symbol $:=$. It must be kept in mind that in contrast to classical mathematical notation an assignment like $x := x + E$ is meaningful in ALGOL, since this simply means that the value of x is increased by the actual value of the expression E .

The Boolean assignment statement is defined by analogy as $V := B$ where B is a Boolean expression and V is a Boolean variable. *Example:*

```
decide := (a = 0) = (b = 0)
```

This gives the variable "decide" the following value:

```
true,  if a = b = 0 or a × b ≠ 0
false, otherwise.
```

The assignment statement may be used also in an extended form: the same value of an expression may be assigned to several variables of the same declared type (see §5, type declarations). *Example:*

```
i := k := p := 1
```

This assignment statement gives the variables i , k and p (of type *real* or *integer*) the value 1.

(c) LABELED STATEMENTS

Any statement can be furnished with a label, which is written in front of the statement and separated from it by a colon. Thus

```
L : S
```

is a labeled statement and may be used in place of any S in the ALGOL definitions. *Example:*

```
15: begin a[k] := 1 + p × k ;
act:   b[k] := k - p
end
```

(d) GO TO STATEMENTS (AR4.3).

Go to statements interrupt the normal sequence of execution of statements. The statement

```
go to DL
```

where D^L is a designational expression, has the operational meaning of a jump to the statement whose label L' is defined by D^L . If D^L is already a label, then this is L' . But if D^L is a switch variable $I[E]$, then the label L' is the label in the k^{th} position of the switch declaration for the identifier I , where k is the integer nearest to the actual value of the expression E (see also the explanations for the switch declarations, §5.c, where an example also is given). If D^L is a conditional designational expression, the label L' is defined accordingly.

It must be kept in mind that after a jump to a statement $L : S$ has occurred, then, beginning with the statement

$L : S$, the statements are again carried out in sequence until a new jump takes place; but no automatic return to the origin of the jump will occur.

An exception has to be added: If the designational expression D^L is not defined, e.g. if the subscript expression of the switch variable lies outside the range from 1 to n , where n is the length of the switch variable, then the go to statement has no effect and the next following statement is carried out.

(e) IF STATEMENTS AND CONDITIONAL STATEMENTS (AR4.5)

The general form of an if statement is

```
if B then Suncond
```

where B is a Boolean variable or expression and S_{uncond} is an unconditional statement. It has the following operational meaning: The statement immediately following **if B then** is executed if and only if the actual value of B is **true**. Thus the if statement occurring in an ALGOL program changes the normal sequence of execution of statements only if the value of B is **false**; in that case the unconditional statement S_{uncond} is skipped, but no other change occurs. *Example:*

```
if k = 0 then
12: begin
    if z + a > 2 then go to 31 ;
13:   k := 0.5 ; z := z + delta ; r := 0
end
```

Here the statement immediately following **if k=0 then** is the compound statement with the label 12. Therefore in case $k \neq 0$ this compound statement is skipped as a whole and the computation is resumed after **end**. If $k=0$, then the compound statement, i.e. the single statements contained in it, are executed.⁴ If $z+a > 2$, then a jump to 31 occurs; otherwise, the three statements following label 13 are executed, after which the computation proceeds with the statement after **end**.

An extended form of an if statement is the conditional statement, which is of the general form:

```
if B then Suncond else S
```

Here B is a Boolean variable or expression, S_{uncond} an unconditional statement, and S an arbitrary statement, i.e. it may be itself a conditional statement. A conditional statement has the following operational meaning: According to the actual value of B one of the two alternative statements S_{uncond} and S is selected. If B has the value **true**, then S_{uncond} is executed and S is skipped; if B has the value **false**, then S_{uncond} is skipped and S is executed. Thus the normal sequence of statements is changed in any case by a conditional statement. *Example:*

```
14: if k ≠ n then
15:   begin z := z + 1 ; y := y / z end
    else
16:   y := y + x ;
17:   ...
```

⁴ A compound statement is unconditional regardless of the statements contained in it.

The same operational effect may be achieved by the following explanatory program:

```

14: if k ≠ n then
15:   begin z := z+1 ; y := y/z ; go to 17 end ;
16: y := y+x ;
17: ...

```

(f) FOR STATEMENTS (AR4.6)

The general form of a for statement is:

for V := ℓ do S

where ℓ represents a list of elements as defined below and S is any statement. The for statement causes the variable V (the running subscript) to run through the actual values of all expressions in the list in succession, and for every value of V the statement S will be executed exactly once. After exhaustion of the list, the normal sequence of execution is resumed, beginning with the statement after S.

In most cases an element of the for list ℓ will be given in the form

E_1 step E_2 until E_3

which is an abbreviation for $E_1, E_1+E_2, E_1+2E_2, \dots, E_1+nE_2$, where n is defined as the largest integer such that (for the actual values of the E's): $n \leq (E_3-E_1)/E_2$. If the resulting n is negative, then the list element is defined as empty; in this case the statement S is not carried out at all for that element.

However, this explanation does not cover the full generality of such an element and is only valid in the case where the arithmetic expressions E_2 and E_3 do not depend on variables changed during the execution of the statement S. A concise description of the operational meaning of the general form of such a for list element is given in (AR 4.6.4.2). *Example:*

for i := 1 step 1 until n do v[i] := 0

The components of a vector v are set to zero for the indices running from 1 to n.

In other cases a for list element may consist of a single arithmetic expression and a for statement may look like

for V := $E_1, E_2, \dots, E_n$ do S

where the E_k stand for arithmetic expressions. The statement S is executed n times while V has the values of $E_1, E_2, \dots, E_n$ consecutively. The values of the arithmetic expressions are computed and assigned to V just before the execution of the statement S. This fact may be important if one or several of the expressions E_k , except the first, depend on variables calculated inside the statement S. *Examples:*

```

for p := 0.1, 0.2, 0.5, 0.8, 0.9, 0.95 do S ;
for k := a, b, a+b do S

```

In the first example, the expressions in the list are only numbers. In the second example, S is executed for k having the values of a, b, and their sum.

A third kind of an element of the for list is the so-called **while** element. It has the general form

E while B

where E is an arithmetic and B a Boolean expression. The statement S which stands under control of such a **while** element is executed for the actual value of E assigned to the running variable V as many times as the Boolean expression B has the value **true**. *Example:*

```

100: x := 1 ; k := 0 ;
101: for k := k+1 while abs(x) > eps ∧ k ≤ n do
      begin v[k] := x := q×x ; m := k end ;
102: ...

```

The two statements labeled by 100 and 101 together have the operational effect that the components of a vector v are assigned the values of a geometric progression with quotient q and starting with $v[1] := q$. This is done as long as the elements of the geometric progression are greater than a tolerance eps and k does not exceed the value of n. In statement 102 (or following) the number m of assigned components is available.

It must be mentioned that the running variable V of a for statement is undefined when the loop is left, because of exhaustion of the for list. Thus no value of the variable k in the last example is available in statement 102 (or following); for this reason the running value of k is assigned to another variable m.

On the other hand, the actual value of the running subscript is defined outside the for statement if and only if the statement is left by a go to statement.

Example 1: A vector v is supposed to have strictly positive components. A program is established to check this assumption, and if it is not true, the index of the first negative component should be available:

```

50: for i := 1 step 1 until n do
51:   if v[i] ≤ 0 then go to nonpos ;
52: ...

```

If all components $v[i]$ are positive, then the computation goes on with statement 52. Otherwise, the for statement is left by the go to statement leading to the statement labeled nonpos. There i is defined and this information may be used.

The most general form of a for list is a concatenation of the three kinds of elements, separated by commas. Thus in the example,

for k := 1 step 1 until i-1, i+1 step 1 until n do S

the variable k runs from 1 to n in steps of 1 with the exception of i ($1 \leq i \leq n$). If i = 1, then the first element is considered to be empty and the same holds for the second element for i = n.

Example 2: Simultaneous computation of $f(x) = f$ and $f'(x) = f1$ for a polynomial $f(x) = \sum_{k=0}^n a[k]x^k$ with Horner's rule.

```

f := f1 := 0 ;
for k := n step -1 until 0 do
begin f1 := f1×x + f ; f := f×x + a[k] end

```

In this example, after setting the values $f = f1 = 0$, the compound statement consisting of the two statements $f1 := \dots$ and $f := \dots$ is executed n+1 times in succession, after which we have the required results.

This example shows that if several statements must be put under control of the same for clause (or the same if clause), they must be enclosed by **begin** and **end**.

(g) DUMMY STATEMENTS (AR4.4)

A dummy statement has no operational effect and acts like an empty order in ordinary programming. It is introduced by putting an additional semicolon. A dummy statement may serve to place a label at a place where it would not be allowed otherwise. *Example:*

```
20: for j := k+2 step 1 until n do
21:   begin alpha := a[j,k]/pivot ;
22:   if alpha = 0 then go to 25 ;
23:   for i := 1 step 1 until n do
24:     a[i,k+1] := -alpha×a[i,j] + a[i,k+1] ;
25:   end j
```

If $\alpha = 0$, then a go to statement refers to the end of the j-loop. The label "25" labels the dummy statement preceding **end j** and introduced by the semicolon at the end of statement 24.

5. Declarations

As explained in (AR5), declarations are interspersed in an ALGOL program to state certain facts. They are needed to make the program self-contained, so that no additional information is required and the computer may understand it. (On the other hand, the human reader of such a program might understand it in most cases without the declarations.) As already stated in §4.a, the declarations are only valid for the block in the head of which they stand.

(a) TYPE DECLARATIONS (AR5.1)

For any simple variable occurring in an ALGOL program a declaration concerning its type must be given. Three different types are possible: **real**, **integer**, **Boolean**. Examples of type declarations are:

```
real a, b, alpha, x, y, z ;
integer i, j, k, n, p ;
Boolean fi, decide, stop
```

If a quantity is declared to be of type **real**, this means that it may be given positive and negative real values including zero. If a quantity occurring in an ALGOL program is essentially integer, it should be declared so by an integer declaration. This has the following operational meaning: If for some reason a noninteger value is assigned to any of the variables listed in the declaration, this is immediately rounded to the nearest integer. But it should be understood that this rounding has only the purpose to round the value of an expression which is theoretically integer-valued to an exact integer, and not to replace the entier function.

Example: In the assignment statement

$$k := n \times (n+1) \times (n+2) / 6$$

the expression on the right side is integer-valued for all integers n , but the computed value may turn out to differ

by a small amount from an integer. If k is declared to be an integer, the value of the expression is in all cases corrected to the nearest integer.

It must be noted, however, that the actual values of expressions occurring in subscript positions are automatically (without integer declaration) rounded to the next integer, but this rounding concerns only the values of the expressions and has no effect whatsoever on the variables in these expressions.

A Boolean variable (taking only the values **true** and **false**) occurring in an ALGOL program must be declared so by a Boolean declaration. On the other hand, Boolean expressions, especially those which are generated by arithmetic relations $E_1 \rho E_2$, must not be declared as Boolean.

(b) ARRAY-DECLARATIONS (AR5.2)

For any subscripted variable occurring in an ALGOL program, exact bounds for the values of the subscripts must be given. This is done by array declarations, which must appear in the block for which they are valid. General form:

$$\text{array } I, I, \dots, I[\ell], I, I, \dots, I[\ell], I, \dots$$

In the list we have several groups of identifiers I , with each group followed by a list of subscript pairs in square brackets. The expressions of a subscript pair are separated by a colon and the pairs in the list are separated by commas.

Each group $I, I, \dots, I[\ell]$ indicates that the variables $I, I, \dots, I$ are subscripted variables with as many subscripts as there are pairs in the list ℓ . Moreover, the first expression of a pair gives the lower and the second expression the upper bound for the subscripts in the corresponding positions. Furthermore, these bounds are common for the group. It must be kept in mind that the expressions in the subscript pairs may depend only on variables which are non-local to the block in which the array declaration stands. Thus in the outermost block of a program the subscript bounds in array declarations must be constant.

All subscripted variables as declared by an array declaration above are understood to be of type **real**. If, on the other hand, the declared variables are of type **integer** or **Boolean**, the array declaration has to be preceded by the corresponding type declarator **integer** or **Boolean**. *Examples:*

```
array a, b [1:m, 1:n], x, y [1:n] ;
integer array p, q [1:n] ;
Boolean array fi [-1:1]
```

Here a and b are real variables with two subscripts each, the first running from 1 to m , the second from 1 to n (rectangular matrices), and x and y are real variables with one single subscript running from 1 to n . p and q are both integer-valued variables whose single subscript runs from 1 to n and fi is declared to be a Boolean variable.

REMARK CONCERNING own: Variables defined by type or array declarations may also be declared to preserve their values when the block is left by preceding the cor-

responding declarations by the declarator own. For further details, see (AR5).

(c) SWITCH DECLARATION (AR5.3)

General form:

switch I := $D_1^L, D_2^L, \dots, D_n^L$

where I is an identifier (the name of the switch) and the D_k^L are designational expressions (see §3.h). In most cases, the D_k^L will simply be labels. With this definition, **go to** I[E] has the operational meaning **go to** D_k^L , where k is the integer nearest to the actual value of E. But if the resulting k lies outside the interval $1 \leq k \leq n$ (n is the number of switch entries), the go to statement is skipped and the normal sequence of operation is resumed with the following statement.

Some of the D_k^L occurring in the switch declaration may again be of the form I[E], in which case we have multiple switches.

As an example, we lengthen the program for computing $f(x)$ and $f'(x)$ by Horner's rule (given as an example in §4.f) for $n \leq 3$:

```
a: begin
    switch Horner := p0, p1, p2, p3 ;
    f := f1 := 0 ;
    go to Horner [n+1] ;
p3: f := f×x + a[3] ; f1 := f1×x + f ;
p2: f := f×x + a[2] ; f1 := f1×x + f ;
p1: f := f×x + a[1] ; f1 := f1×x + f ;
p0: f := f×x + a[0]
end
```

If one tries to use this program for $n > 3$, then **go to** Horner [n+1] will not be executed, since Horner [n+1] is then outside the range of the switch declaration. Therefore the program should check whether $n > 3$ and should give an alarm, or a comment (see AR2.3) should be added to the example above in the form:

comment: This program should not be used for $n > 3$

6. Examples

Though the possibilities of writing programs are somewhat limited because we have not yet treated procedures, we shall give some examples here.

Example 1: The first example concerns the numerical integration of a differential equation of second order with given initial values. We choose the method of Adams' extrapolation, which consists of the following formulae:

$$y(x+h) = y(x) + hy'(x) + h^2[\frac{1}{2}y''(x) + \frac{1}{6}\nabla y''(x)$$

$$+ \frac{1}{8}\nabla^2 y''(x) + \dots]$$

$$y'(x+h) = y'(x) + h[y''(x) + \frac{1}{2}\nabla y''(x)$$

$$+ \frac{5}{12}\nabla^2 y''(x) + \dots]$$

where the $\nabla^k y''(x)$ are the backward differences of y'' at the point x and for the interval h. In contrast to other proposals, we start the integration by an iterative process (statements 2 to 8) which uses the same formulae as the forward integration (statements 10 onwards).

The quantities x_0, y_0, z_0, m, xE, h are supposed to be nonlocal to the block (which is thought of as a part of a larger program) and are therefore considered to be given at the moment of entering this block. Equally the variables x, y, z must be nonlocal quantities to the block, so that they are available outside the block as the final result of the computation.

begin

comment: x_0, y_0, z_0 are the initial values for x, y, y' . m is the order of the method, it must be chosen ≤ 6 . xE is the end of the integration, h is the integration step. $w[0]$ is the second derivative, $w[k]$ its k^{th} backward difference. The values of $x, y, z, w[k]$ for different values of x are not distinguished by a subscript ;

real we, p, q ; **integer** v, r, j ; **Boolean** beta, decide ;
array b, c, w [0:6] ;

```
1: b[0] := 1 ; c[0] := 0.5 ;
   b[1] := 0.5 ; c[1] := 1/6 ;
   b[2] := 5/12 ; c[2] := 1/8 ;
   b[3] := 3/8 ; c[3] := 19/180 ;
   b[4] := 251/720 ; c[4] := 3/32 ;
   b[5] := 95/288 ; c[5] := 863/10080 ;
   b[6] := 19087/60480 ; c[6] := 275/3456 ;
2: for v := 0 step 1 until m do w[v] := 0 ;
3: we := 1010 ; r := m ; decide := true ;
4: go to Adams ;
5: beta := (abs(w[m] - we) > 10-7) ; we := w[m] ;
6: for j := m step -1 until 1 do
7:   for v := 1 step 1 until m-1 do
     w[v] := w[v] - w[v+1] ;
8: if beta then go to 4 ;
9: r := (xE - x0)/h ; decide := false ;
Adams: begin
10: x := x0 ; y := y0 ; z := z0 ;
11: for j := 0 step 1 until r do
   begin
12:   if j = 0 then go to 14 ;
13:   for v := m-1 step -1 until 0 do w[v+1] := w[v] ;
14:   w[0] := f(x,y,z) ;
   comment: f is the function defining the differential
     equation y'' = f(w,y,z). A declaration for this function
     must be added at the top of the program ;
15:   if j = 0 then go to 17 ;
16:   for v := 1 step 1 until m do w[v] := w[v-1] - w[v] ;
17:   p := q := 0 ;
18:   for v := 0 step 1 until m do
19:     begin p := p + b[v]×w[v] ;
20:       q := q + c[v]×w[v]
     end v ;
21:   x := x+h ; y := y + h×(z+q×h) ; z := z + p×h
   end j ;
22: if decide then go to 5
   end Adams
end
```

This method is based on the following principle:

The leading row of backward differences (which are unknown at the beginning) is first filled out with zeros

⁵ It should be noted that between **end** and the next semicolon or next **end** or next **else**, any string of symbols may be written (but not containing **end**, **else** or a semicolon) without any effect on the computation. This serves solely to show the reader which compound statement is closed by the **end** in question, but the machine does not need this additional information.

(statement 2). With this leading row we integrate m steps ahead with the formulae of Adams (statement 4), since r in the compound statement Adams means the number of steps to be integrated. After this we may build up a new difference table from the m^{th} row backwards by keeping the m^{th} difference constant (statements 6 and 7).

In this way we obtain a new leading row of backward differences, with which we again integrate m steps forward. This is repeated until the m^{th} differences of two successive runs are nearly equal (statements 5 and 8; note that "we" is the m^{th} difference of the foregoing run). As soon as β is false, we start integrating ahead a sufficient number of steps to reach x_E (statements 10 and following).

Example 2: Computation of $\tan(x)$ with Lambert's continued fraction (1770).

Starting with $a[0] = 0$, $b[0]=b[1]=1$, $a[1]=x$, the recursion formulae (not in ALGOL!)

$$a[k+1] = (2k+1)a[k] - x^2a[k-1]$$

$$b[k+1] = (2k+1)b[k] - x^2b[k-1]$$

generate two sequences of numbers such that

$$\lim_{k \rightarrow \infty} a[k]/b[k] = \tan(x)$$

exists for any (also complex) x which is not an odd multiple of $\frac{1}{2}\pi$, but even for the poles the sequence behaves reasonably, since then the reciprocal values converge to zero. The continued fraction converges quite fast—even for $x=5$ (with two poles between x and the origin!) we obtain

$$a[12]/b[12] = -3.380\ 515\ 027\dots$$

in place of

$$\tan(5) = -3.380\ 515\ 006\dots$$

There is, however, one difficulty which arises frequently in setting up the program for a problem of that kind: we do not know how many steps it will take in general for x to reach a certain accuracy.⁶ On the other hand, numbers $a[k]$, $b[k]$ are generated by the process, for which subscript ranges must be declared in an array declaration, and for this the number of steps should be known.

However, in examples like this, where $a[k+1]$ and $b[k+1]$ depend only on a limited number of predecessors (general case: $a[k+1] = f(a[k], a[k-1], \dots, a[k-m])$ with fixed m), we may help ourselves by limiting the range of k to a finite interval J , and then, as soon as k reaches one end of J , begin again at the other end, so that $k+1$ and $k-m$ are always in J .

In this problem we would restrict k to the interval from 0 to 21, say, and then, as soon as k reaches 20, redefine $a[0] := a[20]$, $a[1] := a[21]$, and the same for b . If needed, we may combine this with a division of the four

⁶ In this example we can restrict x to a finite interval because of the periodicity of the function. This would also give a limit for k for a given accuracy. We do not make use of this possibility, since it might not exist in other cases.

numbers by the same constant in order to keep them in range.

The question remains of when to stop the computation. Without proof, I say that

$$\text{abs}(x^{2k+1}/(a[k+1] \times a[k] + b[k+1] \times b[k])) < 10^{-10}$$

is a useful criterion and will lead to about 10-digit accuracy. With this, the following ALGOL program results:

```
begin real h,y ; integer r,k ; array a,b,c,d[0:21] ;
1: a[0] := 0 ; b[0] := b[1] := 1 ; a[1] := c[1] := x ;
   y := x ↑ 2 ;
2: for r := 0 step 20 until 1010 do
   begin
3:   for k := 1 step 1 until 20 do
4:     begin
       a[k+1] := (2×(k+r)+1)×a[k] - y×a[k-1] ;
       b[k+1] := (2×(k+r)+1)×b[k] - y×b[k-1] ;
       c[k+1] := y×c[k] ;
       d[k+1] := a[k+1]×a[k] + b[k+1]×b[k] ;
5:     if abs(c[k+1]/d[k+1]) < 10-10 then go to 9
       end k ;
6:     h := abs(a[k+1]) + abs(b[k+1]) ;
7:     c[1] := c[21]/(h×h) ;
8:     a[0] := a[20]/h ; a[1] := a[21]/h ;
       b[0] := b[20]/h ; b[1] := b[21]/h
       end r ;
9:   t := a[k+1]/b[k+1]
   end
```

REMARK: The block is understood to be a part of a larger program. It uses the nonlocal quantities x (the argument) and t (the result $\tan(x)$).

Example 3: This example includes one of the permanent functions: Let $y[0], y[1], \dots, y[100]$ be 100 values of a function $y[k] = f(x_0 + kh)$; then for a given x in the interval $x_0 \leq x \leq x_0 + 100h$, $f(x)$ can be computed approximately by linear interpolation:

```
p := (x - x0)/h ; if p < 0 ∨ p > 100 then go to out of range ;
n := entier(p) ;
f := y[n] + (p-n)×(y[n+1] - y[n])
```

In this example no declarations are given for any of the variables. x_0 , x and h must be given. If the argument x lies outside the given range, the conditional go to statement leads to the statement labeled "out of range", where provision must be made for such a case.

7. Errors in an ALGOL Program

As in ordinary programming, one may make errors in writing an ALGOL program. These errors are more dangerous than in ordinary programming, since the whole translating process must be repeated if the generated machine program turns out to be wrong. Still worse is the effect of errors if such an ALGOL program is published. We distinguish several kinds of errors.

(a) SYNTACTICAL ERRORS

If an ALGOL program actually violates the composition rules, then it is called syntactically wrong. Such errors are in general already detected by the routine which should translate it into machine program. They may also

be found very easily by proofreading, since they are in most cases quite obvious. *Examples:*

Omission of one of a pair of brackets.

Omission of a **begin** or an **end**.

Two operation symbols in succession like $+ \times$.

Omission of a semicolon or other separating symbol.

An error happening sometimes is the omission of the multiplication symbol, since this is usual in mathematical notation, but not allowed in ALGOL.

Underlining of a word other than the word delimiters (see the list of those in AR2).

(b) OPERATIONAL ERRORS

By operational errors we mean errors which destroy the operational meaning of parts of a program. Such errors are much harder to detect; in most cases they will pass the translation routine, but the generated machine program will be defective. On the other hand, a careful reader will be able to detect these errors, even if he is not familiar with the problem to be solved.

Examples: (i) A variable occurs on the right side of an assignment statement dynamically before a value has been assigned to it, or the assignment for such a variable is bypassed by a jump:

```

:
if c = 0 then go to march ;
:
w := 1 + z ;
march: x := sqrt(w) ;
:

```

This is operationally meaningless for $c = 0$, if $w := 1 + z$ is the first statement involving w in that program.

(In the examples treated so far there are many cases where a variable occurs the first time [or exclusively] on the right side of an assignment statement, but those are input variables for which—in an actually used program—values will be assigned by input operations. These input operations have not been treated so far.)

(ii) A subscript exceeds the range which is prescribed by the array declaration.

(iii) A variable declared as Boolean occurs in an arithmetic expression or vice versa.

(c) PROGRAMMING ERRORS

It is of course still possible that a program is syntactically and operationally correct but all the same—because of an oversight—does not describe the numerical method which it should. No rules can be given to prevent errors of this kind. One can only check the ALGOL program carefully, and sometimes only a test run will detect an error. Quite tricky errors, which even a test computation will hardly detect, are those which only slow down the convergence of iteration methods without leading to wrong results.

8. Procedures

Procedures are the subroutines of ALGOL. Their purpose is the same as that of library subroutines of ordinary programming: they serve to simplify ALGOL programs.

As in ordinary programming, we distinguish between the description of a subroutine (procedure declaration) and the call or application of a subroutine (procedure statement or function call).

(a) PROCEDURE DECLARATION (see AR5.4)

A procedure declaration consists of a heading and the statement describing the procedure. The general form of the heading of a procedure declaration is:

procedure $I(p, p, \dots, p)$; **value** ℓ ; (specification part) ;

Here I is an identifier (the name of the procedure), the p 's are the formal parameters of the procedure (in the form of identifiers). In general, these parameters are separated by commas, but one may also replace a comma by a parameter delimiter of the form $)\lambda\lambda\dots\lambda:($ where λ stands for any letter. By inserting such parameter delimiters the meaning of the formal parameters may be explained. They do not have any operational effect.

In the value part, **value** ℓ ; , ℓ represents a list of those formal parameters which have to be treated as local quantities in the procedure body. Thus the operational effect of such a value part is the transfer of the values of all these listed parameters to storage places local in respect to the procedure body. If these formal parameters are assigned new values during execution of the procedure body, these values will not be available outside the procedure. As a consequence, formal parameters the values of which are wanted as results of the procedure must not be listed in the value part. Of course, the value part may be empty.

The specification part gives some information about the type and kind of the formal parameters. In most cases this additional information is not needed and the reader of the program could understand it without additional help, and thus these specifications are quite optional. However, there exist ALGOL translators (ALCOR hardware group) for which all formal parameters must be specified, and anyhow a procedure is easier to read if all specifications are given.

After the heading, the statement which follows is needed to describe the procedure. In general, the statement is a compound statement or even a block if local (temporary) quantities are declared.

Example 1: Computation of the inner product of two vectors a and b with n components each:

```

procedure innerproduct(a,b,n)result: (sigma) ;
  array a,b ; integer n ; real sigma ;
begin integer k ;
  sigma := 0 ;
  for k := 1 step 1 until n do
    sigma := sigma + a[k] × b[k]
end innerproduct

```

The procedure `innerproduct` has the property that it has only one output parameter which is a simple variable, i.e. it produces one single number. In such a case the procedure might be defined as a function by omitting the result parameter `sigma`. But then the output parameter

has to be given the name of the procedure and the procedure declaration must be preceded by a corresponding type declarator (see AR5.4.4):

```
real procedure scalarproduct(a,b,n) ;
  array a,b ; integer n ;
begin real sigma ; integer k ;
  sigma := 0 ;
  for k := 1 step 1 until n do
    sigma := sigma + a[k]×b[k] ;
  scalarproduct := sigma
end scalarproduct
```

REMARKS: Inside the procedure body at least one assignment statement for scalarproduct has to occur. But on the other hand, the variable scalarproduct must not appear on the right side of an assignment statement, because this would mean for its part an activation of the procedure scalarproduct. Therefore the auxiliary variable sigma has to be introduced.

In both examples the formal parameters a, b and n could be listed in the value part. But this is not necessary, because no new values are assigned to these parameters. In the first example, however, sigma must not appear in the value part.

Example 2: Gauss-elimination (without search for pivots) for the solution of $\sum_{k=1}^n a[i,k] \times x[k] + b[i] = 0$ ($i=1,2,\dots,n$). The input parameters are: the matrix $a[i,k]$, the constant terms $b[i]$, the number of equations n. The output parameter is: the solution $x[k]$.

If we denote the coefficients of the reduced equations of Gauss' method by the same identifiers a and b as the originally given elements, we obtain the following procedure:⁷

```
procedure Gauss(a,b,n)result : (x) ;
  array a,b,x ; integer n ;
  comment: The a[i,k] are the coefficients, the b[i] the constant
    terms of the equations  $\sum_{k=1}^n a[i,k] \times x[k] + b[i] = 0$ , and n is
    the number of equations ;
begin integer i,j,k ; real h ;
0: for i := 1 step 1 until n-1 do
1:   for j := i+1 step 1 until n do
2:     begin a[j,i] := -a[j,i]/a[i,i] ;
3:     for k := i+1 step 1 until n do
4:       a[j,k] := a[j,k] + a[j,i]×a[i,k] ;
5:     b[j] := b[j] + a[j,i]×b[i]
6:   end j ;
7: for i := n step -1 until 1 do
8:   begin h := b[i] ;
9:   for j := i+1 step 1 until n do
10:    h := h + x[j]×a[i,j] ;
11:   x[i] := -h/a[i,i]
12: end i
end Gauss
```

We distinguish the two parts: elimination proper (statements 0 to 4), and back substitution (statements 5 to 8). The procedure shows clearly the three typical loops of the elimination: The i-loop, beginning with 0 (counting

⁷ If the elements $a[i,k]$ and $b[i]$ should not be changed by the execution of the procedure, they should be listed in the value part.

the reduction steps), the j-loop, beginning with statement 1 (counting the rows in every reduction step) and the k-loop, beginning with statement 3 (counting the elements in one row of the matrix $a[i,k]$).

It must be noted that this program is not foolproof insofar as some of the $a[i,i]$ which appear as denominators in statements 2 and 8 may vanish (for positive definite symmetric matrices this cannot happen). Similar situations may arise also in other examples treated here.

(b) PROCEDURE STATEMENTS

General form:

$I(p,p,\dots,p)$

I is the name of the procedure and must coincide with the name in the corresponding procedure declaration; the p's are now the actual parameters. The types of the parameters—but not their names—must coincide with those in the corresponding procedure declaration (see the explanations and restrictions in (AR4.7.3 to 4.7.8)).

An example may show the application of the procedure statements:

Let $A = (a[i,k])$ be a matrix with n rows and p columns; we want to orthonormalize the columns, i.e. to decompose A as follows: $A = A_N R$, where A_N is a $(n \times p)$ -matrix with orthonormal columns and R a triangular $(p \times p)$ -matrix. Since $A^T A = R^T A_N^T A_N R = R^T R$, we could obtain R by triangular (Gauss-Cholesky) decomposition of the matrix $A^T A$. The following method is numerically safer, since it avoids the generally ill-conditioned matrix $A^T A$: (the elements of the resulting matrix A_N are again denoted by $a[i,k]$):

```
procedure orth(a,n,p)results : (a,r) ;
  array a,r ; integer n,p ;
  comment: n is the number of rows, p the number of columns
    of the  $(n \times p)$ -matrix a[i,k]. r[i,k] is an upper triangular
     $(p \times p)$ -matrix (zeros below the diagonal) ;
begin integer i,j,k,s ; real u ;
0: for k := 1 step 1 until p do
  begin
1:   for j := 1 step 1 until k-1 do
2:     begin
3:       r[j,k] := 0 ;
4:       for i := 1 step 1 until n do
5:         r[j,k] := r[j,k] + a[i,j]×a[i,k] ;
6:       for s := 1 step 1 until n do
7:         a[s,k] := a[s,k] - r[j,k]×a[s,j]
8:       end j ;
9:       u := 0 ;
10:      for i := 1 step 1 until n do u := u + a[i,k] ↑ 2 ;
11:      r[k,k] := sqrt(u) ;
12:      for s := 1 step 1 until n do
13:        a[s,k] := a[s,k]/r[k,k] ;
14:      for j := k+1 step 1 until p do r[j,k] := 0
15:    end k
16: end orth
```

k counts the number of reduction steps; in the k^{th} step already the $k-1$ first columns of $a[j,k]$ are orthonormal. Then for $j = 1,2,\dots,k-1$ the inner product of the k^{th} with the j^{th} column of $a[j,k]$ is computed (statements 2 and 3) and then the k^{th} column made orthogonal to the

j^{th} (statement 4). In statements 5 to 8, the k^{th} column is normalized and finally in statement 9, the subdiagonal zeros of the k^{th} column of the matrix $r[j,k]$ are filled in.

One sees that this program is itself written as a procedure. This should be done whenever a calculation is self-contained and general enough that it has a chance to be used later as a subroutine. Procedure *orth* certainly fits into this frame, because we can easily solve least square problems with it. The equations

$$\sum_{k=1}^p a[i,k] \times x[k] + v[i] = 0 \quad (i = 1, 2, \dots, n; \quad n \geq p)$$

are solved by

```

procedure lsq(a,v,n,p) results : (x,r) ;
  array a,v,r,x ; integer n,p ;
  comment: p is the number of unknowns, n the number of
    equations of the system  $\sum_{k=1}^p a[i,k] \times x[k] + v[i] = 0$  ( $i=1, \dots, n$ ),
    x[k] is the least square solution and r[k] the result of substituting
    this solution into the equations. The procedure should
    not be applied for  $p > n$  ;
  begin integer i,j,k,s ; real h ;
    array c[1:p,1:p], d[1:p] ;
  1: orth(a,n,p) results : (a,c) ;
  2: for k := 1 step 1 until p do
    begin
  3:   d[k] := 0 ;
    for i := 1 step 1 until n do
      d[k] := d[k] + a[i,k]  $\times$  v[i] ;
  4:   for s := 1 step 1 until n do
     v[s] := v[s] - d[k]  $\times$  a[s,k]
    end k ;
  5: for s := 1 step 1 until n do r[s] := v[s] ;
  6: for i := p step -1 until 1 do
    begin
  7:   h := d[i] ;
  8:   for j := p step -1 until i+1 do
     h := h + x[j]  $\times$  c[i,j] ;
  9:   x[i] := -h/c[i,i]
    end i
  end lsq

```

In this example we have in addition to the array specification in the heading (for the formal parameters) an array declaration at the beginning of the procedure body which concerns variables occurring only inside the procedure. It must be remembered that these variables are not available outside the procedure.

The example shows further that the names of parameters and variables in the procedure declaration are not determinative for the names to be used for the same quantities in the main program. In *lsq*, for instance, *r* denotes the residual vector of the least square solution which has nothing to do with the *r* occurring in the procedure declaration of *orth* and which in *lsq* is denoted by *c*.

In (AR5.4.6) the possibility of adding procedures expressed in machine language (machine oriented procedures) to ALGOL is indicated. In order to show what this may mean, we treat here the development of a function (given by an arbitrary rule for computing its values) into a series

of Chebyshev polynomials for a given interval [7]:

$$f(x) = \frac{1}{2}c_0 + \sum_{k=1}^{\infty} c_k T_k(x,a,b),$$

where

$$T_k(x,a,b) = \cos \left[n \times \arccos \frac{2x-a-b}{b-a} \right].$$

The $T_k(x,-1,1)$ are generally denoted by $T_k(x)$, the $T_k(x,0,1)$ by $T_k^*(x)$.

For $f(x) = 1/(1+3x)$ we have

$$f(x) = \frac{1}{2} + \sum_{k=1}^{\infty} 3^{-k} T_k(x,0,1)$$

which converges quite well in (0,1), whereas the power series diverges for $x \geq 1/3$.

The method of computing the coefficients c_k is given in many textbooks. Numerically we can proceed as follows: For an increasing number of n we compute the exact Newtonian interpolation polynomial for the following $n+1$ points (Chebyshev abscissae):

$$t_k = \frac{1}{2}(a+b) + \frac{1}{2}(b-a)x_k,$$

where

$$x_k = \cos(k\pi/n) \quad k = 0, 1, 2, \dots, n.$$

For these polynomials, the coefficients of the (finite) Chebyshev development are given explicitly as follows:

$$c_k = \frac{2}{n} \left[\frac{1}{2}f(t_0) + \sum_{s=1}^{n-1} f(t_s) x_{s \times k} + \frac{1}{2}(-1)^k f(t_n) \right].$$

Then we increase n until either an upper limits for n is reached, or two successive n 's yield approximately the same coefficients c_k . To avoid the latter happening accidentally when the computed c 's are still far from the true values, we compute the values of the function and the Chebyshev series at a random point in the interval (a,b).

Of course, n need not necessarily run through all integers, but only through a selection (approximately a geometrical sequence of quotient 1.25).

In order to obtain the Chebyshev abscissae for a given n in full machine accuracy, we presume that a machine-oriented procedure,

```

procedure cs(n) results : (x) ; integer n ; array x ;

```

is available, generating the values $x[k] = \cos(k\pi/n)$ for $k = 0, 1, \dots, 2n$. To obtain full machine accuracy special programming techniques are necessary, and thus it is impossible to express the computation in terms of ALGOL.

The same remark holds for the function *random* which generates a random or pseudorandom number lying in the open interval $-1 < \text{random} < 1$. This procedure

```

real procedure random ;

```

must also be available in machine notation. It should be noted that this is at the same time an example of a procedure which has no parameters.

Thus we obtain:

```

procedure Chebyshev(a,b,s,eps,phi,f)results : (c,n)exit : (non-
convergence) ;
  real a,b,eps ; integer s,n ; Boolean phi ;
  real procedure f ; array c ; label nonconvergence ;
  comment: a and b > a are the bounds for the interval. s is an
upper bound for the order up to which the coefficients must
be computed at most. eps is a tolerance for leaving the
procedure. phi decides whether the interpolation poly-
nomial of exact order s is wanted (phi = true) or the
infinite Chebyshev series (phi = false). f is the function to
be developed. c[k] are the coefficients wanted. n is the
order of the approximating polynomial used to meet the
requirements. If the upper bound s has proved insufficient
to fulfill the tolerance, then the procedure is left through
the emergency exit nonconvergence ;
begin real d,g,h,z,y,urandom ; integer k,alpha,v ;
  array x[0:2Xs], u[0:s], w[0:s+1] ;
  1: for k := 1 step 1 until s do c[k] := 0 ;
  2: if phi then n := s else n := 1 ;
  3: cs(n)results:(x) ;
  4: for k := 0 step 1 until n do
    u[k] := f((a+b + (b-a)Xx[k])/2) ;
  5: for k := 0,n do u[k] := u[k]/2 ;
  6: d := g := 0 ;
  7: for k := 0 step 1 until n do
    begin
  8:   g := g + abs(c[k]) ;
  9:   h := 0 ; alpha := 0 ;
  10:  for v := 0 step 1 until n do
    begin
  11:   h := h + x[alpha]Xu[v] ; alpha := alpha + k ;
  12:   if alpha ≥ 2Xn then alpha := alpha - 2Xn
    end v ;
  13:  z := 2Xh/n ; d := d + abs(z - c[k]) ; c[k] := z
    end k ;
  14: if phi then go to 25 ;
  15: y := random ;
  16: urandom := f((a+b + (b-a)Xy)/2) ;
  17: w[n] := w[n+1] := 0 ;
  18: for k := n-1 step -1 until 0 do
    w[k] := 2XyXw[k+1] - w[k+2] + c[k] ;
  19: d := d + abs(w[0] - yXw[1] - 0.5Xc[0] - urandom) ;
  20: g := g + abs(urandom) ;
  21: if d/g < eps then go to 25 ;
  22: if n = s then go to nonconvergence ;
  23: n := entier(1.25Xn + 2) ; if n > s then n := s ;
  24: go to 3 ;
  25: end Chebyshev

```

Explanations referring to the statement labels:

- 1: At the beginning all s+1 coefficients c[k] are filled in as zeros (in order that the comparison of two successive sets of coefficients be meaningful at the very beginning).
- 2: n is given its starting value according to the Boolean variable phi. If phi is **true**, then the interpolation polynomial of order s is wanted. In the opposite case the development is required and thus we start with n = 1 and increase later in statement 23.
- 3: Procedure statement for calculating the values $\cos(k\pi/n)$ as accurately as possible.
- 4: The values of the function f for the n+1 Chebyshev abscissae are computed; these values are called u[k].
- 5: The boundary values of the function are halved in order to simplify the summation in statement 10. This is an example where the running of the subscript is given by a list.
- 6: Initial values for the summations in statements 8, 13, 19 and 20.

- 7: The k-loop begins, k counting the coefficients c[k].
- 8: Summation of the values |c[k]|, where c[k] are the coefficients corresponding to the foregoing value of n. This summation is always meaningful, since the c[k] are defined up to k=s by virtue of statement 1.
- 9: Initial values for the computation of c[k]. Note that the two assignment statements cannot be combined into one because the two variables are of different type.
- 10-12: Summation in order to obtain the c[k]. Alpha is the quantity kXv reduced modulo 2Xn to the interval $0 \leq \alpha < 2Xn$.
- 13: An auxiliary variable z is assigned the new value of c[k]. Then the summation of the values |z - c[k]| takes place, where the c[k] is still the coefficient corresponding to the foregoing value of n. At last c[k] gets its computed value.
- 14: If the interpolation polynomial of exact order s was wanted (phi has the value **true**), the computation is finished and the procedure is left by the go to statement leading to the very end of the procedure.
- 15, 16: A random number denoted by y is generated by invoking the function random, and the function f is computed for a random point of the interval (a,b).
- 17, 18: Clenshaw's recursion formula for the evaluation of the Chebyshev series at the random point.
- 19: The absolute discrepancy of the function and the series at the random point is added to d.
- 20: Furthermore g is increased by the absolute value of the function at the random point.
- 21: If d/g, which is something like the relative error of the coefficients, fulfills the tolerance, then the procedure is left.
- 22: If, on the other hand, n has already reached its maximum value s (with phi = **false**), then the given tolerance is too small for the upper bound s, the process did not converge, and thus the procedure is left by the exit label nonconvergence.
- 23: If n < s and d/g > eps, then n is increased. Although n is declared to be an integer (by the specification in the procedure heading) the entier function should be used for rounding the expression. If the increased n exceeds s, then it is reduced.
- 24: After this we start anew with statement 3.
- 25: A dummy statement is introduced by the semicolon after the last statement in order to be able to put a label to which a go to statement (statements 14 and 21) can refer.

There remain a few words to be said about the application of such a procedure, because of the free function f and the exit label, nonconvergence, occurring in the declaration.

If in an ALGOL program the procedure is called by the statement

```

Chebyshev(-1,1,100,10-5,false)proc:(rho)result:(c,eta)exit:
(color)

```

then this means that the Chebyshev coefficients of the function rho must be computed for the interval (-1,1) with a tolerance of 10^{-5} and with an n equal at most to 100, and that the computation in case of nonconvergence has to proceed with the statement labeled with color (and not with the statement following the procedure statement). This requires that in the same ALGOL program there must be a statement with the label color and a function declaration for the function rho. The function must be defined by a type procedure declaration

```

real procedure rho(x) ; real x ;
.....

```

Without much explanation we give here the ALGOL program for the numerical inversion of matrices with the method of Gauss-Jordan as proposed by H. Rutishauser [8]. The program described uses pivotal search and exchange of the pivotal row and column with the k^{th} row and column. Thus in the k^{th} Jordan step the k^{th} diagonal element becomes the pivot. This makes the determination of the pivot in the remaining matrix simpler but makes a final reordering of the matrix necessary.

```

procedure gjr(a,n,eps) result : (a) exit : (singular) ;
  array a ; integer n ; real eps ; label singular ;
  comment : n is the order of the matrix a[i,k] to be inverted.
  eps is a tolerance for acceptance of the singularity of the
  given matrix and singular is the emergency exit in case of
  a singular matrix ;
begin integer i,j,k ; real pivot,z ;
  array b,c[1:n] ; integer array p,q[1:n] ;
  1: for k := 1 step 1 until n do
    begin
      comment : determination of the pivot element ;
      2: pivot := 0 ;
      3: for i := k step 1 until n do
        4: for j := k step 1 until n do
          5: if abs(a[i,j]) > abs(pivot) then
            6: begin pivot := a[i,j] ; p[k] := i ; q[k] := j
              end ;
        7: if abs(pivot) ≤ eps then go to singular ;
      comment : exchange of the pivotal row with the  $k^{\text{th}}$ 
      row ;
      8: if p[k] ≠ k then
        9: for j := 1 step 1 until n do
          10: begin z := a[p[k],j] ; a[p[k],j] := a[k,j] ;
            a[k,j] := z
          end j ;
      comment : exchange of the pivotal column with the  $k^{\text{th}}$ 
      column ;
      11: if q[k] ≠ k then
        12: for i := 1 step 1 until n do
          13: begin z := a[i,q[k]] ; a[i,q[k]] := a[i,k] ;
            a[i,k] := z
          end i ;
      comment : Jordan step ;
      14: for j := 1 step 1 until n do
        15: begin
          16: if j = k then
            17: begin b[j] := 1/pivot ; c[j] := 1 end
          else
            18: begin b[j] := -a[k,j]/pivot ; c[j] := a[j,k] end ;
          19: a[k,j] := a[j,k] := 0
          end j ;
        20: for i := 1 step 1 until n do
          21: for j := 1 step 1 until n do
            22: a[i,j] := a[i,j] + c[i] × b[j]
          end k ;
      comment : reordering of the matrix ;
      23: for k := n-1 step -1 until 1 do
        begin
          24: if p[k] ≠ k then
            25: for i := 1 step 1 until n do
              26: begin z := a[i,p[k]] ; a[i,p[k]] := a[i,k] ;
                a[i,k] := z
              end i ;
            27: if q[k] ≠ k then
              28: for j := 1 step 1 until n do
                29: begin z := a[q[k],j] ; a[q[k],j] := a[k,j] ;
                  a[k,j] := z
                end j
            end k
        end gjr

```

APPENDIX

9. Input-Output Operations

In the ALGOL report nothing is said about input-output operations. But each computation has to start with some initial values which depend on the specific problem to be treated and so have to be given through some input medium into the machine. On the other hand, the desired results of the computation have to be transmitted to the world outside of the machine by means of output installations. Therefore each ALGOL program which actually has to be run on a computer will necessarily contain statements concerning input and output operations. Such operations have not been treated so far in this paper, but they must be defined by procedures which of course have to be written in machine code (see AR5.4.6). Examples of such machine oriented procedures are:

(a) Suppose that there exists a standard input medium (paper tape, magnetic tape, cards) and that all input data needed by the program should be read in by this means. Thus the principal result of the procedure

real procedure read ;

will be the next following number standing on the input medium. Normally the procedure is applied in assignment statements like

n := read ; m := read ;

where the variables n and m are given their actual values.

(b) Suppose that there exists a typewriter for printing the results. Then a procedure for printing one value is for instance:

procedure print(V)

The procedure statement

print(a[i,k])

will cause the printing of the actual value of a[i,k].

Apart from the output procedure print(V) a procedure controlling the line feed of the typewriter might be desirable for listing the results. Thus we need, e.g.

procedure newline ;

An example may show the use of these three procedures. A matrix A = (a_{ik}) of order n should be inverted by applying the procedure gjr (see the end of §8):

```

begin integer n,i,j ; real eps ;
  n := read ; eps := read ;
  begin
    array a[1:n,1:n] ;
    for j := 1 step 1 until n do
      for i := 1 step 1 until n do
        a[i,j] := read ;
    gjr(a,n,eps) result:(a) exit:(indef) ;
    for j := 1 step 1 until n do
      begin newline ;
        for i := 1 step 1 until n do
          begin newline ; print(a[i,j]) end i
        end j ;
      go to omega ;
    indef: newline ; print(-1) ;
    omega: end
  end

```


The program assumes that the actual values of the order n , the tolerance ϵ and the elements of the matrix (column by column) are prepared on the input medium. In case of nonsingularity the inverted matrix is printed column by column, each column separated from the other by an additional empty space. Otherwise only the number -1 is printed to indicate the singularity of the given matrix.

Furthermore, the example uses four procedures as non-local quantities. How these procedures are entered in relation to the program depends very much on the internal organization of a computer and how the specific translator for it is built. But this compiler oriented question lies beyond the scope of the present paper.

Further and more complicated examples of input-output procedures can be invented according to the special equipment of the computer and the purpose which they have to fulfill. Even such input and output facilities which do not exist at the present time, but will be available in the future, can be handled by introducing appropriate procedures. Therefore it must be mentioned here that there is no need to introduce new elements to ALGOL for

such purposes, which might become obsolete as soon as new peripheral equipment is introduced.

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IV

COLLECTED ALGORITHMS

(in numerical order)

1. QUADI

R. J. Herbord

National Bureau of Standards, Washington 25, D. C.

comment QuadI is useful when integration of several functions of same limits at same time using same point rule is desired. The interval (a,b) is divided into m equal subintervals for an n-point quadrature integration. p is the number of functions to be integrated. w_k and u_k are normalized weights and abscissas respectively, where $k=1,2,3,\dots,n$. u_k must be in ascending order. $P(B,j) = (c)$ is a procedure which must be supplied by the programmer. It evaluates (c) the function (as indicated by j) for B. I_j is the result of integration for function j.;

procedure QuadI (a,b,m,n,p, $w_k,u_k,P(B,j) = (c)$) =: (Ij)

begin

QuadI: h := (b-a)/m

for j := 1(1)p ; $I_j := 0$

A := a-h/2

for i := 1(1)m

L1

begin A := A+h

for k := 1(1)n

L2

begin B := A+(h/2)× u_k

for j := 1(1)p

L3:

begin P(B,j) =: (c)

$I_j := I_j + w_k \times c$ **end** L3 ; **end** L2

end L1

for j := 1(1)p

$I_j := (h/2) \times I_j$

return

integer (j,k,i)

end QuadI

2. ROOTFINDER

J. Wegstein

National Bureau of Standards, Washington 25, D. C.

comment This procedure computes a value of $g=x$ satisfying the equation $x=f(x)$. The procedure calling statement gives the function, an initial approximation $a \neq 0$ to the root, and a tolerance parameter ϵ for determining the number of significant figures in the solution. This accelerated iteration or secant method is described by the author in *Communications*, June, 1958.;

procedure Root(f(), a, ϵ) =: (g)

begin

Root b := a ; c := f(b) ; g := c

if (c=a) ; **return**

d := a ; b := c ; e := c

Hob:

c := f(b)

g := (d×c-b×e)/(c-e-b+d)

if (abs((g-b)/g) ≤ ϵ) ; **return**

e := c ; d := b ; b := g ; **go to** Hob

end

CERTIFICATION

2. ROOTFINDER, J. Wegstein, *Communications ACM*, February, 1960

Henry C. Thacher, Jr.,* Argonne National Laboratory, Argonne, Illinois

Rootfinder was coded for the Royal-Precision LGP-30 Computer, using an interpretive floating point system with 28 bits of significance. The translation from ALGOL was made by hand. Provision was made to terminate the iteration after ten cycles if convergence had not been secured.

The program was tested against the following functions:

(1)	$f(x) = (x+1)^{1/3}$	(Root = 1.3247180)
(2)	$f(x) = \tan x$	
(3.α)	$f(x) = 2\pi\alpha + \tan^{-1} x$	(α = 1, 2, 3, 4)
(4.α)	$f(x) = \sinh \alpha x$	(α = -1.2, -0.5, 0.5, 1.2)

Selected results were as follows:

f(x)	α	ε	x_{k-1}	x_k	
1	1.3	10^{-7}	1.3247233	1.3258637	(1)
1	1.3	10^{-5}		1.3247165	(1)
2	5	10^{-3}	-.4674691	-.36021288	(1, 2)
2	4	10^{-3}	+.84880381	+.69496143	(1, 2)
3.1	1	10^{-5}		7.7252531	
3.2	2	10^{-5}		14.066155	
3.3	3	10^{-5}		20.371026	
3.4	4	10^{-5}		26.665767	

(1) No convergence after 10 iterations. Underlined figures are incorrect.

(2) For this function, $f'(0) = 1$; so convergence is not to be expected at this root. However, the algorithm did not find any other root.

It should be noted that the convergence criterion used fails for a zero root. The provision to terminate after a given number of cycles is therefore essential. Also, double precision is desirable.

REMARK ON ALGORITHM 2

ROOTFINDER (J. Wegstein, *Communications ACM*, February, 1960)

HENRY C. THACHER, JR.,* Argonne National Laboratory, Argonne, Illinois

$$\frac{y_k - Y}{y_{k-1} - Y} = \frac{(y_{k-2} - Y)f''}{2(f' - 1) + (y_{k-1} - y_{k-2})f''} + O(y_{k-1} - Y)^3$$

where Y is the desired root, and the derivatives f' and f'' are evaluated there. Convergence is thus second order, provided that $|f''| |y_{k-1} - Y| < 2 |f' - 1|$.

The algorithm is, however, somewhat unstable numerically because of the factor $f(y_{k-1}) - f(y_{k-2}) - y_{k-1} + y_{k-2}$ in the denominator.

Experience has shown that the minimum for ϵ is about one half the precision being used. Provision to indicate when round-off errors are causing random oscillations of g would be a desirable addition.

The criterion used for terminating the iteration renders the algorithm unsuitable for a zero root. A preliminary test for a zero root would be desirable. In addition, the algorithm should include provision for exit after a stated number of iterations.

Algorithm 15 appears to offer advantages along these lines.

* Work supported by the U. S. Atomic Energy Commission. This algorithm has the convergence factor

REMARKS ON ALGORITHMS 2 AND 3 (*Comm. ACM*, February 1960), ALGORITHM 15 (*Comm. ACM*, August 1960) AND ALGORITHMS 25 AND 26 (*Comm. ACM*, November 1960)

J. H. WILKINSON

National Physical Laboratory, Teddington.

Algorithms 2, 15, 25 and 26 were all concerned with the calculation of zeros of arbitrary functions by successive linear or quadratic interpolation. The main limiting factor on the accuracy attainable with such procedures is the condition of the method of evaluating the function in the neighbourhood of the zeros. It is this condition which should determine the tolerance which is allowed for the relative error. With a well-conditioned method of evaluation quite a strict convergence criterion will be met, even when the function has multiple roots.

For example, a real quadratic root solver (of a type similar to Algorithm 25) has been used on ACE to find the zeros of triple-diagonal matrices T having $t_{ii} = a_i$, $t_{i+1,i} = b_{i+1}$, $t_{i,i+1} = c_{i+1}$. As an extreme case I took $a_1 = a_2 = \dots = a_6 = 0$, $a_6 = a_7 = \dots = a_{10} = 1$, $a_{11} = 2$, $b_i = 1$, $c_i = 0$ so that the function which was being evaluated was $x^5(x-1)^5(x-2)$. In spite of the multiplicity of the roots, the answers obtained using floating-point arithmetic with a 46-bit mantissa had errors no greater than 2^{-4} . Results of similar accuracy have been obtained for the same problem using linear interpolation in place of the quadratic. This is because the method of evaluation which was used, the two-term recurrence relation for the leading principal minors, is a very well-conditioned method of evaluation. Knowing this, I was able to set a tolerance of 2^{-4} with confidence. If the same function had been evaluated from its explicit polynomial expansion, then a tolerance of about 2^{-7} would have been necessary and the multiple roots would have been obtained with very low accuracy.

To find the zero roots it is necessary to have an absolute tolerance for $|x_{r+1} - x_r|$ as well as the relative tolerance condition. It is undesirable that the preliminary detection of a zero root should be necessary. The great power of rootfinders of this type is that, since we are not saddled with the problem of calculating the derivative, we have great freedom of choice in evaluating the function itself. This freedom is encroached upon if we frame the rootfinder so that it finds the zeros of $x = f(x)$ since the true function $x - f(x)$ is arbitrarily separated into two parts. The formal advantage of using this formulation is very slight. Thus, in Certification 2 (June 1960), the calculation of the zeros of $x = \tan x$ was attempted. If the function $(-x + \tan x)$ were used with a general zero finder then, provided the method of evaluation was, for example

$$x = n\pi + y$$

$$\tan x - x = -n\pi + \frac{\frac{y^3}{3} - \frac{y^5}{30} - \dots}{\cos y},$$

the multiple zeros at $x = 0$ could be found as accurately as any of the others. With a slight modification of common sine and cosine routines, this could be evaluated as

$$-n\pi + \frac{(\sin y - y) - y(\cos y - 1)}{1 + (\cos y - 1)}$$

and the evaluation is then well-conditioned in the neighbourhood of $x = 0$. As regards the number of iterations needed, the restriction to 10 (Certification 2) is rather unreasonably small. For example, the direct evaluation of $x^\infty - 1$ is well conditioned, but starting with the values $x = 2$ and $x = 1.5$ a considerable

number of iterations are needed to find the root $x = 1$. Similarly a very large number are needed for Newton's method, starting with $x = 2$. If the time for evaluating the derivative is about the same as that for evaluating the function (often it is much longer), then linear interpolation is usually faster, and quadratic interpolation much faster, than Newton.

In all of the algorithms, including that for Bairstow, it is useful to have some criterion which limits the permissible change from one value of the independent variable to the next [1]. This condition is met to some extent in Algorithm 25 by the condition S4, that $\text{abs}(f_{\text{prt}}) < \text{abs}(x_2 \times 10)$, but here the limitation is placed on the permissible increase in the value of the function from one step to the next. Algorithms 3 and 25 have tolerances on the size of the function and on the size of the remainders r_1 and r_0 respectively. They are very difficult tolerances to assign since these quantities may take very small values without our wishing to accept the value of x as a root. In Algorithm 3 (*Comm. ACM* June 1960) it is useful to return to the original polynomial and to iterate with each of the computed factors. This eliminates the loss of accuracy which may occur if the factors are not found in increasing order. This presumably was the case in Certification 3 when the roots of $x^5 + 7x^4 + 5x^3 + 6x^2 + 3x + 2 = 0$ were attempted. On ACE, however, all roots of this polynomial were found very accurately and convergence was very fast using single-precision, but the roots emerged in increasing order. The reference to slow convergence is puzzling. On ACE, convergence was fast for all the initial approximations to p and q which were tried. When the initial approximations used were such that the real root $x = -6.3509936103$ and the spurious zero were found first, the remaining two quadratic factors were of lower accuracy, though this was, of course, rectified by iteration in the original polynomial. When either of the other two factors was found first, then all factors were fully accurate even without iteration in the original polynomial [1].

REFERENCE

- [1] J. H. WILKINSON. The evaluation of the zeros of ill-conditioned polynomials Parts I and II. *Num. Math.* 1 (1959), 150-180.

3. SOLUTION OF POLYNOMIAL EQUATION BY BAIRSTOW-HITCHCOCK METHOD

A. A. GRAU

Oak Ridge National Laboratory, Oak Ridge, Tenn. —

procedure

BAIRSTOW (n, a[, eps0, eps1, eps2, eps3, K] = :
(m, x[, y[, nat[, ex[]]);

comment The Bairstow-Hitchcock iteration is used to find successively pairs of roots of a polynomial equation of degree n with coefficients a_i ($i = 0, 1, \dots, n$) where a_n is the constant term. On exit from the procedure, m is the number of pairs of roots found, $x[i]$ and $y[i]$ ($i = 1, \dots, m$) are a pair of real roots if $\text{nat}[i] = 1$, the real and imaginary parts of a complex pair if $\text{nat}[i] = -1$, and $\text{ex}[i]$ indicates which of the following conditions was met to exit from the iteration loop in finding this pair:

1. Remainders, r_1 , r_0 , become absolutely less than eps1 .
2. Corrections, incrp , incrq , become absolutely less than eps2 .

3. The ratios, incrp/p , incrq/q , become absolutely less than eps3 .

4. The number of iterations becomes K .

In the last case, the pair of roots found is not reliable and no further effort to find additional roots is made. The quantity eps0 is used as a lower bound for the denominator in the expressions from which incrp and incrq are found;

```

begin
integer      (i, j, k, n1, n2, m1) ;
array        (b, c[0 : n+1]) ;
BAIRSTOW    for i := 0(1)n ; bi := ai
              bn+1 := 0 ; n2 := entire((n+1)/2)
              n1 := 2×n2
              for m1 := 1(1)n2 ; begin p := 0 ; q := 0
step:         for k := 1(1)K ; begin
              for i := 0(1)n1 ; ci := bi
              for j := n1-2, n1-4 ; begin
              for i := 0(1)j ; begin
              ci+1 := ci+1 - p × ci
              ci+2 := ci+2 - q × ci end end
              r0 := cn1 ; r1 := cn1-1
              s0 := cn1-2 ; s1 := cn1-3
              v0 := -q × s1 ; v1 := s0 - s1 × p
              det0 := v1 × s0 - v0 × s1
              if (abs(det0) < eps0) ; begin
              p := p+1 ; q := q+1 ; go to step end
              det1 := s0 × r1 - s1 × r0
              det2 := r0 × v1 - v0 × s1
              incrp := det1/det0 ; incrq := det2/det0
              p := p + incrp ; q := q + incrq
              if (abs(r0) < eps1) ; begin
              if (abs(r1) < eps1) ; begin
              exm1 := 1 ; go to next end end
              if (abs(incrp) < eps2) ; begin
              if (abs(incrq) < eps2) ; begin
              exm1 := 2 ; go to next end end
              if (abs(incrp/p) < eps3) ; begin
              if (abs(incrq/q) < eps3) ; begin
              exm1 := 3 ; go to next end end end
              exm1 := 4
next:         S := p/2 ; T := S2 - q
              if (T ≥ 0) ; begin T := sqrt(T)
              natm1 := 1 ; xm1 := S + T
              ym1 := S - T end
              if (T < 0) ; begin natm1 := -1 ; xm1 := S
              ym1 := sqrt(-T) end
              if (exm1 := 4) ; go to out
              for j := 0(1)(n1-2) ; begin
              bj+1 := bj+1 - p × bj
              bj+2 := bj+2 - q × bj ; end
              n1 := n1 - 2 ; if (n1 < 1)
out:          begin m := m1 ; return end
              if (n1 < 3) ; begin
              m1 := m1 + 1 ; exm1 := 1
              p := b1/b0 ; q := b2/b0
              go to next end
end end

```

CERTIFICATION

3. SOLUTION OF POLYNOMIAL EQUATION BY BAIRSTOW-HITCHCOCK METHOD, A. A. Grau, *Communications ACM*, February, 1960.

Henry C. Thacher, Jr.,* Argonne National Laboratory, Argonne, Illinois.

Bairstow was coded for the Royal-Precision LGP-30 computer, using an interpretive floating point system (24.2) with 28 bits of significance. The translation from ALGOL was made by hand.

The following minor corrections were found necessary.

a. $\text{det } 2 := r0 \times v1 - v0 \times s1$ should be $\text{det } 2 := r0 \times v1 - v0 \times r1$

b. $S := p/2$ should be $S := -p/2$.

After these were made, the program ran smoothly for the following equations:

$$x^4 - 3x^3 + 20x^2 + 44x + 43 = 0 \quad x = -.97063897 \pm 1.0058076i$$

$$x = -2.4706390 \pm 4.6405330i$$

$$x^6 - 2x^5 + 2x^4 + x^3 + 6x^2 - 6x + 8 = 0$$

$$x = 0.50000000 \pm 0.86602539i$$

$$x = 1.00000000 \pm 1.0000000i$$

$$x = 1.50000000 \pm 1.3228756i$$

$$x^5 + x^4 - 8x^3 - 16x^2 + 7x + 15 = 0$$

$$x = .000000005, ** - 0.99999999$$

$$x = 3.0000000, 0.99999999$$

$$x = -2.00000000 \pm 1.0000000i$$

With the equation $x^5 + 7x^4 + 5x^3 + 6x^2 + 3x + 2 = 0$ convergence was slow, and full accuracy was not obtained. However, the equation with reciprocal roots, $2x^5 + 3x^4 + 6x^3 + 5x^2 + 7x + 1 = 0$, converged rapidly.

* Work supported by the U. S. Atomic Energy Commission.

** Spurious zero real roots are introduced for equations of odd order.

CERTIFICATION OF ALGORITHM 3
SOLUTION OF POLYNOMIAL EQUATION BY
BAIRSTOW-HITCHCOCK (A. A. Grau, *Comm. ACM*
Feb. 1960)

JOHN HERNDON

Stanford Research Institute, Menlo Park, California

Bairstow was transliterated into BALGOL and tested on the Burroughs 220. The corrections supplied by Thatcher, *Comm. ACM*, June 1960, were incorporated. Results were correct for equations for which the method is suitable. $x^4 - 16 = 0$ is one of those which gave nonsensical results. Seven-digit results were obtained for 12 test equations, one of which was $x^6 - 2x^5 + 2x^4 + x^3 + 6x^2 - 6x + 8 = 0$.

CERTIFICATION OF ALGORITHM 3 SOLUTION OF POLYNOMIAL EQUATIONS BY BAIRSTOW HITCHCOCK METHOD (A. A. Grau, *Comm. ACM*, February, 1960)

JAMES S. VANDERGRAFT
Stanford University, Stanford, California

Bairstow was coded for the Burroughs 220 computer using the Burroughs ALGOL. Conversion from ALGOL 60 was made by hand on a statement-for-statement basis. The integer declaration had to be extended to include n, k, n, NAT, EX, and the corrections noted in the certification by Henry C. Thacher, Jr., *Communications ACM*, June, 1960, were incorporated.

By selecting the input parameters carefully, all branches of the routine were tested and the program ran smoothly. The following polynomials equations were solved:

$$\begin{aligned}x^5 - 14x^4 + 49x^2 - 36 &= 0, x = \pm 1.0000000 \\&x = \pm 1.9999998 \\&x = \pm 3.0000001 \\x^5 - 30x^4 + 273x^3 - 820x^2 + 576 &= 0, x = \pm 1.0000000 \\&x = \pm 2.0000000 \\&x = \pm 2.9999999 \\&x = \pm 4.0000001\end{aligned}$$

Several minor errors were found in the certification by Mr. Thacher. The constant term in the first polynomial should be 54 instead of 43, the second pair of roots for that polynomial should be $+ 2.470639 \pm 4.6405330i$, and the second pair of roots for the second polynomial should be $-1.0 \pm i$.

SEE REMARKS ALGORITHM 2

4. BISECTION ROUTINE

S. Gorn

University of Pennsylvania Computer Center
Philadelphia, Pa.

comment This procedure evaluates a function at the end-points of a real interval, switching to an error exit (fools exit) FLSXT if there is no change of sign. Otherwise it finds a root by iterated bisection and evaluation at the midpoint, halting if either the value of the function is less than the free variable ϵ or two successive approximations of the root differ by less than $\epsilon 1$. ϵ should be chosen of the order of error in evaluating the function (otherwise time would be wasted), and $\epsilon 1$ of the order of desired accuracy. $\epsilon 1$ must not be less than two units in the last place carried by the machine or else indefinite cycling will occur due to round-off on bisection. Although this method is of 0 order, and therefore among the slowest, it is applicable to any continuous function. The fact that no differentiability conditions have to be checked makes it, therefore, an 'old work-horse' among routines for finding real roots which have already been isolated. The free variables $y1$ and $y2$ are (presumably) the end-points of an interval within which there is an odd number of roots of the real function F . α is the temporary exit for the evaluation of F ;

procedure Bisecc($y1, y2, \epsilon, \epsilon 1, F()$, FLSXT) =: (x)

begin

Bisecc: $i := 1$; $j := 1$; $k := 1$; $x := y2$
 α : $f := F(x)$; **if** ($\text{abs}(f) \leq \epsilon$) ; **return**
go to γ_1

First val: $i := 2$; $f1 := f$; $x := y1$; **go to** α
Succ val: **if** ($\text{sign}(f) = \text{sign}(f1)$) ; **go to** δ_i ; **go to** γ_1
Sec val: $j := 2$; $k := 2$
Midpoint: $x := y1/2 + y2/2$; **go to** α
Reg δ : $y2 := x$
Precision: **if** ($\text{abs}(y1 - y2) \geq \epsilon 1$) ; **go to** Midpoint
return
Reg γ : $y1 := x$; **go to** Precision
integer (i, j, k)
switch $\gamma :=$ (First val, Succ val)
switch $\delta :=$ (FLSXT, Reg δ)
switch $\gamma :=$ (Sec val, Reg γ)

end Bisecc

CERTIFICATION OF ALGORITHM 4 BISECTION ROUTINE (S. Gorn, *Comm. ACM*, March 1960)

PATTY JANE RADER,* Argonne National Laboratory,
Argonne, Illinois

BISEC was coded for the Royal-Precision LCP-30 computer, using an interpretive floating point system (24.2) with 28 bits of significance.

The following minor correction was found necessary.

α : **go to** γ_1 should be **go to** γ_1

After this correction was made, the program ran smoothly for $F(x) = \cos x$, using the following parameters:

y_1	y_2	ϵ	α	Results
0	1	.001	.001	FLSXT
0	2	.001	.001	1.5703
1.5	2	.001	.001	1.5703
1.55	2	.1	.1	1.5500
1.5	2	.001	.1	1.5625

These combinations test all loops of the program.

5. BESSEL FUNCTION I, SERIES EXPANSION

Dorothea S. Clarke

General Electric Co., FPLD, Cincinnati 15, Ohio

comment Compute the Bessel function $I_n(X)$ when n and X are within the bounds of the series expansion. The procedure calling statement gives n , X and an absolute tolerance δ for determining the point at which the terms of the summation become insignificant. Special case: $I_0(0) = 1$;

$I(n, X, \delta) =: (Is)$

procedure
begin

I : $s := 0$; $\text{sum} := 0$
if ($n \neq 0$) ; **go to** STRT
if ($X = 0$) ; **begin** $Is := 1$; **return end**
 $\text{summ} := 1$; **go to** SURE

STRT:

if ($s = 0$) ; **go to** HRE
for

$t := 1(1)s$
 $\text{sfac} := \text{sfac} \times t$
HRE: $\text{snfac} := \text{sfac}$
for $t := s + 1(1)s + n$
 $\text{snfac} := \text{snfac} \times t$
 $\text{summ} := \text{sum} + (X/2)^{n+2s} / (\text{sfac} \times \text{snfac})$

SURE: **if**

($\delta < \text{abs}(\text{summ} - \text{sum})$)
 $s := s + 1$; $\text{sum} := \text{summ}$; **go to** STRT **end**
 $Is := \text{summ}$; **return**

end

6. BESSEL FUNCTION I, ASYMPTOTIC EXPANSION

Dorothea S. Clarke
General Electric Co., FPLD, Cincinnati 15, Ohio

comment Compute the Bessel Function $I_n(X)$ when n and X are within the bounds of the asymptotic expansion. The procedure calling statement gives n , X and an absolute tolerance δ for determining the point at which the terms of the summation become insignificant;

procedure $I(n, X, \delta) = (IA)$

begin

$I:$ $r := 1$; $pe := (4 \times n^2 - 1) / (8 \times X)$
 $sum := -pe$

Repeat: $r := r + 1$
 $pe := pe \times ((2 \times n)^2 - (2 \times r - 1)^2) / (r \times 8 \times X)$
 $(\delta < abs(pe))$

if $sum := sum + (-1)^r \times pe$; **go to Repeat** **end**

begin $IA := (1 + sum) \times (exp(X) / sqrt(2 \times \pi \times X))$
return

end

7. EUCLIDIAN ALGORITHM

Robert Claussen
General Electric Co., Cincinnati 15, Ohio

comment Every pair of numbers a , b not both zero have a positive greatest common divisor: gcd;

procedure $EUC(a, b) = (gcd)$

begin

$EUC:$

if $(a = 0)$
begin $gcd := b$; **return end**

if $(b = 0)$
begin $gcd := a$; **return end**

$r2 := a$
 $r1 := b$

here: $g := r2 / r1$

comment Assumption is made that truncation takes place in the above statement;
 $r := r2 - r1 \times g$
 $(r = 0)$

if $gcd := r1$; **return end**

begin $r2 := r1$
 $r1 := r$
go to here end

integer (g)

end

ALGORITHM 8

EULER SUMMATION

3 (May 1960), 318 P. NAUR

procedure $euler(fct, sum, eps, tim)$; **value** eps, tim ;
integer tim ; **real procedure** fct ; **real** sum, eps ;
comment $euler$ computes the sum of $fct(i)$ for i from zero up to infinity by means of a suitably refined euler transformation. The summation is stopped as soon as tim times in succession the absolute value of the terms of the transformed series are found to be less than eps . Hence, one should provide a function fct with one integer argument, an upper bound eps , and an integer tim . The output is the sum sum . $euler$ is particularly efficient in the case of a slowly convergent or divergent alternating series ;

```
begin integer i, k, n, t ; array m[0:15] ; real mn, mp, ds ;
i := n := t := 0 ; m[0] := fct(0) ; sum := m[0]/2 ;
nextterm: i := i+1 ; mn := fct(i) ;
for k := 0 step 1 until n do
begin mp := (mn+m[k])/2 ; m[k] := mn ;
mn := mp end means ;
if (abs(mn) < abs(m[n])) ^ (n < 15) then
begin ds := mn/2 ; n := n+1 ; m[n] :=
mn end accept
else ds := mn ;
sum := sum + ds ;
if abs(ds) < eps then t := t+1 else t := 0 ;
if t < tim then go to nextterm
end euler
```

CERTIFICATION OF ALGORITHM 8

EULER SUMMATION [P. Naur et al. *Comm. ACM* 3, May 1960]

HENRY C. THACHER, JR.*
Argonne National Laboratory, Argonne, Ill.
* Work supported by the U. S. Atomic Energy Commission

The body of *euler* was tested on the LGP-30 computer using the Dartmouth SCALP translator. No errors were detected.

The program gave excellent results when used to derive the coefficients for the expansion of $\ln(1+x)$ in shifted Chebyshev polynomials from the first ten terms of the power series. For $n = 0, 1, 2, 3, 4$, the coefficient of x^i in the power series was multiplied by the coefficient of $T_n^*(x)$ in the expression of x^i in terms of the $T_n^*(x)$. The product, for $i = 1, 2, \dots, 10$ was used as $fct(i)$ in the program. Results for $n = 0$ were as follows:

i	$fct(i)$	ds	sum
1	+0.50000000	—	—
2	-0.18750000	+0.07812500	+0.3281250
3	+0.10416667	+0.05729166	+0.3854167
4	-0.068359375	-0.005940758	+0.3794759
5	+0.049218750	-0.001928713	+0.3775471
6	-0.037597656	-0.001357019	+0.3761900
7	+0.029924665	+0.0001742393	+0.3763642
8	-0.024547577	+0.0000571311	+0.3764212
9	+0.020607842	+0.0000395427	+0.3764607
10	-0.017619705	-0.0000055069	+0.3764551
True Value ¹			+0.3764528129.....

Errors less than 0.2×10^{-8} were also found for $n = 1, 2, 3, 4, 5, 6, 7, 8$ and 9

This technique appears to be a useful supplement to direct telescoping (Algorithms 37 and 38) and to the methods recommended by Clenshaw¹, for slowly convergent power series.

¹ Clenshaw, C. W., *Chebyshev Series for Mathematical Functions*. National Physical Laboratory Math Tables, Vol. 5, London, H.M.S.O. (1962).

ALGORITHM 9 RUNGE-KUTTA INTEGRATION

3 (May 1960), 318 P. NAUR

procedure $RK(x, y, n, FKT, eps, eta, xE, yE, fi)$; **value** x, y ;
integer n ; **Boolean** fi ; **real** x, eps, eta, xE ; **array** y, yE ; **procedure** FKT ;
comment : RK integrates the system $y_k' = f_k(x, y_1, y_2, \dots, y_n)$ ($k = 1, 2, \dots, n$) of differential equations with the method of Runge-Kutta with automatic search for appropriate length of integration step. Parameters are: The initial values x and $y[k]$ for x and the unknown functions $y_k(x)$. The order n of the system. The procedure $FKT(x, y, n, z)$ which represents the system to be integrated, i.e. the set of functions f_k . The tolerance values eps and eta which

govern the accuracy of the numerical integration. The end of the integration interval x_E . The output parameter y_E which represents the solution at $x=x_E$. The Boolean variable fi , which must always be given the value **true** for an isolated or first entry into RK. If however the functions y must be available at several mesh-points $x_0, x_1, \dots, x_n$, then the procedure must be called repeatedly (with $x=x_k, x_E=x_{k+1}$, for $k=0, 1, \dots, n-1$) and then the later calls may occur with $fi=false$ which saves computing time. The input parameters of FKT must be x, y, n , the output parameter z represents the set of derivatives $z[k]=f_k(x, y[1], y[2], \dots, y[n])$ for x and the actual y 's. A procedure comp enters as a non-local identifier ;

begin

```
array z,y1,y2,y3[1:n] ; real x1,x2,x3,H ; Boolean out ;
integer k,j ; own real s,Hs ;
```

```
procedure RK1ST(x,y,h,x_e,y_e) ; real x,h,x_e ; array
y,y_e ;
```

```
comment : RK1ST integrates one single RUNGE-KUTTA
with initial values  $x, y[k]$  which yields the output
parameters  $x_e=x+h$  and  $y_e[k]$ , the latter being the
solution at  $x_e$ . Important: the parameters  $n, FKT, z$ 
enter RK1ST as nonlocal entities ;
```

begin

```
array w[1:n], a[1:5] ; integer k,j ;
a[1] := a[2] := a[5] := h/2 ; a[3] := a[4] := h ;
x_e := x ;
for k := 1 step 1 until n do y_e[k] := w[k] := y[k] ;
for j := 1 step 1 until 4 do
```

begin

```
FKT(x_e,w,n,z) ;
x_e := x+a[j] ;
for k := 1 step 1 until n do
begin
w[k] := y[k]+a[j]*z[k] ;
y_e[k] := y_e[k] + a[j+1]*z[k]/3
end k
end j
```

end RK1ST ;

Begin of program:

```
if fi then begin H := x_E - x ; s := 0 end else H := Hs ;
out := false ;
```

AA: if $(x+2.01 \times H - x_E) > 0 \equiv (H > 0)$ then

```
begin Hs := H ; out := true ; H := (x_E - x)/2
end if ;
```

```
RK1ST(x,y,2 \times H,x1,y1) ;
```

BB: RK1ST(x,y,H,x2,y2) ; RK1ST(x2,y2,H,x3,y3) ;

```
for k := 1 step 1 until n do
if comp(y1[k],y3[k],eta) > eps then go to CC ;
```

```
comment : comp(a,b,c) is a function designator, the value
of which is the absolute value of the difference of the
mantissae of a and b, after the exponents of these
quantities have been made equal to the largest of the ex-
ponents of the originally given parameters a,b,c ;
```

```
x := x3 ; if out then go to DD ;
for k := 1 step 1 until n do y[k] := y3[k] ;
if s=5 then begin s := 0 ; H := 2 \times H end if ;
s := s+1 ; go to AA ;
```

CC: H := 0.5 \times H ; out := false ; x1 := x2 ;

```
for k := 1 step 1 until n do y1[k] := y2[k] ;
go to BB ;
```

DD: for k := 1 step 1 until n do y_E[k] := y3[k]

end RK

* This RK-program contains some new ideas which are related to ideas of S. GILL, A process for the step-by-step integration of differential equations in an automatic computing machine, *Proc. Camb. Phil. Soc.* Vol. 47 (1951) p. 96; and E. FRÖBERG, On the solution of ordinary differential equations with digital computing machines, *Fysiograf. Sällsk. Lund, Förh.* 20 Nr. 11 (1950) p. 136-152. It must be clear, however, that with respect to computing time and round-off errors it may not be optimal, nor has it actually been tested on a computer.

10. EVALUATION OF THE CHEBYSHEV POLYNOMIAL $T_n(X)$ BY RECURSION

G. M. Galler

National Bureau of Standards, Washington 25, D. C.

comment

This procedure computes the Chebyshev polynomial $T_n(X) = \cos(n \times \cos^{-1}(X))$ for any given real argument, X , and any order, n , by the recursion formula below;

real procedure

real

begin real

```
Ch(n, X) ;
X ; integer n ;
a, b, c ; integer i ;
a := 1 ; b := X ;
if n = 0 then c := a else if n = 1 then
c := b else for i := 2 step 1 until n do
begin c := 2 \times X \times b - a ;
a := b ; b := c
end
Ch := c
end
```

CERTIFICATION OF ALGORITHM 10

CHEBYSHEV POLYNOMIAL $T_n(x)$ (Galler, *Comm.*

ACM, June, 1960)

JOHN HERNDON

Stanford Research Institute, Menlo Park, California

When transliterated into BALGOL and tested on the Burroughs 220, $Ch(n, x)$ gave better than 7-digit accuracy for $n = 0, 1, 4, 8$ and $x = .01, .2, .7$. It gave answers when $x > 1$ which corresponded to the value of the series with x substituted.

11. EVALUATION OF THE HERMITE POLYNOMIAL $H_n(X)$ BY RECURSION

G. M. Galler

National Bureau of Standards, Washington 25, D. C.

comment

This procedure computes the Hermite polynomial $H_n(X) = (-1)^n \times e^{X^2} \times (d^n/dX^n(e^{-X^2}))$ for any given real argument, X , and any order, n , by the recursion formula below;

real procedure

integer

begin real

```
He(n, X) ;
n ; real X ;
a, b, c ; integer i ;
a := 1 ; b := 2X
if n = 0 then c := a else if n = 1 then
c := b else for i := 1 step 1 until n-1 do
begin c := 2 \times X \times b - 2 \times i \times a ;
a := b ; b := c
end
He := c
end
```

12. EVALUATION OF THE LAGUERRE POLYNOMIAL $L_n(X)$
BY RECURSION
G. M. GALLER
National Bureau of Standards, Washington 25 D. C.

comment This procedure computes the Laguerre polynomial
 $L_n(X) = e^X \times (d^n/dX^n(X^n \times e^{-X}))$ for any given real argument, X, and any order, n, by the recursion formula below;

real procedure La(n, X) ;
integer n ; **real** X ;
begin real a, b, c ; **integer** i ;
a := 1 ; b := 1 - X ;
if n = 0 then c := a else if n = 1 then
c := b else for i = 1 step 1 until n-1 do
begin c := (1 + 2 × i - X) × b - (i ↑ 2) × a ;
a := b ; b := c
end
La := c
end

13. EVALUATION OF THE LEGENDRE POLYNOMIAL $P_n(X)$
BY RECURSION
G. M. GALLER
National Bureau of Standards, Washington 25 D. C.

comment This procedure computes the Legendre polynomial
 $P_n(X) = (1/(2^n \times n!)) \times d^n/dX^n(X^2 - 1)^n$ for any given real argument, X, and any order, n, by the recursion formula below;

real procedure Le(n, X) ;
integer n ; **real** X ;
begin real a, b, c ; **integer** i ;
a := 1 ; b := X ;
if n = 0 then c := a else if n = 1 then
c := b else for i = 1 step 1 until n-1 do
begin c := b × X + (i/(i+1)) × (X × b - a) ;
a := b ; b := c
end
Le := c
end

CERTIFICATION OF ALGORITHM 13
LEGENDRE POLYNOMIAL $P_n(x)$ (Galler, *Comm.*
ACM, June 1960)

JOHN HERNDON
Stanford Research Institute, Menlo Park, California

When transliterated into BALGOL and tested on the Burroughs 220, Le(n, x) gave 7-digit accuracy for n = 0, 1, 4, 9 and X = .01, .2, .7, 1.9, 5.0.

ALGORITHM 14.
COMPLEX EXPONENTIAL INTEGRAL

A. Beam
National Bureau of Standards, Washington 25, D. C.

procedure EKZ(x, y, k, ε, u, v, n) ; **real** x, y, k, ε, u, v ;
integer n ;

comment EKZ computes $w(z, k) = u + iv = z^k e^z \int_z^\infty e^{-t} dt / t^k$
from the continued fraction representation found in H. S. Wall, *Continued Fractions*, Chap. 18 (D. Van Nostrand, New York, 1948). Input parameters are x, y, k, and ε where $z = x + iy$. Successive convergents are computed as follows: For n = 2, 3, 4, ..., $D_n = z/(z + M \times D_{n-1})$, $R_n = (D_n - 1)R_{n-1}$, $C_n = C_{n-1} + R_n$, where M is $k + (n-2)/2$ or $(n-1)/2$ according to whether n is even or odd, and $D_1 = R_1 = C_1 = 1$. Computation is stopped when C_n and C_{n-1} agree to the significance specified by ε. The corresponding index n is available after use of the procedure. This method is valid in the entire complex plane except for the origin and the negative real axis. Convergence is too slow to be practical for $|z| < .05$. Also for some range within the half-strip $|y| < 2$, $x < 0$ (this range depends on k). The method is valid for complex k, but only real k is considered in this procedure;

begin **real** t1, t2, t3, M, K, c, a, d, b, g, h, ε1 ;
integer m ;
comment R = a + ib, D = c + id, C = g + ih ;
ε1 := ε ↑ 2 ;
u := c := a := 1 ; v := d := b := 0 ;
n := 1 ; K := k - 1 ;
BACK: g := u ; h := v ; n := n + 1 ;
m := n ÷ 2 ;
if 2 × m = n then M := m + K else M := m ;
t1 := x + M × c ; t2 := y + M × d ;
t3 := t1 ↑ 2 + t2 ↑ 2 ;
c := (x × t1 + y × t2) / t3 ;
d := (y × t1 - x × t2) / t3 ;
t1 := c - 1 ; t2 := a ;
a := a × t1 - d × b ; b := d × t2 + t1 × b ;
u := g + a ; v := h + b ;
if (a ↑ 2 + b ↑ 2) / (u ↑ 2 + v ↑ 2) > ε1 then go to BACK ;
end EKZ

CERTIFICATION OF ALGORITHM 14
COMPLEX EXPONENTIAL INTEGRAL (A. Beam,
Comm. ACM, July, 1960)

P. J. RADER AND HENRY C. THACHER, JR.*
Argonne National Laboratory, Argonne, Illinois

EKZ was programmed by hand for the Royal-Precision LGP-30 computer, using a 28-bit mantissa floating-point interpretive system (24.2 modified). To facilitate comparison with existing tables (National Bureau of Standards Applied Mathematics Series 51 and 37), the real and imaginary parts of $E_k(z)$ were computed from u and v. Results are shown in the following table. In all cases, the values agreed with tabulated values within the tolerance specified.

x	y	k	ε	n
1×10^{-8}	1.0	1	10^{-1}	7
1×10^{-8}	1.0	1	10^{-2}	14
1×10^{-8}	1.0	1	10^{-3}	24
1×10^{-8}	1.0	1	10^{-4}	37

1×10^{-8}	1.0	1	10^{-6}	52
1×10^{-8}	1.0	1	10^{-6}	70
1×10^{-8}	1.0	1	10^{-7}	90
1×10^{-8}	1.0	1	10^{-8}	114
1×10^{-8}	2.0	1	10^{-6}	37
1×10^{-8}	3.0	1	10^{-6}	26
1×10^{-8}	4.0	1	10^{-6}	21
1.0	1×10^{-8}	1	10^{-6}	40
1.0	1.0	1	10^{-6}	34
1.0	2.0	1	10^{-6}	26
1.0	3.0	1	10^{-6}	21
2.0	1×10^{-8}	1	10^{-6}	23
2.0	1.0	1	10^{-6}	22
2.0	2.0	1	10^{-6}	20
2.0	3.0	1	10^{-6}	17
3.0	1×10^{-8}	1	10^{-6}	17
3.0	1.0	1	10^{-6}	17
3.0	2.0	1	10^{-6}	16
3.0	3.0	1	10^{-6}	15
4.0	0.0	0	10^{-6}	20
4.0	0.0	1	10^{-6}	15
4.0	0.0	2	10^{-6}	16
4.0	0.0	3(1)14	10^{-6}	17
4.0	0.0	15, 16	10^{-6}	16

It thus appears that the algorithm gives satisfactory accuracy, but that in certain ranges of the variables, the time required may be excessive for extensive use.

ALGORITHM 15

ROOTFINDER II (Modification of Algorithm 2. ROOTFINDER, J. Wegstein, *Communications ACM*, February, 1960)

HENRY C. THACHER, JR.,* Argonne National Laboratory, Argonne, Illinois

```

procedure ROOT II (f, a, eps, n, g, c, m); integer n, m;
real procedure f; real a, eps, g, c;
comment ROOT II computes a value of  $g = y$  satisfying
the equation  $y = f(y)$ . The iteration will converge
to Y providing that at some time in the iteration a  $g$  is
reached such that  $\text{abs}(g - Y) \times \text{abs}(d(df/dy)/dy) < 2 \times \text{abs}((df/dy) - 1)$ ,
where the derivatives are evaluated at Y. Input includes (1)  $f$ ,
a procedure for computing  $f(y)$ , (2)  $a$ , an initial approximation
to the root, (3)  $\text{eps}$ , a tolerance for the relative error in  $g$ ,
and (4)  $n$ , a maximum number of iterations to be performed.
Output includes: (1)  $g$ , the required root, (2)  $c = f(g) - g$ ,
(3)  $m$ , a parameter indicating the success of the procedure.
If the tolerance was not met,  $m < 0$ .  $|m - 1|$  gives the number
of times that the correction to  $g$  exceeded the preceding one,
an indication of instability. ;

begin integer j; real b, d, h;
m := 1; if f(0) = 0 then begin g := 0;
go to return end
else g := f(a); b := d := c := a - g;
if c = 0 then go to return else
for j := 1 step 1 until n do begin c := f(g) - g;

```

```

if (abs(c/g) < eps) then go to return else h :=
b/c;
if h < 0 or h > 2 then m := m + 1 else
d := d/(h - 1); b := c; g := g + d end
iteration
comment if the system is known to be stable, the if clause
of the last statement can be omitted;
m := - m return end

```

CERTIFICATION OF ALGORITHM 15

ROOTFINDER II (Revision by Henry C. Thacher, Jr., *Communications ACM*, August, 1960)

HENRY C. THACHER, JR.,* Argonne National Laboratory, Argonne, Illinois

The revision of ROOTFINDER suggested in the preceding remark was programmed by hand for the Royal Precision LGP-30 computer, using a 28-bit mantissa floating point interpretive system (24.2).

The program was tested for the following equations:

- (1.k) $f(y) = \arctan y + k\pi$ ($k = 0, 1, 2, 3, 4, 6, 8$)
(2) $f(y) = (y^3 + 1)^{1/3}$
(3) $f(y) = y^3 - 1$ } These both have the root 1.3247180428
(4.k) $f(y) = \sinh \alpha_k y$
(5.k) $f(y) = \cosh \alpha_k y$ ($\alpha_1 = -1.2, \alpha_2 = -0.5, \alpha_3 = 0.5, \alpha_4 = 1.2$)

Typical results of these tests were as follows:

$f(y)$	ϵ	a	g	$[f(g) - g] \times 10^7$	Remarks
1.0	10^{-8}	1.0000	0.0000000	0.00	
1.1	10^{-8}	3.1415	4.4934094	0.15	
1.2	10^{-8}	6.2832	7.7252518	0.60	
1.3	10^{-8}	9.4248	10.904122	0.00	
1.4	10^{-8}	12.5664	14.066194	0.30	
1.6	10^{-8}	18.8496	20.371303	0.60	
1.8	10^{-8}	25.1327	26.666054	0.60	
1.2	10^{-8}	1.3	1.3247179	0.00	
1.2	10^{-8}	0.5	1.3247179	0.00	
3	10^{-8}	9.0	4.4804900	197.74×10^7	Diverged 2 times, not converged after 20 iter.
3	10^{-8}	5.0	1.3482797	$.51 \times 10^7$	Converged in less than 20 iter.
3	10^{-8}	3.0	1.3247180	0.0	Diverged 2 times. Term. with $h = 1$.
3	10^{-8}	2.0			
3	10^{-8}	1.1	1.3247180	1384.24	Diverged 9 times. Converged after 20 iter.
3	10^{-8}	1.0			Terminated when g became 0.
3	10^{-8}	0.8	1.3247180	0.00	Diverged 4 times. Conv. in less than 20.
3	10^{-8}	0.6	1.6161598	4.39×10^7	Diverged 2 times. No conv. after 20.
4.k	10^{-8}	1.0	0.00000000	0.00000000	For all k.
5.1, 5.4	10^{-8}	1.0	0.09179585	0.793×10^7	Diverged 7 times. No conv. after 20 iter.
5.2, 5.3	10^{-8}	1.0	1.11787755	0.037	

Function (3) is of particular interest, since it does not converge for most algorithms. With the Wegstein iteration, convergence was obtained, or would have been obtained with a few more iterations for a wide range of initial guesses.

REMARK ON ALGORITHM 15

ROOTFINDER II (Henry C. Thacher, Jr., *Comm. ACM*, August 1960)

GEORGE E. FORSYTHE AND JOHN G. HERRIOT, Stanford University, Stanford, California

As pointed out by Lieberstein (*Comm. ACM*, January 1959, p. 5), this algorithm is precisely the Newton method of chords or the scant method applied to $g(x) = f(x) - x = 0$. Thus convergence is not of second order but rather (for simple roots) of order $\frac{1}{2}(\sqrt{5} - 1) = 1.618$, as shown by Jeeves (*Comm. ACM*, August 1958, pp. 9-10). In the first portion of the algorithm b, c, d , should be set equal to $g - a$ instead of $a - g$ in order to be consistent with

the iteration portion. Doing this will usually cut down the number of iterations. Not only is a preliminary test for a zero root desirable but the possibility that g may be zero at any stage of the iteration should be considered in writing the return criterion. The possibility that $h = 1$ should also be checked and appropriate action taken. Algorithm 26 takes care of these matters and also corrects some minor errors in Algorithm 15. This method is certainly not the best rootfinder that could be written.

SEE ALGORITHM 2

ALGORITHM 16 CROUT WITH PIVOTING

GEORGE E. FORSYTHE

Stanford University, Stanford, California

```

real procedure INNERPRODUCT(u,v) index : (k) start : (s)
    finish : (f);
    value s, f; integer k, s, f; real u, v;
    comment INNERPRODUCT forms the sum of  $u(k) \times v(k)$  for  $k = s, s+1, \dots, f$ . If  $s > f$ , the value of INNERPRODUCT is zero. The substitution of a very accurate inner product procedure would make CROUT more accurate;

begin
    real h;
     $h := 0$ ; for  $k := s$  step 1 until  $f$  do  $h := h + u \times v$ ;
     $INNERPRODUCT := h$ 
end INNERPRODUCT;

procedure CROUT (A, b, n, y, pivot, INNERPRODUCT);
    value n; array A, b, y, pivot; integer n, pivot;
    real procedure INNERPRODUCT;
    comment This is Crout's method with row interchanges, as formulated in reference [1], for solving  $Ay = b$  and transforming the augmented matrix  $[A|b]$  into its triangular decomposition  $LU$  with all  $L[k, k] = 1$ . If  $A$  is singular we exit to 'singular,' a non-local label.  $pivot[k]$  becomes the current row index of the pivot element in the  $k$ -th column. Thus enough information is preserved for the procedure SOLVE to process a new right-hand side without repeating CROUT. The accuracy obtainable from CROUT would be much increased by calling CROUT with a more accurate inner product procedure than INNERPRODUCT;

begin
    integer k, i, j, imax, p; real TEMP, quot;
    for  $k := 1$  step 1 until  $n$  do
1: begin
         $TEMP := 0$ ;
        for  $i := k$  step 1 until  $n$  do
2: begin
             $A[i, k] := A[i, k] - INNERPRODUCT(A[i, p], A[p, k], p, 1, k-1)$ ;
            if  $abs(A[i, k]) > TEMP$  then
3: begin
                 $TEMP := abs(A[i, k])$ ;  $imax := i$ 
            end 3
        end 2;
         $pivot[k] := imax$ ;
        comment We have found that  $A[imax, k]$  is the largest pivot in column  $k$ . Now we interchange rows  $k$  and  $imax$ ;
        if  $imax \neq k$  then

```

```

4: begin for  $j := 1$  step 1 until  $n$  do
5: begin
         $TEMP := A[k, j]$ ;  $A[k, j] := A[imax, j]$ ;
         $A[imax, j] := TEMP$ 
    end 5;
     $TEMP := b[k]$ ;  $b[k] := b[imax]$ ;  $b[imax] := TEMP$ 
end 4;
    comment The row interchange is done. We proceed to the elimination;
    if  $A[k, k] = 0$  then go to singular;
    for  $i := k+1$  step 1 until  $n$  do
         $quot := 1.0/A[k, k]$ ;  $A[i, k] := quot \times A[i, k]$ 
    end;
    for  $j := k+1$  step 1 until  $n$  do
         $A[k, j] := A[k, j] - INNERPRODUCT(A[k, p], A[p, j], p, 1, k-1)$ ;
         $b[k] := b[k] - INNERPRODUCT(A[k, p], b[p], p, 1, k-1)$ 
    end 1;
    comment The triangular decomposition is now finished, and we do the back substitution;
    for  $k := n$  step -1 until 1 do
         $y[k] := (b[k] - INNERPRODUCT(A[k, p], y[p], p, k+1, n)/A[k, k])$ 
    end CROUT;

procedure SOLVE (B, c, n, z, pivot, INNERPRODUCT);
    value n; array B, c, z, pivot; integer n, pivot;
    real procedure INNERPRODUCT;
    comment SOLVE assumes that a matrix  $A$  has already been transformed into  $B$  by CROUT, but that a new column  $c$  has not been processed. SOLVE solves the system  $Az = c$ , and the output  $z$  of SOLVE is precisely the same as the output  $y$  of the procedure statement CROUT (A, c, n, y, pivot, INNERPRODUCT). However, SOLVE is faster, because it does not repeat the triangularization of  $A$ ;

begin
    integer k; real TEMP;
    for  $k := 1$  step 1 until  $n$  do
        begin
             $TEMP := c[pivot[k]]$ ;  $c[pivot[k]] := c[k]$ ;  $c[k] := TEMP$ ;  $c[k] := c[k] - INNERPRODUCT(B[k, p], c[p], p, 1, k-1)$ 
        end;
        for  $k := n$  step -1 until 1 do
             $z[k] := (c[k] - INNERPRODUCT(B[k, p], z[p], p, k+1, n)/B[k, k])$ 
        end SOLVE

```

REFERENCE

- [1] J. H. WILKINSON, theory and practice in linear systems, pp. 43-100 of JOHN W. CARR III (editor), *Application of Advanced Numerical Analysis to Digital Computers*, (Lectures given at the University of Michigan, Summer 1958, College of Engineering, Engineering Summer Conferences, Ann Arbor, Michigan [1959]).

REMARK ON ALGORITHM 16

CROUT WITH PIVOTING (G. E. Forsythe, *Comm. ACM*, 3 (Sept. 1960), 507-8.)

HENRY C. THACHER, JR.,* Argonne National Laboratory, Argonne, Illinois

This procedure contains the following errors:

a. In SOLVE, the expression
 $c[k] := c[k] - \text{INNERPRODUCT}$
 $(B[k, p], c[p], p - 1, k - 1)$

should read:

$c[k] := c[k] - \text{INNERPRODUCT}$
 $(B[k, p], c[p], p, 1, k - 1)$

b. In CROUT, the specification part should read:

array A, b, y ; **integer** n ; **integer array** pivot ;

c. In SOLVE, the specification part should read:

array B, c, z ; **integer** n ; **integer array** pivot ;

The efficiency of the algorithm will be improved by the following changes:

a. In the elimination phase of CROUT, replace

for i := k + 1 **step** 1 **until** n **do**

begin quote := 1.0/A[k, k] ; A[i, k] := quot XA[i, k] **end** ;

by

quot := 1.0/A[k, k] ; **for** i := k + 1 **step** 1 **until** n **do**
A[i, k] := quot XA[i, k] ;

b. Omit INNERPRODUCT from the formal parameter list in both CROUT and SOLVE, and declare INNERPRODUCT either locally, or globally. This avoids any reference to INNERPRODUCT in the calling sequence produced by a compiler.

It is also to be noted that a minor modification of CROUT allows it to be used to evaluate the determinant of A.

All of these suggestions are included in a later algorithm.

REMARK ON ALGORITHM 16

CROUT WITH PIVOTING (G. Forsythe, *Communications ACM*, September, 1960)

GEORGE E. FORSYTHE

Stanford University, Stanford, California

QUERY

Perhaps the most basic procedure for an ALGOL library of matrix programs is an inner product procedure. The procedure Innerproduct given on page 311 of [1] is fairly difficult to comprehend, and probably poses great difficulties for most translating routines. I merely copied its form in writing a modified inner product routine for [2].

My query is: How should one write an inner product procedure in ALGOL?

REFERENCES

1. PETER NAUR (editor), J. W. BACKUS, ET AL., Report on the algorithmic language ALGOL 60, *Comm. Assoc. Comp. Mach.* 3 (1960), 299-314.
2. GEORGE E. FORSYTHE, CROUT with pivoting in ALGOL 60, *Comm. Assoc. Comp. Mach.* 3 (1960), 507-508.

ALGORITHM 17

TRDIAG

C. F. SPRAGUE III

General Atomic Division of General Dynamics Corp., San Diego, California

procedure trdiag (a,b,c,d) order : (n) result : (x);
value n;
comment this procedure gives the solution to the tri-diagonal system of linear algebraic equations:
 $a_1x_1 + b_1x_1 + d_1 = 0$
 $a_ix_{i+1} + b_ix_i + c_ix_{i-1} + d_i = 0, i = 2, 3, \dots, n-1$
 $b_nx_n + c_nx_{n-1} + d_n = 0.$
This method is often used to obtain solutions to second order difference equations;
begin array gamma [1 : n-1]; **integer** i; **real** y;
gamma [1] := -a[1]/b[1];
x[1] := -d[1]/b[1];
for i := 2 **step** 1 **until** n-1 **do**
begin
y = b[i] + c[i] X gamma [i - 1];
gamma [i] := -a[i]/y; x[i] := -(c[i] X x[i-1] + d[i])/y **end**;
x[n] := -(c[n] X x[n-1] + d[n])/(b[n] + c[n] X gamma [n-1]);
for i := n **step** -1 **until** 2 **do**
x[i - 1] := x[i] X gamma [i - 1] + x[i - 1]
end trdiag

ALGORITHM 18

RATIONAL INTERPOLATION BY CONTINUED FRACTIONS

R. W. FLOYD

Armour Research Foundation, Chicago, Illinois

comment This procedure fits to m given points (x_i, y_i) a continued fraction in the form

$a_1 + (x - x_1)/(a_2 + (x - x_2)/(a_3 + (x - x_3)/\dots(x - x_{m-1})/a_m)\dots)$

It also simplifies the continued fraction to a rational function $(N_0 + N_1x + \dots + N_{deg}x^{deg})/(D_0 + D_1x + \dots + D_{deg}x^{deg})$,

where deg is at most $m \div 2$;

procedure confr(m,x,y,a,N,D);
real array x,y,a,N,D; **integer** m;
begin **real** aa,xx,T; **integer** i,j,k; **real array** P,Q[0 : m $\div$ 2]
switch sw := sw1, sw2;
for j := 1 **step** 1 **until** m **do**
begin aa := y[j]; xx := x[j];
for i := 1 **step** 1 **until** j-1 **do**
aa := (xx - x[i])/(aa - a[i]); a[j] := aa
end;
k := 1; P[0] := 1; Q[0] := a[1];
mult : **for** j := 1 **step** 1 **until** m $\div$ 2 **do** P[j] := Q[j] := 0;
for i := 2 **step** 1 **until** m **do**
begin **for** j := i $\div$ 2 **step** -1 **until** 1 **do**
begin T := a[i] X Q[j] - x[i-1] X P[j] + P[j-1];
P[j] := Q[j]; Q[j] := T
end; T := a[i] X Q[0] - x[i-1] X P[0];
P[0] := Q[0]; Q[0] := T
end; **go to** sw[k];
sw1 : **for** j := 0 **step** 1 **until** m $\div$ 2 **do** N[j] := Q[j];
k := 2; P[0] := 0; Q[0] := 1; **go to** mult;
sw2 : **for** j := 0 **step** 1 **until** m $\div$ 2 **do** D[j] := Q[j]
end procedure

CERTIFICATION OF ALGORITHM 18 RATIONAL INTERPOLATION BY CONTINUED FRACTIONS

[R. W. Floyd, *Comm. ACM.*, Sept. 1960]
HENRY C. THACHER, JR.*
Reactor Engineering Div., Argonne National Lab.,
Argonne, Ill.

* Work supported by the U. S. Atomic Energy Commission

The body of procedure *confr* was tested with the ALGOL translator system written for the LGP-30 computer by the Dartmouth College Computer Center. No syntactical errors were found in the procedure body, except for a missing semicolon after the array declaration. The translated algorithm gave satisfactory results when tested on values of $(4x+1)/(x+4)$ at any three of the points $x = 1, 2, 3, 4$. When all four points were used, a division overflow occurred in the statement **for** $i := 1$ **step** 1 **until** $j-1$ **do** $aa := (xx - x[i])/(aa - a[i])$; which forms the reciprocal differences. An overflow of this type will occur whenever $y[j]$ is approximated to high accuracy by one of the continued fractions based only on the points $x[i]$, $i = 1, 2, \dots, k$ with k less than j . Unless $i = j-1$, the difficulty may be overcome by setting aa equal to the largest real representable in the computer whenever division overflow would occur. When $i = j-1$, the difficulty is irretrievable, and the data points must be reordered.

ALGORITHM 19 BINOMIAL COEFFICIENTS

RICHARD R. KENYON
Computing Laboratory, Purdue University, Lafayette,
Indiana

comment This procedure computes binomial coefficients $C_m^n = n!/m!(n-m)!$ by the recursion formula $C_{i+1}^n = (n-1)C_i^n/(i+1)$ starting from $C_0^n = 1$;

integer procedure $C(m, n)$;
integer m, n ;
begin **integer** i, a, b ;
 $a := 1$;
 if $2 \times m > n$ **then** $b := n - m$ **else**
 $b := m$;
 for $i := 0$ **step** 1 **until** b **do**
 begin $a := (n - i) \times a \div (i + 1)$ **end**
 $C := a$
end Binomial Coefficients

CERTIFICATION OF ALGORITHM 19 BINOMIAL COEFFICIENTS [Richard R. Kenyon, *Comm. ACM* Oct., 1960]

RICHARD GEORGE*
Particle Accelerator Div., Argonne National Lab., Ar-
gonne, Ill.

* Work supported by the U. S. Atomic Energy Commission.

This procedure was tested on the LGP-30, using the compiler ALGOL-30 from Dartmouth College Computation Center. The following changes were found necessary:

(1) Within the **comment**, the line

$$C_{i+1}^n = (n-1)C_i^n/(i+1)$$

should be

$$C_{i+1}^n = (n-i)C_i^n/(i+1)$$

(2) The line defining the iteration loop
 for $i := 0$ **step** 1 **until** b **do**
should be
 for $i := 0$ **step** 1 **until** $b-1$ **do**
(3) The sequence
 end $C := a$ **end**
should be
 end; $C := a$ **end**

REMARK ON ALGORITHM 19
BINOMIAL COEFFICIENTS (Richard R. Kenyon,
Comm. ACM, Oct. 1960)
RICHARD STECK
Armour Research Foundation, Chicago 16, Ill.

The **for** clause of Algorithm 19 should read:

for $i := 0$ **step** 1 **until** $b-1$ **do**

With this correction the algorithm was certified on the Armour Research Foundation UNIVAC 1105.

The recursion formula stated in the **comment** should read:

$$C_{i+1}^n = (n-i) C_i^n / (i+1).$$

ALGORITHM 20 REAL EXPONENTIAL INTEGRAL S. PEAVY

National Bureau of Standards, Washington 25, D.C.

real procedure Expint (x) ; **real** x ;
comment $-E_1(-x) = \int_x^\infty (e^{-u}/u) du$ is computed for
 $x > 0$ by approximation formulas. For
 $0 < x < 1$ the approximation is from E. E.
Allen, Note 169, *MTAC* 56, pg 240 (1954).
The second approximation formula is for
 $1 \leq x < \infty$ and is from C. Hastings, Jr.,
"Approximations For Digital Computers"
(Princeton University Press, Princeton,
New Jersey, 1955). The absolute error
 $\epsilon(x)$ is $|\epsilon(x)| < 2 \times 10^{-7}$ for $0 < x < 1$
and $|\epsilon(x)| < 2 \times 10^{-8}$ for $1 \leq x < \infty$;

begin **real** y, w, z ;
 if $x < 1$ **then**
 $z := (((.00107857 \times x - .00976004) \times x$
 $+ .005519968) \times x - .24991055) \times x$
 $+ .99999193) \times x - .57721566 - \ln(x)$
 else begin
 $y := ((x + 8.5733287401) \times x$
 $+ 18.059016973) \times x + 8.6347608925) \times x$
 $+ .2677737343$;
 $w := (((x + 9.5733223454) \times x$
 $+ 25.6329561486) \times x$
 $+ 21.0996530827) \times x + 3.9584969228$;
 $z := \exp(-x) / x \times (y/w)$ **end**
 Expint := z **end**

CERTIFICATION OF ALGORITHM 20 REAL EXPONENTIAL INTEGRAL (S. Peavy, *Comm.* *ACM*, Oct. 1960)

WILLIAM J. ALEXANDER* and HENRY C. THACHER, JR.*
Argonne National Laboratory, Argonne, Illinois

Expint (x) was programmed for the LGP-30 computer, using both a 7S floating-point compiler (ACT III) and an 8S floating-point interpretive code (24.2). Constants given to more than 7S (or to 8S for the 24.2 program) were rounded to 7S (or 8S).

After changing the constant .005519968 to .05519968, both programs gave acceptable accuracy over the range tested.

The 8S (24.2) program was compared with the 9D values given for $-E_i(-x)$ in Mathematical Tables Project, *Tables of Sine, Cosine, and Exponential Integrals, Volume II* (1940) for the set of values $x = 0.1(0.1)1.0(1.0)10.0$. The largest discrepancy found was -16×10^{-8} for $x = 0.1$. For x greater than 1, all values tested were good to 8S.

For computing real values of the exponential integral, this algorithm is much faster than EKZ (Algorithm 13). For $x < 1$, the ratio of speeds was of the order of 20.

REMARK ON ALGORITHM 20

REAL EXPONENTIAL INTEGRAL (S. Peavy, *Comm. ACM*, October 1960)

S. PEAVY

National Bureau of Standards, Washington, D. C.

A printing error has been called to our attention by J. A. Beutler of E. I. duPont de Nemours and Co. Lines 15 through 17 of Algorithm 20 should read

```
z := (((.00107857 × x - .00976004) × x
      + .05519968) × x - .24991055) × x
      + .99999193) × x - .57721566 - ln (x)
```

ALGORITHM 21

BESSEL FUNCTION FOR A SET OF INTEGER ORDERS

W. BÖRSCH-SUPAN

National Bureau of Standards, Washington 25, D. C.

```
procedure BESSELSETINT (x, n, ε, J) ; value x, n, ε ;
  real x, ε ; integer n ; real array J ;
  comment: This procedure computes the values of the Bessel
  functions  $J_p(x)$  for real argument  $x$  and the set of all integer
  orders from 0 up to  $n$  and stores these values into the array  $J$ ,
  whose subscript bounds should include the integers from 0 up
  to  $n$ .  $n$  must be nonnegative.
```

The computation is done by applying the recursion formula backward from $p = k$ down to $p = 0$ as described in *MTAC 11* (1957), 255-257. k is chosen to yield errors less than 10^{-5} approximately after the first application of the recursion. The recursion is repeated with a larger k until the difference between the results of the two last recursions doesn't exceed the given bound $\epsilon > 0$. The steps in increasing k are chosen in such a way that the errors decrease at least by a factor of approximately 10^{-5} . There is no protection against overflow. ;

```
begin real dist, rec0, rec1, rec2, sum, max, err ;
  integer k, p ; Boolean s ; real array Jbar[0:n] ;
  if x = 0 then
    begin J[0] := 1 ; for p := 1 step 1 until n do J[p] := 0 ;
      go to Exit
    end ;
  dist := if abs(x) ≥ 8 then 5 × abs(x) ↑ (1/3) else 10 ;
  k := entier ((if abs(x) ≥ n then abs(x) else n) + dist) + 1 ;
  s := false ;
```

```
Rec: rec0 := 0 ; rec1 := 1 ; sum := 0 ;
  for p := k step -1 until 1 do
    begin J[if p > n + 1 then n else p - 1] := rec2 :=
      2 × p/x × rec1 - rec0 ;
```

```
if p = 1 then sum := sum + rec2
else if p ÷ 2 × 2 ≠ p then sum :=
  sum + 2 × rec2 ;
rec0 := rec1 ; rec1 := rec2
```

```
end recursion ;
```

```
Norm: for p := 0 step 1 until n do J[p] := J[p]/sum ;
  if s then
```

```
  begin max := 0 ;
    for p := 0 step 1 until n do
      begin err := abs (J[p] - Jbar[p]) ;
        if err > max then max := err
      end . maximum error ;
    if max ≤ ε then go to Exit
```

```
  end then
```

```
  else s := true ;
```

```
  for p := 0 step 1 until n do Jbar[p] := J[p] ;
  k := entier (k + dist) ;
  go to Rec ;
```

```
Exit: end BESSELSETINT
```

ALGORITHM 22

RICCATI-BESSEL FUNCTIONS OF FIRST AND SECOND KIND

H. OSER

National Bureau of Standards, Washington 25, D. C.

```
procedure RICCATIBESSEL (x, n, eps, S, C) ;
```

```
  value x, n, eps ;
```

```
  real x, eps; integer n; real array S, C ;
```

comment: RICCATIBESSEL computes $S_k(x) = (\pi x/2)^{1/2} J_{k+1/2}(x)$ and $C_k(x) = -(\pi x/2)^{1/2} Y_{k+1/2}(x)$ for real $x \neq 0$ and all integer values of k from 0 through n with a prescribed (absolute) accuracy ϵ . The computation is done by using the recursion relations of the cylinder functions. For $\text{abs}(x) > n$ both $S_k(x)$ and $C_k(x)$ are computed by using the recursions for ascending orders. For $n > \text{abs}(x)$ the functions $S_k(x)$ are obtained by using the recursion in descending orders. (See STEGUN-ABRAMOWITZ, *MTAC 11*, 1957, 255-257). Reaching out two different intervals beyond the order n , the two vectors $S_k(x)$ and $S_k^*(x)$ are checked if the maximum component of their difference meets the tolerance ϵ . If this is not the case a maximum of 10 iterations is set up to achieve the required absolute accuracy. Initial values $S_{k_{\max}}$ and $S_{k_{\max}-1}$ for the backward iteration are computed from the corresponding values $C_{k_{\max}-1}$ and $C_{k_{\max}}$. No check of accuracy is done in case $n < \text{abs}(x)$. Both $C_k(x)$ and $S_k(x)$ are affected in this case by errors of the same order of magnitude as the subroutines for $\sin(x)$ and $\cos(x)$;

```
begin real r1, r2, r3, r4, r5, r6, step, acc, max, a, b, d1, d2 ;
```

```
  integer i, k, l, imax ;
```

```
  real array W[0:n] ;
```

```
  switch P := initial, improve ;
```

```
  acc := 106 ;
```

```
  step := 103 ;
```

```
  imax := 10 ;
```

comment: These constants may be chosen differently, but caution has to be taken because of overflow. acc sets an initial iteration to give roughly a 6-place accuracy. Subsequent iterations should improve the result to 3 more places each ;


```

i := 1 ;
if x = 0 then go to exit1 ;
if n < abs(x) then
case1: begin r1 := -sin(x) ; r2 := r4 := C[0] := cos(x) ;
            r5 := S[0] := sin(x) ;
            for k := 1 step 1 until n do
                begin C[k] := r3 := (2×k-1) × r2/x - r1 ;
                     S[k] := r6 := (2×k-1) × r5/x - r4 ;
                     r1 := r2 ; r2 := r3 ;
                     r4 := r5 ; r5 := r6
                end k ; go to finish
            end case1 ;
case2: l := 1 ; r1 := -sin(x) ; r2 := C[0] := cos(x) ;
        for k := 1 step 1 until n do
            begin C[k] := r3 := (2×k-1) × r2/x - r1 ;
                 r1 := r2 ;
                 r2 := r3
            end ;
        a := n ;
loop: for k := 1+n step 1 until if abs(x) ≤ 11
      then l2+a else 2×a+1 do
    begin r3 := (2×k-1) × r2/x - r1 ;
          if abs(r3/C[n]) > acc then go to S ;
          r1 := r2 ;
          r2 := r3 ;
          comment: This loop is most liable to cause
                   overflow ;
    end loop ;
    k := if abs(x) ≤ 11 then l2+a else 2×a + 1 ;
    r2 := r1 ;
S:   r6 := x ↑ 2/(4×k ↑ 2×r2) ;
    r5 := 1/r3 ;
    go to P[l] ;
initial: for k := k step -1 until 2 do
        begin W[if k > n+2 then n else k-2] := r4 :=
              (2×k-1) × r5/x - r6 ;
              r6 := r5 ;
              r5 := r4
        end ;
        d1 := r5/x - r6 ;
        d2 := if abs(W[0]) ≥
              abs(d1) then sin(x)/W[0] else cos(x)/d1 ;
        for k := 0 step 1 until n do
            W[k] := d2×W[k] ;
        acc := step × acc ;
        l := 2 ;
        a := a + step ↑ (1/3) ;
        r2 := C[n] ;
        r1 := C[n-1] ;
        go to loop ;
improve: for k := k step -1 until 2 do
        begin S[if k > n+2 then n else k-2] := r4 :=
              (2×k-1) × r5/x - r6 ;
              r6 := r5 ;
              r5 := r4
        end k ;
        d1 := r5/x - r6 ;
        d2 := if abs(S[0]) ≥
              abs(d1) then sin(x)/S[0] else cos(x)/d1 ;
        max := 0 ;
        for k := 1 step 1 until n do
            begin S[k] := d2×S[k] ;
                 b := abs(S[k] - W[k]) ;
                 if b > max then max := b
            end ;
        if max < eps then go to finish ;

```

```

for k := 0 step 1 until n do W[k] := S[k] ;
acc := step × acc ;
if i ≥ imax then go to exit2 ;
i := i+1 ; a := a + step ↑ (1/3) ;
r2 := C[n] ; r1 := C[n-1] ; go to loop ;
exit1: go to finish ; comment: x = 0 ;
exit2: go to finish ;
comment: maximum number of iterations reached ;
finish: end RICCATIBESSEL

```

ALGORITHM 23

MATH SORT

WALLACE FEURZEIG

Laboratories for Applied Science, University of Chicago,
Chicago, Ill.

```

procedure MATHSORT (INVEC, OUTVEC, TOTEVEC,
n, k, SETFUNC) ; value n, k ;
array INVEC, OUTVEC ;
integer array TOTEVEC ;
integer procedure SETFUNC ;
integer n, k ;

```

begin comment MATHSORT is a fast sorting algorithm which produces a monotone rearrangement of an arbitrarily ordered set of n numbers (represented by the vector INVEC) by a surprising though familiar device. The resultant sorted set is represented by the vector OUTVEC. The key field, i.e. the ordered set of bits (or bytes) on which the sort is to be done, is obtained by some extraction-justification function denoted SETFUNC. The key field allows the representation of k possible values denoted 0, 1, ..., k-1.

The procedure determines first of all the exact frequency distribution of the set with respect to the key, i.e. the number of elements of INVEC with key field value precisely equal to j for all j between 0 and k-1. The cumulative frequency distribution TOTEVEC [i] = $\sum_{j=0}^i$ (Number of elements of INVEC with key value = j) is then computed for $0 \leq i \leq k-1$. This induces the direct assignment (storage mapping function) of each element of INVEC to a unique cell in OUTVEC. This assignment (like the determination of the frequency distribution) requires just one inspection of each element of INVEC. Thus the algorithm requires only 2n "look and do" operations plus k-1 additions (to get the cumulative frequency distribution).

The algorithm can be easily and efficiently extended to handle alphabetic sorts or multiple key sorts. To sort on another key the same algorithm is applied to each new key field with the new INVEC designated as the last induced ordering (i.e. the current OUTVEC). The algorithm has been used extensively at LAS on binary as well as decimal machines both for internal memory sorts and (with trivial modification) for large tape sorts ;

```

for i := 1 step 1 until n do
    TOTEVEC[SETFUNC(INVEC[i])] := TOTEVEC
    [SETFUNC(INVEC[i])] + 1 ;
for i := 1 step 1 until k-1 do
    TOTEVEC[i] := TOTEVEC[i] + TOTEVEC[i-1] ;
for i := 1 step 1 until n do
    begin OUTVEC[TOTEVEC[SETFUNC(INVEC[i])]]
        := INVEC[i] ;
        TOTEVEC[SETFUNC(INVEC[i])] :=
        TOTEVEC[SETFUNC(INVEC[i])] - 1 ;
    end
end

```

end MATHSORT.

CERTIFICATION OF ALGORITHM 23

MATHSORT (Wallace Feurzeig, *Comm. ACM*, Nov., 1960)

RUSSELL W. RANSHAW

University of Pittsburgh, Pittsburgh, Pa.

The MATHSORT procedure as published was coded for the IBM 7070 in FORTRAN. Two deficiencies were discovered:

1. The TOTVEC array was not zeroed within the procedure. This led to some difficulties in repeated use of the procedure.

2. Input vectors already in sort on nonsort fields were unsorted. That is, given the sequence.

31, 21, 32, 22, 33,

Mathsort would produce, for a sort on the 10's digit:

22, 21, 33, 32, 31,

which is definitely out of sequence.

The following modified form of the procedure corrects these difficulties. Note the transformation of symbols.

```

procedure MATHSORT (I, O, T, n, k, S); value n, k;
  array I, O; integer array T; integer procedure S;
  integer n, k;
begin
  for i := 0 step 1 until k - 1 do T[i] := 0;
  for i := 1 step 1 until n do T[S(I[i])] := T[S(I[i])] + 1;
  for i := k - 2 step -1 until 0 do T[i] := T[i] +
    T[i + 1];
  for i := 1 step 1 until n do
    begin
      O[n + 1 - T[S(I[i])]] := I[i];
      T[S(I[i])] := T[S(I[i])] - 1;
    end
end MATHSORT.
```

Using the MATHSORT procedure ten times and having the procedure S supply each digit in order, 1000 random numbers of 10 digits each were sorted into sequence in 31 seconds. The method of locating the lowest element, interchanging with the first element, and continuing until the entire list has been so examined yielded a complete sort on the same 1000 random numbers in 227 seconds. Using the Table-Lookup-Lowest command in the 7070 yielded 56 seconds for the same set of random numbers.

ALGORITHM 24

SOLUTION OF TRI-DIAGONAL LINEAR EQUATIONS

B. LEAVENWORTH

American Machine & Foundry Co., Greenwich, Conn.

```

procedure TRIDAG (n, A, B, C, D); integer n;
array A, B, C, D;
comment: This procedure1 finds the solution of an  $n \times n$  system
of linear equations whose matrix is in tridiagonal form, that
is,  $a_{ij} = 0$  for  $|i - j| \geq 2$ . Parameters are: the main diagonal
 $B_n$ , the diagonal just below  $A_r$ , the diagonal just above  $C_r$ ,
the right-hand side  $D$ : (where  $p = 1, \dots, n$  and  $r = 1, \dots, n - 1$ )
and the matrix order  $n$ . The solution vector replaces
the input vector  $D$  and the vector  $B$  is also destroyed in the
process;
begin
  real w; integer j;
  D[1] := D[1]/B[1]; w := B[1];
  for j := 2 step 1 until n do
```

```

    begin B[j - 1] := C[j - 1]/w; w := B[j] - A[j - 1]
      × B[j - 1];
      D[j] := (D[j] - A[j - 1] × D[j - 1])/w end;
  for j := 1 step 1 until n - 1 do
    D[n - j] := D[n - j] - B[n - j] × D[n - j + 1]
  end TRIDAG
```

¹ D. W. PEACEMAN AND H. H. RACHFORD, JR., The Numerical Solution of Parabolic and Elliptic Differential Equations, *Journal of the Soc. for Ind. and Applied Math.* Vol. 3 March 1955.

ALGORITHM 25

REAL ZEROS OF AN ARBITRARY FUNCTION

B. LEAVENWORTH

American Machine and Foundry Co., Greenwich, Conn.

```

procedure ZEROS(n, C, FUNCTION, m, ep1, ep2, ep3, eta);
integer n, m; real ep1, ep2, ep3, eta; array C;
procedure FUNCTION;
```

comment: This procedure finds the real zeros of an arbitrary function using Muller's method^{1, 2} and is adapted from a FORTRAN code by Frank.³ Each iteration determines a zero of the quadratic passing through the last three function values. Parameters include the number of roots desired n . If C_i is zero, starting values are $-1, 1, 0$ respectively. If $C_i = \beta$ then the starting values are $.9\beta, 1.1\beta, \beta$. The procedure FUNCTION(rt , frt) must be supplied to evaluate the function value frt , given the argument rt . m is the maximum number of iterations permitted. $ep1$ is the relative convergence criterion on successive iterates. $ep2$ is the absolute convergence criterion on the function value. eta is the spread for multiple roots, that is, if $|rt - C_i| < ep3$ where C_i is a previously found root, then rt is replaced by $rt + eta$;

```

begin integer L, jk, i, mm; real p, p1, p2, x0, x1, x2, rt,
  frt, fp1, d, dd, di, h, bi, den, dn, dm, tem;
  switch S: S1, S2, S3, S4;
  for L := 1 step 1 until m do
    begin jk := 0; if C[L] = 0 then go to initial else
      go to assign;
    initial: p := -1; p1 := 1; p2 := 0; go to start;
    assign: p := .9 × C[L]; p1 := 1.1 × C[L]; p2 := C[L];
    start: rt := p; go to fn;
    enter: go to S[if jk < 4 then jk else 4];
    S1: rt := p1; x0 := fp1; go to fn;
    S2: rt := p2; x1 := fp1; go to fn;
    S3: x2 := fp1; h := if C[L] = 0 then -1
      else -.1 × C[L]; d := -.5;
    loop: dd := 1 + d; bi := x0 × d ↑ 2 - x1 × dd ↑ 2 × x2 ×
      (dd + d);
      den := bi ↑ 2 - 4 × x2 × d × dd × (x0 × d - (x1 × dd) + x2);
      if den ≤ 0 then den := 0 else den := sqrt(den);
      dn := bi + den; dm := bi - den;
      if abs(dn) ≤ abs(dm) then den := dm else den := dn;
      if den = 0 then den := 1;
      di := -2 × x2 × dd / den; h := di × h; rt := rt + h;
      go to if abs(h/rt) < ep1 then call else fn;
    S4: if abs(fp1) < abs(x2 × 10) then
      begin x0 := x1; x1 := x2; x2 := fp1; d := di;
        go to loop end else begin di := di × .5; h := h × .5;
          rt := rt - h; go to fn end;
    fn: jk := jk + 1; if jk < m then mm := 1 else mm := 0;
    call: FUNCTION(rt, frt); if mm = 1 then go to compute
      else go to root;
```

```

compute: fprt := frt ;
  for i := 2 step 1 until L do
    begin tem := rt - C[i-1] ; if abs(tem) < ep3 then go to
    change else fprt := fprt/tem end
test: if abs(frt) < ep2 ^ abs(fprt) < ep2 then go to root
  else go to enter ;
change: rt := rt + eta ; jk := jk - 1 ; go to fn ;
root: C[L] := rt end L
end ZEROS

```

¹ D. E. MULLER, A Method for Solving Algebraic Equations Using an Automatic Computer, *MTAC 10* (1956).

² W. L. FRANK, Finding Zeros of Arbitrary Functions, *J. ACM* 5 (1958).

³ W. L. FRANK, RWGRT, General Root Finder 704 FORTRAN Source Language Subroutine SHARE Distribution # 635. Parameters used by Frank are: $ep1 = 10^{-6}$, $ep2 = 10^{-20}$, $ep3 = 10^{-20}$, $eta = 10^{-3}$.

REMARK ON ALGORITHM 25

REAL ZEROS OF AN ARBITRARY FUNCTION
(B. Leavenworth, *Comm. ACM*, November 1960)

ROBERT M. COLLINGE

Burroughs Corporation, Pasadena, California

On attempting to use this algorithm, I discovered the two following errors:

- (1) The line following the SWITCH statement should read:
for L := 1 step 1 until n do
- (2) The line starting with the label loop: should read:
loop: dd := 1 + d ; bi = $x_0 \times d \uparrow 2 - x_1 \times dd \uparrow 2$
+ $x_2 \times (dd + d)$;

With these two modifications incorporated the algorithm was translated into the language of the Burroughs Algebraic Compiler and has been used successfully on the Burroughs 220 Computer.

SEE ALGORITHM 2

ALGORITHM 26

ROOTFINDER III (Modification of Algorithm 15.
Rootfinder II, Henry C. Thacher, Jr., *Comm. ACM*,
August 1960)

JOHN G. HERRIOT, Stanford University, Stanford, California

procedure ROOTIII (f, a, eps, n, g, c, m) ; **integer** n, m ;
real procedure f ; **real** a, eps, g, c ;

comment ROOTIII computes a value of $g = y$ satisfying the equation $y = f(y)$. The iteration will converge to Y providing that at some time in the iteration a g is reached such that $\text{abs}(g - Y) \times \text{abs}(d(df/dy)/dy) < 2 \times \text{abs}((df/dy) - 1)$, where the derivatives are evaluated at Y. Input includes: (1) f, a procedure for computing f(y), (2) a, an initial approximation to the root, (3) eps, a tolerance for the relative error in g, and (4) n, a maximum number of iterations to be performed. Output includes: (1) g, the required root, (2) $c = f(g) - g$, (3) m, a parameter indicating the success of the procedure. If the tolerance was not met $m < 0$. The number $|m| - 1$ gives the number of times that the correction to g exceeded the preceding one. If $f(y) - y$ has the same value for two successive approximations to g, then $h = 1$, and we exit to "alarm", a nonlocal label. Alarm should provide a means of deciding whether g is an acceptable root or not. ;

```

begin integer j ; real b, d, h ;
m := 1 ; j := 0 ; c := 0 ;
if f(0) = 0 then begin g := 0 ;
go to return end ;
g := f(a) ; b := d := c := g - a ;
if c = 0 then go to return ;
for j := 1 step 1 until n do
begin c := f(g) - g ;
if  $\text{abs}(c) \leq \text{abs}(g) \times \text{eps}$  then go to return ;
h := b/c ;
if h = 1 then go to alarm ;
if  $h > 0 \wedge h < 2$  then m := m + 1 ;
d := d/(h - 1) ; b := c ; g := g + d
end iteration ;
m := - m ; return : end

```

SEE ALGORITHM 2

ALGORITHM 27

ASSIGNMENT

ROLAND SILVER

MIT Lincoln Laboratory,* Lexington, Massachusetts

procedure Assignment(d, n, x) ; **value** n ; **integer** n ;
array d ; **integer array** x ;
comment: Assignment determines that permutation x of the
integers [1:n] for which the sum $(i := 1(1)n)$ of
the elements $d[i, x[i]]$ of the $n \times n$ matrix d is a
minimum. $n \geq 2$. For more complete information
see: An Algorithm for the Assignment Problem,
Roland Silver, *Comm. ACM*, Nov. 1960, p. 605 ;

```

begin
switch Switch := NEXT, L1, NEXT1, MARK ;
array a[1:n, 1:n] ;
integer array c[1:n], cb[1:n], lambda[1:n], mu[1:n],
r[1:n], y[1:n] ;
integer cbl, cl, cl0, i, j, k, l, rl, rs, sw ;
comment:
INITIALIZE ;
for i := 1 step 1 until n do
begin min := d[i, 1] ;
for j := 2 step 1 until n do if d[i, j] < min then min
:= d[i, j] ;
for j := 1 step 1 until n do a[i, j] := d[i, j] - min
end i ;
for j := 1 step 1 until n do
begin min := a[1, j] ;
for i := 2 step 1 until n do if a[i, j] < min then min
:= a[i, j] ;
for i := 1 step 1 until n do a[i, j] := a[i, j] - min
end j ;
for i := 1 step 1 until n do x[i] := y[i] := 0 ;
for i := 1 step 1 until n do
begin
for j := 1 step 1 until n do
begin
if  $a[i, j] \neq 0 \vee x[i] \neq 0 \vee y[j] \neq 0$  then go to J1 ;
x[i] := j ; y[j] := i
end j ;
end i ;
J1: comment: Start labeling ;
rl := cl := 0 ; rs := 1 ;
for i := 1 step 1 until n do

```

```

begin mu[i] := lambda[i] := 0 ;
if x[i] ≠ 0 then go to I1 ;
rl := rl + 1 ; r[rl] := i ; mu[i] := -1
I1: end i ;
LABEL: comment: Label and scan ;
i := r[rs] ; rs := rs + 1 ;
for j := 1 step 1 until n do
begin if a[i, j] ≠ 0 or lambda[j] ≠ 0 then go
to J2 ;
lambda[j] := i ; cl := cl + 1 ; c[cl] := j ;
if y[j] = 0 then go to MARK ;
rl := rl + 1 ; r[rl] := y[j] ; mu[y[j]] := i
J2: end j ;
if rs ≤ rl then go to LABEL ;
comment:
RENORMALIZE ;
sw := 1 ; cl0 := cl ; cbl := 0 ;
for j := 1 step 1 until n do
begin if lambda[j] ≠ 0 then go to J3 ;
cbl := cbl + 1 ; cb[cbl] := j
J3: end j ;
min := a[r[i], cb[i]] ;
for k := 1 step 1 until rl do
begin
for l := 1 step 1 until cbl do if a[r[k], cb[l]] ≤ min
then min := a[r[k], cb[l]]
end k ;
for i := 1 step 1 until n do
begin if mu[i] ≠ 0 then go to I2 ;
for l := 1 step 1 until cl0 do a[i, c[l]] := a[i, c[l]] + min ;
go to I3 ;
I2: for l := 1 step 1 until cbl do
begin a[i, cb[l]] := a[i, cb[l]] - min ;
go to Switch[sw] ;
NEXT: if a[i, cb[l]] ≠ 0 ∨ lambda[cb[l]] ≠ 0 then go to L1 ;
lambda[cb[l]] := i ;
if y[cb[l]] = 0 then
begin j := cb[l] ; sw := 2 ; go to L1 end ;
cl := cl + 1 ; c[cl] := cb[l] ;
rl := rl + 1 ; r[rl] := y[cb[l]] ;
L1: end l ;
I3: end i ;
go to Switch[sw + 2] ;
NEXT1: if cl0 = cl then go to LABEL ;
for i := cl0 + 1 step 1 until cl do mu[y[c[i]]] := c[i] ;
go to LABEL ;
MARK: comment: mark new column and permute ;
y[j] := i := lambda[j] ;
if x[i] = 0 then begin x[i] := j ; go to
START end ;
k := j ; j := x[i] ; x[i] := k ;
go to MARK
end Assignment

```

* Operated with support from the U. S. Army, Navy and Air Force.

[NOTE: The reader should distinguish between the letter l and the figure 1, both of which appear in the above algorithm.—Ed.]

CERTIFICATION OF ALGORITHM 27 ASSIGNMENT [Roland Silvers, *Comm. ACM* 3, Nov. 1960].

ROBERT D. WITTY
Burroughs Corp., Detroit, Mich.

Assignment was successfully run on the Burroughs B5000 using Burroughs extended ALGOL 60.

Input Array

60	0	0	76	0	0
0	40	18	0	60	24
60	16	2	4	0	40
0	27	18	3	55	75
0	40	62	16	11	53
28	4	10	84	0	16

Solution Vector: X(6, 4, 3, 1, 5, 2)

The following changes were made in the algorithm prior to its successful run:

```

FROM MIN := a[r[i], cb[i]];
TO MIN := a[r[1], cb[1]];
FROM if X[i] = 0 then begin X[i] := j;
go to START end;
TO if X[i] = 0 then begin X[i] := j;
for i := 1 step 1 until N do begin if X[i] = 0 then go
to START;
end; go to EXIT; end;
FROM end ASSIGNMENT
TO EXIT: end; ASSIGNMENT

```

CERTIFICATION OF ALGORITHM 27 ASSIGNMENT [Roland Silver, *Comm. ACM*, Nov. 1960] ALBERT NEWHOUSE University of Houston, Houston, Texas

The ASSIGNMENT algorithm was translated into MAD and successfully run on the IBM 709/7094 after the following corrections were made:

All references to array *a* and *d* refer to the same array, i.e. change all *a*[*i*, *j*] to *d*[*i*, *j*]. Furthermore:

(a) 3rd line after LABEL: comment: Label and scan;
should read

```
begin if d[i, j] ≠ 0 ∨ lambda[j] ≠ 0 then go
```

(b) first line after J3: end j;
should read

```
min := d[r[1], cb[1]];
```

(c) line I2:
should read

```
I2: for l := 1 step 1 until cbl do
```

Since there is no provision made for this algorithm to end the following additions were made:

(1) in the integer declaration add the variable: *flag*

(2) first line after START: comment: ...
add the line

```
flag := n;
```

(3) first line before I1: end i;
change to read

```
rl := rl + 1; r[rl] := i; mu[i] := -1; flag := flag - 1
```

(4) add a line after I1: end i;
if flag = n then go to FINI;

(5) change the last line of the algorithm to read:

```
FINI: end Assignment
```

In order to obtain the minimum value of the $\sum_{i=1}^n a_{ix_i}$ (in the following called total) the following additions may be made:

Add a real variable *total* and
 (A) new line after *INITIALIZE*;
 total := 0;
 (B) new line after the first *end i*;
 total := *total* + *min*;
 (C) new line after the first *end j*;
 total := *total* + *min*;
 (D) after the line *end k*; after *J3: end j*;
 add the line
 total := *total* + (*rl+cbl-n*) × *min*;

ALGORITHM 28 LEAST SQUARES FIT BY ORTHOGONAL POLYNOMIALS

JOHN G. MACKINNEY

General Kinetics Incorporated, Arlington 6, Virginia

```

procedure LSFIT (f, x1, xm, m, k, alpha, beta, sigma, s, p) ;
  value x1, xm, m, k ; real x1, xm ; integer
    m, k ;
  real array f, alpha, beta, sigma, s, p ;
comment LSFIT accepts m values of the function f at equal
  intervals of the abscissa from x1 through xm, and obtains in
  p[0] through p[k] the coefficients of the best polynomial ap-
  proximation of degree k or less (least squares) as programmed
  by George E. Forsythe, Journal SIAM 5, no. 2, June 1957,
  with only minor variations. The output values alpha [1:k],
  beta [0:k], and s [0:k] enable the user to make final adjust-
  ments to the results, according to the statistic sigma [0:k].
  LSFIT uses the procedure POLYX (a, b, c, d, n) to trans-
  form its results from the interval (-2, 2) to the interval (x1,
  xm) ;
begin integer i, j ; real dummy, x, xone, deltax, delsq,
  omega, lastw, thisw ;
  real array cthisp, cpoly [0:k], clastp [-1:k],
  lastp, thisp [1:m] ;
  Boolean swx ;
comment Initialization ;
  swx := true ; beta [0] := clastp [0] := clastp [-1] :=
  delsq := omega := 0 ;
  cthisp [0] := 1 ; thisw := m ;
  for i := 1 step 1 until m do
    begin delsq := delsq + f[i]2 ;
      thisp [i] := 1 ; lastp [i] := 0 ;
      omega := omega + f[i] end ;
  s [0] := cpoly [0] := omega/thisw ;
  delsq := delsq - s [0] × omega ;
  sigma [0] := delsq/(m-1) ;
comment Transformation of abscissa ; i := m + 2 ;
  if 2×i = m then deltax := 4/(m-1) else deltax :=
  4/m ; xone := -2 ;
comment Main Computation loop ;
  for i := 0 step 1 until k-1 do
    begin dummy := 0 ; x := xone ;
      1: for j := 1 step 1 until m do
        begin dummy := dummy + x × thisp [j] ↑ 2 ;
          x := x + deltax end ;
        2: alpha [i + 1] := dummy/thisw ;
          lastw := thisw ;
          thisw := omega := 0 ;
          x := xone ;
        3: for j := 1 step 1 until m do
          begin dummy := beta [i] × lastp [j] ;
            lastp [j] := thisp [j] ;

```

```

      thisp [j] := (x - alpha [i + 1]) × thisp [j]
      - dummy ;
      thisw := thisw + thisp [j] ↑ 2 ;
      omega := omega + f [j] × thisp [j] ;
      x := x + deltax end ;
    4: beta [i + 1] := thisw / lastw ;
      s[i + 1] := omega / thisw ;
      delsq := delsq - s[i + 1] × omega ;
      sigma [i + 1] := delsq / (m - i - 1) ;
      if swx then go to 6 ;
    5: cpoly [i + 1] := 0 ; go to 9 ;
comment Termination of main loop when higher power will
  not improve fit ;
    6: if sigma [i + 1] < sigma [i] then go to 7 ;
      swx := false ; go to 5 ;
comment Recursion for polynomial coefficients ;
    7: for j := 0 step 1 until i do
      begin dummy := clastp [j] × beta [i] ;
        clastp [j] := cthisp [j] ;
        cthisp [j] := clastp [j - 1] - alpha [i + 1] × cthisp [j] - dummy ;
        cpoly [j] := cpoly [j] + s [i + 1] × cthisp [j] end ;
      8: cpoly [i + 1] := s [i + 1]
        cthisp [i + 1] := 1 ;
      9: clastp [i + 1] := 0 end of main
  computation loop, transformation of polynomial follows ;
  begin real a, b ;
    a := deltax × (m - 1) / (xm - x1) ;
    b := xone - a × x1 ;
    POLYX (a, b, cpoly, p, k) end
end of LSFIT

```

REMARK ON ALGORITHM 28
 LEAST-SQUARES FIT BY ORTHOGONAL POLYNOMIALS (John G. MacKinney, *Comm. ACM* 3 (Nov. 1960))

D. B. MACMILLAN

Knolls Atomic Power Laboratory, General Electric Co., Schenectady, N. Y.

The algorithm obtains the coefficients of the fitted polynomial of lowest degree such that an increase in the degree would cause an increase in the statistic sigma (sigma squared in Forsythe's notation). A significant decrease in sigma, as one goes from a fitted polynomial to one of higher degree, indicates that the increase in degree causes an improvement in the fit to the function underlying the data, rather than merely following more closely the random variations about that function introduced by the physical measurement process.

If one of the orthogonal polynomials, say the one of *i*th degree, is missing from the underlying function, and some of the orthogonal polynomials of higher degree are present, then the fitted polynomial of *i*th degree will not be a real improvement over that of (*i* - 1)-th degree, but higher order fitted polynomials will be a real improvement. For example, in one of our recent routine problems the coefficient of the second degree orthogonal polynomial was quite small, and the first few values of sigma, starting with sigma (1), were .255, .264, .062, .046, .048. The algorithm would have chosen the first degree fitted polynomial as "best", but the third and fourth degree fitted polynomials were clearly better than it.

This loophole may be plugged by modifying the algorithm so it computes the coefficients of the polynomial of lowest degree *j* for which it is true that

$$\sigma(i + 1) \geq \sigma(i)$$

and that

$$\sigma(j) \geq .6 \sigma(i) \quad j = i+2, i+3, \dots, k,$$

(.6 was chosen arbitrarily).

ALGORITHM 29
POLYNOMIAL TRANSFORMER
JOHN G. MACKINNEY
 General Kinetics Inc., Arlington 6, Virginia

```

procedure POLYX (a, b, c, d, n) ; value a, b, n ; integer
  n ; real a, b ;
  real array c, d ;
comment POLYX computes coefficients d0, d1, ..., dn of the
  transformed polynomial p(t) given c0, c1, ...,
  cn of p(x) where x = at + b ;
begin integer i, j, k ; real array z, w [0:n] ;
  w[0] := z[0] := 1 ; d[0] := c[0] ;
  for i := 1 step 1 until n do
    begin w[i] := 1 ; z[i] := b × z[i - 1] ;
      d[0] := d[0] + c[i] × z[i] ;
    end of initialization ;
    for j := 1 step 1 until n do
      begin w[0] := w[0] × a ; d[j] := c[j] × w[0] ;
        k := 1 ;
        for i := j + 1 step 1 until n do
          begin w[k] := a × w[k] + w[k - 1] ;
            d[j] := d[j] + c[i] × w[k] × z[k] ;
          end ;
          k := k + 1 end ;
    end ;
  end of POLYX polynomial transformer

```

ALGORITHM 30
NUMERICAL SOLUTION OF THE POLYNOMIAL
EQUATION

K. W. ELLENBERGER
 Missile Division, North American Aviation, Downey,
 California

```

procedure ROOTPOL (n, a, L, F, u, v, CONV) ;
  value n, a, L, F ; integer L, F, n ;
  array a, u, v, CONV ;
comment The Bairstow and Newton correction formulae are
  used for a simultaneous linear and quadratic iterated synthetic
  division. The coefficients of a polynomial of degree n are given as
  ai (i = 0, ..., n) where an is the constant term. The coeffi-
  cients are scaled by dividing them by their geometric mean.
  The Bairstow or Newton iteration method will nearly always
  converge to the number of figures carried, F, either to root
  values or to their reciprocals. If the simultaneous Newton and
  Bairstow iteration fails to converge on root values or their
  reciprocals in L iterations, the convergence requirement will be
  successively reduced by one decimal figure. This program antici-
  pates and protects against loss of significance in the quadratic
  synthetic division. (Refer to "On Programming the Numerical
  Solution of Polynomial Equations," by K. W. Ellenberger,
  Commun. ACM 3 (Dec. 1960), 644-647.) The real and imaginary
  part of each root is stated as u[i] and v[i], respectively, together
  with the corresponding constant, CONVi, used in the con-
  vergence test. This program has been used successfully for over
  a year on the Bendix G15-D (InterCard System) and has recently
  been coded for the IBM 709 (Fortran System);
  begin integer i, j, m ; array h, b, c, d, e[-2:n] ;
  real t, K, ps, qs, pt, qt, s, rev, r ;
ROOTPOL: b-1 := b-2 := c-1 := c-2 := d-1 := d-2 := e-1 :=
  e-2 := 0 ;
  for j := 0 step 1 until n do hj := aj ; t := 1 ;
  K := 10F ;

```

```

ZROTEST: if hn = 0 then
  begin un := 0 ; vn := 0 ; CONVn := K ;
    n := n - 1 ; go to ZROTEST
  end ;
INIT: if n = 0 then go to RETURN ;
  ps := qs := pt := qt := s := 0 ;
  rev := 1 ; K := 10F ;
  if n = 1 then
    begin r := -h1/h0 ; go to LINEAR
  end ;
  for j := 0 step 1 until n do
    begin
      if hj = 0 then s := s else s := s + log(abs(hj))
    end ; s := s10 ;
    for j := 0 step 1 until n do hj := hj/s ;
    if abs(h1/h0) < abs(hn-1/hn) then
      begin t := -t ; m := entier ((n+1)/2) ;
        for j := 0 step 1 until m do
          begin s := hj ; hj := hn-j ; jn-j := s
        end ;
      end ;
      if qs ≠ 0 then
        begin p := ps ; q := qs ; go to ITERATE
      end ;
      if hn-2 = 0 then
        begin q := 1 ; p := -2
      end else
        begin q := h/hn-2 ; p := (hn-1 - q × hn-2)/hn-2
      end ;
      if n = 2 then go to QADRTIC ; r := 0 ;
ITERATE: for i := 1 step 1 until L do
  begin
BAIRSTOW: for j := 0 step 1 until n do
    begin bj := hj - p × bj-1 - q × bj-2 ;
      cj := bj - p × cj-1 - q × cj-2
    end ;
    if nn-1 = 0 then go to BNTEST ;
    if bn-1 = 0 then go to BNTEST ;
    if abs(hn-1/bn-1) < K then go to NEWTON ;
    bn := hn - q × bn-2 ;
    if bn = 0 then go to QADRTIC ;
    if K < abs(hn/bn) then go to QADRTIC ;
NEWTON: for j := 0 step 1 until n do
    begin dj := hj + r × dj-1 ; ej := dj + r × ej-1
    end ;
    if dn = 0 then go to LINEAR ;
    if K < abs(hn/dn) then go to LINEAR ;
    cn-1 := -p × cn-2 - q × cn-3 ;
    s := cn-2 - cn-1 × cn-3 ;
    if s = 0 then
      begin p := p - 2 ; q := q × (q + 1)
    end else
      begin p := p + (bn-1 × cn-2 - bn × cn-3)/s ;
        q := q + (-bn-1 × cn-1 + bn × cn-2)/s
      end ;
    if en-1 = 0 then r := r - 1 else r := r - dn/en-1
  end ; ps := pt ; qs := qt ; pt := p ;
  qt := q ;
  if rev < 0 then K := K/10 ; rev = -rev ;
  go to REVERSE ;
LINEAR: if t < 0 then r := 1/r ; un := r ; vn := 0 ;
  CONVn := K ; n := n - 1 ;
  for j := 0 step 1 until n do hj := dj ;
  if n = 0 then go to RETURN ;
  go to BAIRSTOW ;
QADRTIC: if t < 0 then
  begin p := p/q ; q := 1/q
  end ;
  if 0 < (q - (p/2)2) then

```

```

begin un := un-1 := -p/2 ;
s := sqrt (q - (p/2)2) ; vn := s ;
vn-1 := -s
end else
begin s := sqrt ((p/2)2 - q) ;
if p < 0 then un := -p/2 + s
else un := -p/2 - s ; un-1 := q/un ;
vn := vn-1 := 0
end ; CONVn := CONVn-1 := K ;
n := n-2 ;
for j := 0 step 2 until n do hj := bj ;
go to INIT ;

```

RETURN: end

CERTIFICATION OF ALGORITHM 30 NUMERICAL SOLUTION OF THE POLYNOMIAL EQUATION (K. W. Ellenberger, *Comm. ACM*, Dec. 1960)

WILLIAM J. ALEXANDER
 Argonne National Laboratory, * Argonne, Ill.

ROOTPOL was coded by hand for the LGP-30 using the ACT-III Compiler with 24 bits of significance. The following corrections were found necessary.

- (a) b₋₁ := b₋₂ := c₋₁ := c₋₂ := d₋₁ := d₋₂ := e₋₁ := e₋₂ := 0 should be
 b₋₁ := b₋₂ := c₋₁ := c₋₂ := d₋₁ := e₋₁ := h₋₁ := 0
- (b) m := entier ((n+1)/2) should be
 m := entier ((n-1)/2)
- (c) j_{n-1} := s should be h_{n-1} := s
- (d) q := h/h_{n-2} should be h_n/h_{n-2}
- (e) c_j := b_j - p × c_{j-1} - q × c_{j-2} should be
 c_j := b_j - p × c_{j-1} - q × c_{j-2}
- (f) if n_{n-1} = 0 then go to BNTEST should be
 if h_{n-1} = 0 then go to BNTEST
- (g) s := sqrt (q - (p/2)²) should be
 s := sqrt (q - (p/2)²)
- (h) for j := 0 step 2 until n do h_j := b_j should be
 for j := 0 step 1 until n do h_j := b_j
- (i) go to BAIRSTOW should be go to ITERATE

The following correction was found necessary in the given example (Refer to "On Programming the Numerical Solution of Polynomial Equations," by K. W. Ellenberger, *Comm. ACM* 3, Dec., 1960):

$$f(x) = (.10098) 10^8 x^4 - (.98913) 10^6 x^3 + (.10000) 10^6 x + (.10000) 10^1 = 0 \text{ should be}$$

$$f(x) = (.10098) 10^8 x^4 - (.98913) 10^6 x^3 - (.10990) 10^6 x^2 + (.10000) 10^6 x + (.10000) 10^1 = 0$$

With these corrections the results obtained agree with those given in the example.

For equations of higher order it was found necessary to avoid repeated scaling of the reduced equation in order to prevent floating point overflow. The range on the exponent in the ACT III system is $-32 \leq e \leq 31$.

Further floating point overflow difficulties were experienced when certain coefficients in the reduced equation became small but not zero. The following additions were made to avoid this fault:

- (a) for j := 0 step 1 until n do h_j := d_j was replaced by
 for j := 0 step 1 until n do begin if abs (h_j/d_j) < K then
 h_j := d_j else h_j := 0 end
- (b) for j := 0 step 1 until n do h_j := b_j was replaced by
 for j := 0 step 1 until n do begin if abs (h_j/b_j) < K then
 h_j := b_j else h_j := 0 end

With the above changes the following results were obtained:

$$x^4 - 3x^3 + 20x^2 + 44x + 54 = 0$$

$$x = -.9706390 \pm 1.005808i$$

$$x = 2.470639 \pm 4.640533i$$

$$x^4 - 2x^3 + 2x^2 + x^2 + 6x^2 - 6x + 8 = 0$$

$$x = -.9999999 \pm .9999999i$$

$$x = 1.500000 \pm 1.322876i$$

$$x = .5000002 \pm .8660251i$$

$$x^5 + x^4 - 8x^3 - 16x^2 + 7x + 15 = 0$$

$$x = 3.000001$$

$$x = -2.000000 \pm 1.000001i$$

$$x = -.9999997$$

$$x = .9999998$$

CERTIFICATION OF ALGORITHM 30 NUMERICAL SOLUTION OF THE POLYNOMIAL EQUATION [K. W. Ellenberger, *Comm. ACM* 3 (Dec. 1960), as corrected in the previous Certification by William J. Alexander, *Comm. ACM* 4 (May 1961)]

KALMAN J. COHEN

Graduate School of Industrial Administration, Carnegie
 Institute of Technology, Pittsburgh, Pa.

The ROOTPOL procedure originally published by Ellenberger as corrected and modified by Alexander was coded for the Bendix G20 in 20-GATE. Some serious errors were found in the third and fourth lines above the statement labelled "REVERSE" in Ellenberger's Algorithm which were not mentioned in Alexander's Certification. First, the function "log" is not a standard function in ALGOL 60; it is clear from the context, however, that Ellenberger intends this to be the logarithm function to the base 10. Second, Ellenberger's Algorithm failed to divide the accumulated sum of the logarithms by n+1 before taking the antilogarithm.

The correct, and slightly simplified, manner in which the third and fourth lines above the statement labelled "REVERSE" should read is:

```

if hj ≠ 0 then s := ln(abs(hj))
end; s := s/(n+1); s := exp(s);

```

With these corrections, the numerical results obtained essentially agree with those reported by Alexander.

ALGORITHM 31 GAMMA FUNCTION

ROBERT M. COLLINGE

Burroughs Corporation, Pasadena, California

real procedure Gamma (x); real x;

comment For x in the range $2 \leq x \leq 3$ an approximating polynomial is used. In this range the maximum absolute error $\epsilon(x)$ is $|\epsilon(x)| < 0.25 \times 10^{-7}$. For $x > 3$ we write $\Gamma(x) = (x-1)(x-2) \dots (x-n)\Gamma(x-n)$ where $2 \leq (x-n) \leq 3$, and for $x < 2$ we write

$$\Gamma(x) = \frac{\Gamma(x+n)}{x(x+1) \dots (x+n-1)} \text{ where } 2 \leq (x-n) \leq 3. \text{ For } x = 0$$

or a negative integer $\Gamma(x)$ is set equal to a large value 10^{90} .

begin

real h, y;

h := 1.0; y := x;

A1: if y = 0 then h := 10⁹⁰

else if y = 2.0 then go to A2

else if y < 2.0 then begin

h := h/y; y := y + 1.0; go to A1 end


```

else if y ≥ 3.0 then begin
y := y - 1.0; h := h × y; go to A1 end
else begin y := y - 2.0;
h := (((((((0.0016063118 × y + .0051589951) × y
+ .0044511400) × y + .0721101567) × y
+ .0821117404) × y + .4117741955) × y
+ .4227874605) × y + .9999999758) × h end;

```

A2: Gamma := h end Gamma.

CERTIFICATION OF ALGORITHM 31

GAMMA FUNCTION [R. M. Collinge, *Comm. ACM*, Feb. 61]

PETER G. BEHREZ

Mathematikmaskinnämnden, Stockholm, Sweden

GAMMA was successfully run on FACIT EDB using FACIT-ALGOL 1, which is a realization of ALGOL 60 for FACIT EDB. No changes in the program were necessary. The relative error was as stated in the comment of GAMMA about 10^{-4} .

ALGORITHM 32

MULTINT

R. DON FREEMAN JR.

Michigan State University, East Lansing, Michigan

```

real procedure MULTINT (n, Low, Upp, Funev, s, P, u, w);
value n;
real procedure Low, Upp, Funev; array s, u,
w; integer n;

```

comment MULTINT will perform a single, double, triple, ..., T-order integration depending on whether $n=1, 2, \dots, T$. The result is:

$$\text{MULTINT} = \int_{\text{Low}(1)}^{\text{Upp}(1)} \text{Funev}(1, x_1) dx_1 \int_{\text{Low}(2, x_1)}^{\text{Upp}(2, x_1)} \text{Funev}(2, x_1, x_2) dx_2 \dots \int_{\text{Low}(n, x_1, \dots, x_{n-1})}^{\text{Upp}(n, x_1, \dots, x_{n-1})} \text{Funev}(n, x_1, \dots, x_n) dx_n$$

The variable of integration is $x[j]$. $j=1$ refers to the outermost integral, $j=n$, the innermost integral. The code divides each interval equally into $s[j]$ subintervals and performs a P-point Gaussian integration on each subinterval with weight functions $w[k[j]]$ and abscissas $u[k[j]]$. P is the size of the arrays of weight functions and abscissas and must be provided by the main code along with these arrays.

Since the values $x[1], x[2], \dots, x[n]$, are stored in an array, as are a, b, c, d, r , it is necessary to substitute an integer for the upper bound T of these arrays before the program is executed. This means, for example, if 3 is substituted for T, then the procedure will not do a 4th order integral unless it is retranslated with $T \geq 4$.

The values of the lower and upper bounds and functions must of course be specified at the time of use. If each of these constituted a separate procedure, it would require writing and translating 3n different procedures. This is eliminated by grouping them into Low, Upp, and Funev which compute the lower and upper bounds and value of the functions respectively in each of the j th integrals. Since these are each essentially a collection of "subprocedures," the first statement of each should be a switch directing the code to the "subprocedure" which is used in the j th integral. Note that, for example, $\text{Low}(3, x)$ is formally a function of $x[1], x[2], \dots, x[T]$; this is done merely because it is more convenient to make $\text{Low}(j, x)$ formally a function of the whole array x for all j . Actually of course $\text{Low}(3, x)$ would be a function of $x[1]$ and $x[2]$ only;

```

begin real array a, b, c, d, r, x[1:T];
integer array k, h[1:T]; real f; integer j, m;
for j := 1 step 1 until T do
x[j] := 0.0;
m := 1;
r[n+1] := d[n+1] := 1.0;
setup: for j := m step 1 until n do
begin
a[j] := Low(j, x);
b[j] := Upp(j, x);
d[j] := (b[j] - a[j]) / s[j];
c[j] := a[j] + 0.5 × d[j];
x[j] := c[j] + 0.5 × d[j] × u[1];
r[j] := 0.0;
h[j] := k[j] := 1; end;
j := n;
sum: f := Funev(j, x);
r[j] := r[j] + r[j+1] × d[j+1] × f × w[k[j]];
if (k[j] < P) then go to labk;
if (h[j] < s[j]) then go to labh;
j := j - 1;
if (j = 0) then go to exit;
go to sum;
labh: h[j] := h[j] + 1;
c[j] := a[j] + (h[j] - 0.5) × d[j];
k[j] := 1;
go to initialx;
labk: k[j] := k[j] + 1;
initialx: x[j] := c[j] + 0.5 × d[j] × u[k[j]];
if (j = n) then go to sum;
m := j + 1;
go to setup;
exit: MULTINT := r[1] × d[1] × 0.5 ↑ n; end

```

CERTIFICATION OF ALGORITHM 32

MULTINT [R. Don Freeman, *Comm. ACM*, Feb. 1961]

HENRY C. THACHER, JR.*

Reactor Engineering Div., Argonne National Laboratory, Argonne, Ill.

* Work supported by the U. S. Atomic Energy Commission.

The procedure was transcribed into the ACT-III language for the LGP-30 computer, and was tested on the integrals:

$$(1) \int_0^1 \int_0^1 \int_0^1 \int_0^1 k[\cos u - 7u \sin u - 6u^2 \cos u + u^3 \sin u] dw dx dy dz = \sin k$$

where $u = kxyz$, and

$$(2) \int_0^1 \int_0^{\sqrt{1-x^2}} \int_0^{\sqrt{1-x^2-y^2}} \frac{dz dy dx}{x^2 + y^2 + (z - k)^2} = \pi \left(2 + \frac{1}{2} \left(\frac{1}{k} - k \right) \log \left| \frac{1+k}{1-k} \right| \right)$$

The ALGOL procedures for the second integral are:

```

real procedure Low (j, x);
Low := 0;
real procedure Upp(j, x); comment z ≡ x[3], y ≡ x[2], x ≡
x[1];
begin
integer i; real temp;
temp := 1.0;
for i := j - 1 step - 1 until 1 do
temp := temp - x[i] × x[i];
Upp := sqrt(temp)
end;

```

```

real procedure Funev(j,x);
comment The real parameter k is global;
Funev := if j < 3 then 1.0 else 1/(x[1]×x[1]+x[2]×x[2]+(x[3]-k)
↑ 2);

```

The first integral was tested only with $s[j] = 1$, and with various Gaussian formulas for integrals over the interval $(-1, +1)$. Results were as follows:

k	$\pi/2$	π	$3\pi/2$	2π
true	1.000000	0.000000	-1.000000	0.000000
p = 2	0.993704	-0.0333603	+0.020166	6.881490
p = 3	1.000032	0.0000848	-1.061651	-0.597419
p = 4	0.999999	0.0000001	-0.998407	+0.0027035
p = 5	1.000000	-0.0000002	-1.000028	-0.0007857

For the second integral, two values of $s = s[1] = s[2] = s[3]$ were used, and two values of p . Results were as follows:

k	$1/2$		2	
true	11.46027376		1.10609687	
s	1	2	1	2
p = 2	5.454460	11.838651	1.0368770	1.1184305
p = 3	9.361666	12.408984	1.1343551	1.1094278

The effect of the pole at $(0,0,k)$ is obvious.

For the algorithm to run in any compiler, the semicolon following $x[T]$; in the fourth line above the end of the comment must be deleted. The array bounds on the arrays r and d must be increased to $[1 : T+1]$.

For a system which permits variable array bounds, the introduction of the integer T appears superfluous. For such a system, T may be replaced by n throughout with a probable gain in efficiency. For most translators, the presence of undefined elements in an array will not cause difficulties, provided these elements do not appear in an expression before they are assigned a value.

The statement "for $j := 1$ step 1 until T do $x[j] := 0.0$;" is thus superfluous. The semicolon before the end which precedes the label "sum" also appears unnecessary.

In spite of these minor corrections, the algorithm appears to be extremely convenient for multiple quadratures over arbitrary regions using the Cartesian product of any explicit one-dimensional formula (and not merely a Gaussian formula) for integrating over the range $[-1, 1]$. If endpoints are used in the formula, it will, of course, repeat the calculation for each section of the range.

ALGORITHM 33

FACTORIAL

M. F. LIPP

RCA Digital Computation and Simulation Group,
Moorestown, New Jersey

```

real procedure Factorial (n) ;
value n ; integer n ;
comment This procedure makes use of the implicitly defined
recursive property of Algol to compute n! ;
begin Factorial := if n = 0 then 1. else n× Factorial (n-1)
end

```

ALGORITHM 34 GAMMA FUNCTION

M. F. LIPP

RCA Digital Computation and Simulation Group,
Moorestown, New Jersey

```

real procedure Gamma (x) ; real x ;
comment This procedure generalizes the recursive factorial
routine, finding  $\Gamma(1+x)$  for reasonable values of  $x$ . Accuracy
vanishes for large  $x$  ( $|x| > 10$ ) and for negative  $x$  with small
fractional parts. For  $x$  being a negative integer the impossible
value zero is given ;
begin test: if x < 0 then go to minus else if x < 1 then
begin integer i ; real y ; array a [1:8] ;
a [1] := -.57719165 ;
a [2] := .98820589 ; a [3] := -.89705694 ;
a [4] := .91820686 ;
a [5] := -.75670408 ; a [6] := .48219939 ;
a [7] := -.19352782 ;
a [8] := .03586834 ; y := a [1] ;
for i := 2 step 1 until 8 do y := y × x + a [i] ;
Gamma := y end hastings
else Gamma := x × Gamma (x-1) ; go to endgam ;
minus: if x = -1 then Gamma := 0 else
Gamma := Gamma (x+1) / x ;
endgam : end gam

```

REMARK ON ALGORITHM 34

GAMMA FUNCTION [M. F. Lipp, *Comm. ACM* 4
(Feb. 1961)]

MARGARET L. JOHNSON AND WARD SANGREN
Computer Applications, Inc., San Diego, Calif.

The coefficients used in the calculation of the Hasting's polynomial are used in reverse order. The algorithm should have
 $a[1] = -.19352782$; $a[2] = .48219939$; $a[3] = -.75670408$;
 $a[4] = .91820686$; $a[5] = -.89705694$; $a[6] = .98820589$;
 $a[7] = -.57719165$; $a[8] = 1.0$;
 $y = .03586834$;
for $i := 1$ step 1 until 8 do $y := y \times x + a[i]$;

Further, since $\Gamma(x) = \Gamma(1+x)$, the divisor x in the statement labeled minus should be $x+1$.

ALGORITHM 35

SIEVE

T. C. Wood

RCA Digital Computation and Simulation Group, Moorestown, New Jersey

```

procedure Sieve (Nmax) Primes: (p) ;
integer Nmax; integer array p ;
comment Sieve uses the Sieve of Eratosthenes to find all prime
numbers not greater than a stated integer Nmax
and stores them in array p. This array should be
of dimension 1 by entier (2 × Nmax/ln (Nmax)) ;
begin integer n, i, j ;
p[1] := 1 ; p[2] := 2 ; p[3] := 3 ;
for n := 3 step 2 until Nmax do
i := 3 ;
L1: go to if p[i] ≤ sqrt (n) then a1 else a2 ;
a1: go to if n/p[i] = n ÷ p[i] then b1 else b2 ;
b2: i := i + 1 ; go to L1 ;
a2: p[j] := n ; j := j + 1 ;
b1: end end

```

CERTIFICATION OF ALGORITHM 35

SIEVE (T. C. Wood, *Comm. ACM*, March 1961)

P. J. BROWN

University of North Carolina, Chapel Hill, N. C.

SIEVE was transliterated into GAT for the UNIVAC 1105 and successfully run for a number of cases.

The statement:

go to if $n/p[i] = n \div p[i]$ then b1 else b2;

was changed to the statement:

go to if $n/p[i] - n \div p[i] < .5/N_{\max}$ then b1 else b2;

Roundoff error might lead to the former giving undesired results.

CERTIFICATION OF ALGORITHM 35

SIEVE [T. C. Wood, *Comm. ACM*, Mar. 1961]

J. S. HILLMORE

Elliott Bros. (London) Ltd., Borehamwood, Herts., England

The statement:

go to if $n/p[i] = n \div p[i]$ then b1 else b2;

was changed to the statement:

go to if $(n \div p[i]) \times p[i] = n$ then b1 else b2;

This avoids any inaccuracy that might result from introducing real arithmetic into the evaluation of the relation.

The modified algorithm was successfully run using the Elliott ALGOL translator on the National-Elliott 803.

ALGORITHM 36

TCHBYCHEFF

A. J. GIANNI

RCA Digital Computation and Simulation Group, Moorestown, New Jersey

procedure tchebycheff (t, x, m, ℓ) ;

real array t, x ; **integer** ℓ , m ;

comment given a set of $m+1$ values of x stored in a one-dimensional array whose subscripts run from 0 thru m at least, construct a table of $t_n(x)$, $n = 0, 1, \dots, \ell$ and store it in the two-dimensional array t, where you find $t_n(x[m])$ as $t[n, m]$;

begin integer i, k, n ;

for k := 0 step 1 until m do **begin** t[0, k] := 1 ;

t[1, k] := x[k] **end** ;

for n := 2 step 1 until ℓ do for i = 0 step 1

until m do

t[n, i] := $2 \times x[i] \times t[n-1, i] - t[n-2, i]$

end tcheby

ALGORITHM 37

TELESCOPE 1

K. A. BRONS

RCA Advanced Programming Group, Pennsauken, N. J.

procedure Telescope1 (N, L, eps, limit, c) ; **value** limit, L ;
integer N ; **real** L, eps, limit ; **array** c ;

comment : Telescope 1 takes an Nth degree polynomial approxi-

mation $\sum_{k=0}^N c_k x^k$ to a function which was valid to

within $\text{eps} \geq 0$ over an interval (0, L) and reduces it, if possible, to a polynomial of lower degree, valid to within $\text{limit} > 0$. The initial coefficients c_k are replaced by the final coefficients, and the deleted coefficients are replaced by zero. The initial eps is replaced by the final bound on the error. N is replaced by the degree of the reduced polynomial. N and eps must be variables.

This procedure computes the coefficients given in the Techniques Department of the ACM Communications, Vol. 1, No. 9, from the recursion formula

$$a_{k-1} = -a_k \frac{k \cdot L \cdot (2k-1)}{2(N+k-1) \cdot (N-k+1)} ;$$

begin integer k ; **array** d[0:N] ;

start : if $N < 1$ then go to exit ; d[N] := -c[N] ;

for k := N step -1 until 1 do

d[k-1] := $-d[k] \times L \times k \times (k-0.5) /$

$((N+k-1) \times (N-k+1))$;

if $\text{eps} + \text{abs}(d[0]) < \text{limit}$ then

begin eps := $\text{eps} + \text{abs}(d[0])$;

for k := N step -1 until 0 do c[k] := c[k] + d[k] ;

N := N - 1 ; go to start **end** ;

exit : **end**

CERTIFICATION OF ALGORITHM 37

TELESCOPE 1 [K. A. Brons, *Comm. ACM*, Mar., 1961]

HENRY C. THACHER, JR.*

Reactor Engineering Div., Argonne National Lab., Argonne, Ill.

* Work supported by the U. S. Atomic Energy Commission.

The body of *Telescope 1* was compiled and tested on the LGP-30 using the ALGOL 60 translator system developed by the Dartmouth College Computer Center. No syntactical errors were found, and the program ran satisfactorily. The 10th degree polynomial obtained by truncating the exponential series was telescoped using $\text{lim} = .1_{10} - 2$ and $L = 1.0$. The result was $N = 3$, $\text{eps} = .2103005_{10} - 3$, and coefficients $+ .9997892$, $-.9930727$, $+ .4636493$, $-.1026781$. The error curve for the telescoped polynomial was computed for $x = 0(.02)1.0$. The error extrema were bounded by eps to within 0.5%. The discrepancy is within the range of input conversion and round-off error.

CERTIFICATION OF ALGORITHM 37

TELESCOPE 1 [K. A. Brons, *Comm. ACM*, Mar. 1961]

JAMES F. BRIDGES

Michigan State University, East Lansing, Mich.

This procedure was tested on the CDC 160A, using 160A FORTRAN. The 10th degree polynomial obtained by truncating the series $\exp(-x)$ was telescoped using $L = 1$ and $\text{lim} = 0.001$. The result was $N = 3$, $\text{eps} = .21061862_{10} - 3$ and coefficients $+0.99978965$, -0.99307236 , $+0.46364955$, -0.10267767 . The error curve was computed for $x = 0(0.02)1.0$ and no error exceeded eps, the worst error being 2% of eps less than eps.

This result is in close agreement with that of Henry C. Thatcher, Jr. in his Certification (*Comm. ACM*, Aug. 1962). Mr. Thatcher has pointed out that he inadvertently referred to the series for $\exp(-x)$ as the "exponential series" thereby inferring the positive series $\exp(+x)$. There is also a typographical error in his eps. It should be $+0.2103505_{10} - 3$.

ALGORITHM 38

TELESCOPE 2

K. A. BRONS

RCA Advanced Programming, Pennsauken, N. J.

procedure Telescope 2 (N, L, eps, limit, c) ; **value** limit, L ;
integer N ; **real** L, eps, limit ; **array** c ;
comment Telescope 2 takes an Nth degree polynomial approximation $\sum_{k=0}^N c_k x^k$ to a function which was valid to within $\text{eps} \geq 0$ over an interval $(-L, L)$ and reduces it, if possible, to a polynomial of lower degree, valid to within $\text{limit} > 0$. The initial coefficients c_k are replaced by the final coefficients, and deleted coefficients are replaced by zero. The initial eps is replaced by the final bound on the error, and N is replaced by the degree of the reduced polynomial. N and eps must be variables. This procedure computes the coefficients given in the Techniques Department of the ACM Communications, Vol. 1, No. 9, from the recursion formula

$$a_{k+1} = -a_k \frac{k \cdot L^2 (k-1)}{(N+k-2) \cdot (N-k+2)} ;$$

start: **begin** **integer** k ; **real** s ; **array** d[0:N] ;
if N < 2 **then go to** exit ; d[N] := -c[N] ;
for k := N **step** - 2 **until** 2 **do**
d[k-2] := -d[k] $\times L^2 \times k \times (k-1) /$
 $((N+k-2) \times (N-k+2)) ;$
if (N/2) - entier (N/2) = 0 **then** s := d[0] **else**
s := d[1]/N ;
if eps + abs(s) < limit **then begin**
eps := eps + abs(s) ;
for k := N **step** - 2 **until** 0 **do**
c[k] := c[k] + d[k] ;
N := N - 1 ; **go to** start **end** ;
exit: **end**

CERTIFICATION OF ALGORITHM 38

TELESCOPE 2 [K. A. Brons, *Comm. ACM*, Mar., 1961]

JAMES F. BRIDGES

Michigan State University, East Lansing, Mich.

This procedure was tested on the CDC 160A using 160A FORTRAN. The 10th degree polynomial obtained by truncating the series expansion of $\exp(+x)$ was telescoped using $L = 1.0$ and $\text{lim} = 0.001$. The result was $N = 4$, $\text{eps} = 0.59159949_{10} - 3$ and coefficients $+1.0000447$, $+0.99730758$, $+0.49919675$, $+0.17734729$, $+0.043793910$. Errors were calculated for $x = -1.0(0.02)1.0$. The only error to exceed eps was at $x = 1.0$ and was within 0.6% of eps.

ALGORITHM 39

CORRELATION COEFFICIENTS WITH MATRIX MULTIPLICATION

PAPKEN SASSOUNI

Burroughs Corporation, Pasadena, California

procedure NORM (x) number of rows: (m) number of columns:
(n) normalized output: (y) standard deviations:
(s) ;

value m, n ; **integer** m, n ; **array** x, y, s ;

comment Given an observation matrix [x] consisting of observations x_{ij} on a population, NORM will calculate

$$y_{ij} = \frac{x_{ij} - \bar{x}_j}{\sqrt{\sum_{i=1}^m (x_{ij} - \bar{x}_j)^2}} \quad \text{for } i = 1, \dots, m \quad j = 1, \dots, n$$

and the standard deviations

$$s_j = \sqrt{\frac{\sum_{i=1}^m (x_{ij} - \bar{x}_j)^2}{m}}$$

where $\bar{x}_j$ is the mean of observations on the j-th factor ;

begin **integer** i, j ; **real** r, h, c, b ;
r := sqrt (m) ; **for** j := 1 **step** 1 **until** n **do**
h := 0 ;
for i := 1 **step** 1 **until** m **do**
h := h + x[i, j] ; h := h/m ; b := 0 ;
for j := 1 **step** 1 **until** m **do**
c := x[i, j] - h ; b := b + c² ; y[i, j] := c
end 2 ;
b := sqrt (b) ;
for i := 1 **step** 1 **until** m **do**
y[i, j] := y[i, j]/b ; s[j] := b/r
end 1
end NORM ;

comment The normalization is now completed, and we are ready to compute the correlation matrix ;

procedure TRANSMULT (y) number of rows: (m) number of columns: (n) symmetrical square matrix result: (z) ;

value m, n ; **integer** m, n ; **array** y, z ;

comment This procedure multiplies two matrices, the first being the transpose of the second. The result is a symmetrical matrix with respect to the main diagonal, therefore only the lower part of it, including the main diagonal, is computed. The upper half is obtained by equating corresponding elements;

begin **integer** i, j, k ; **real** h ;
for j := 1 **step** 1 **until** n **do**
for i := j **step** 1 **until** n **do**
h := 0 ;
for k := 1 **step** 1 **until** m **do**
h := h + y[k, i] $\times$ y[k, j] ; z[i, j] := h ;
if i $\neq$ j **then** z[j, i] := h
end i
end TRANSMULT. [z] is the square matrix of the correlation coefficients of the initial observation matrix [x]

ALGORITHM 40 CRITICAL PATH SCHEDULING

B. LEAVENWORTH

American Machine & Foundry Co., Greenwich, Conn.

procedure CRITICALPATH (n, I, J, DIJ, ES, LS, EF, LF, TF, FF) ;

integer n ; **integer array** I, J, DIJ, ES, LS, EF, LF, TF, FF ;

comment: Given the total number of jobs n of a project, the vector pair I_k, J_k representing the kth job, which is thought of as an arrow connecting event I_k to event J_k ($I_k < J_k$, $k = 1 \dots n$), and a duration vector $(DIJ)_k$, CRITICAL-PATH determines the earliest starting time $(ES)_k$, latest starting time $(LS)_k$, earliest completion time $(EF)_k$, latest completion time $(LF)_k$, the total float $(TF)_k$, and the free float $(FF)_k$. I_k must be 1 and the I_k, J_k must be in ascending order. For example, if the first three jobs are labelled (1, 2), (1, 3), (3, 4), then the I, J vectors are (1, 1, 3) and (2, 3, 4) respectively. The critical path is given by each arrow whose total float is zero. The following non-local labels are used for exits: out1 — I_k not less than J_k ; out2 — I_k out of sequence ; out3 — I_k missing;

begin

integer k, index, max, min ; **integer array** ti, te [1:n] ;
index := 1 ;

for k := 1 **step** 1 **until** n **do**

begin

if $I[k] \geq J[k]$ **then go to** out1 ;

if $I[k] < \text{index}$ **then go to** out2 ;

if $I[k] > \text{index} \wedge I[k] \neq \text{index} + 1$ **then go to** out3 ;

if $I[k] = \text{index} + 1$ **then** index := $I[k]$;

C: end ;

for k := 1 **step** 1 **until** n **do**

ti[k] := te[k] := 0 ;

for k := 1 **step** 1 **until** n **do**

begin

max := $ti[I[k]] + DIJ[k]$;

if $ti[J[k]] = 0 \vee ti[J[k]] < \text{max}$ **then**

ti[J[k]] := max ;

A: end ti ;

te[J[n]] := ti[J[n]] ;

for k := n **step** -1 **until** 1 **do**

begin

min := $te[J[k]] - DIJ[k]$;

if $te[I[k]] = 0 \vee te[I[k]] > \text{min}$ **then**

te[I[k]] := min ;

B: end te ;

for k := 1 **step** 1 **until** n **do**

begin

ES[k] := $ti[I[k]]$;

LS[k] := $te[J[k]] - DIJ[k]$;

EF[k] := $ti[I[k]] + DIJ[k]$;

LF[k] := $te[J[k]]$;

TF[k] := $te[J[k]] - ti[I[k]] - DIJ[k]$;

FF[k] := $ti[J[k]] - ti[I[k]] - DIJ[k]$;

end

end CRITICALPATH

REFERENCES

- (1) JAMES E. KELLEY, JR. AND MORGAN R. WALKER, "Critical-Path Planning and Scheduling," 1959 Proceedings of the Eastern Joint Computer Conference.
- (2) M. C. FRISHBERG, "Least Cost Estimating and Scheduling — Scheduling Phase Only," IBM 650 Program Library File No. 10.3.005.

CERTIFICATION OF ALGORITHM 40

CRITICAL PATH SCHEDULING (B. Leavenworth,

Comm. ACM, Mar. 1961)

NEAL P. ALEXANDER

Union Carbide Olefins Company, South Charleston, West Virginia

The Critical Path Scheduling algorithm was coded in FORTRAN for the IBM 7070. The following changes were made:

(a) $ti[k] := te[k] := 0$;

should be

$ti[k] := 0$;

$te[k] := 9999$;

(b) **if** $te[I[k]] = 0 \vee te[I[k]] > \text{min}$ **then**

should be

if $te[I[k]] > \text{min}$ **then**

This change permits a value of 0 to be calculated for $te[I[k]]$ and remain as the minimum value.

In the statement

if $ti[J[k]] = 0 \vee ti[J[k]] < \text{max}$ **then**

the part of the statement " $ti[J[k]] = 0$ " is redundant and can be omitted.

CERTIFICATION OF ALGORITHM 40

CRITICAL PATH SCHEDULING [B. Leavenworth,

Comm. ACM 4 (Mar. 1961), 152; 4 (Sep. 1961), 392;

5 (Oct. 1962), 513]

IRVIN A. HOFFMAN (Recd 7 Feb. 1964)

Woodward Governor Co., Rockford, Ill.

The Critical Path Scheduling algorithm was coded in FAST for the NCR315. The modifications suggested by Alexander [Comm. ACM 4 (Sept. 1961)] were included. Results were correct in all tested cases. However, the example of the I, J vectors given in the comment is incorrect, as it would cause the exit out3 — I_k missing.

[EDITOR'S NOTE. There are also two semicolons which should be removed from the comment of Algorithm 40.—G.E.F.]

CERTIFICATION OF ALGORITHM 40

CRITICAL PATH SCHEDULING [B. Leavenworth,

Comm. ACM (Mar. 1961)]

LARS HELLBERG

Facit Electronics AB, Solna, Sweden.

The Critical Path Scheduling algorithm was transliterated into FACIT-ALGOL-1 and tested on the FACIT EDB. The modifications suggested by Alexander [Comm. ACM (Sept. 1961)] were included. Results were correct in all tested schedules.

ALGORITHM 41

EVALUATION OF DETERMINANT

JOSEF G. SOLOMON

RCA Digital Computation and Simulation Group, Moorestown, New Jersey

real procedure Determinant (A,n);

real array A; **integer** n;

comment This procedure evaluates a determinant by triangularization;

```

begin real    Product, Factor, Temp; array B[1:n, 1:n],
              C[1:n, 1:n];
integer      Count, Sign, i, j, r, y;
              Sign := 1; Product := 1;
for          i := 1 step 1 until n do for j := 1 step 1 until
              n do
begin        B[i,j] := A[i,j]; C[i,j] := A[i,j] end;
for          r := 1 step 1 until n-1 do
begin        Count := r-1;
              zerocheck: if B[r,r] ≠ 0 then go to resume;
              if Count < n-1 then Count := Count + 1
              else go to zero;
for          y := r step 1 until n do
begin        Temp := B[Count+1,y]; B[Count+1,y] :=
              B[Count,y]; B[Count,y] := Temp end;
              Sign := - Sign; go to zerocheck;
              zero: Determinant := 0; go to return;
              resume: for i := r+1 step 1 until n do
begin        Factor := C[i,r] / C[r,r];
              for j := r+1 step 1 until n do
begin        B[i,j] := B[i,j] - Factor × C[r,j] end end;
              i := r+1 step 1 until n do
              for j := r+1 step 1 until n do C[i,j] := B[i,j]
              end;
              for
                  i := 1 step 1 until n do Product := Product
                  × B[i,i]; Determinant := Sign × Product;
              return: end

```

CERTIFICATION OF ALGORITHM 41

EVALUATION OF DETERMINANT [Josef G. Solomon, RCA Digital Computation and Simulation Group, Moorestown, N. J.]

BRUCE H. FREED

Dartmouth College, Hanover, N. H.

When Algorithm 41 was translated into SCALP for running on the LGP-30, the following corrections were found necessary:

1. In the "y" loop after "B[Count,y] := Temp" and before the "end" insert
"Temp := C[Count+1,y];
C[Count+1,y] := C[Count,y];
C[Count,y] := Temp"
2. "Sign" is an ALGOL word when uncapitalized. However, many systems (if not all) do not recognize the difference between small and capital letters. For this reason "Sign" was changed to "ssign" for the LGP-30 run (and in the revision which follows later).

The following addition might be made in the specification as a concession to efficiency: "value A,n".

The following changes might be made to make the Algorithm less wordy:

1. for "Ssign := 1; Product := 1;"
put "Ssign := Product := 1;"
2. for "begin B[i,j] := A[i,j]; C[i,j] := A[i,j] end;"
put "B[i,j] := C[i,j] := A[i,j];"
3. for "begin B[i,j] := B[i,j] - Factor × C[r,j] end end;"
put "B[i,j] := B[i,j] - Factor × C[r,j] end;"

The above corrections and changes were made and the program was run with the correct results, as follows:

$$A = \begin{pmatrix} 10.96597 & 35.10765 & 96.72356 \\ 2.35765 & -84.11256 & .87932 \\ 18.24689 & 22.13579 & 1.11123 \end{pmatrix}$$

Determinant = .1527313e06

Hand calculation on a desk calculator gives the value of the determinant for the above matrix as 152,731.3600.

$$A = \begin{pmatrix} 1.0 & 3.0 & 3.0 & 1.0 \\ 1.0 & 4.0 & 6.0 & 4.0 \\ 1.0 & 5.0 & 10.0 & 10.0 \\ 1.0 & 6.0 & 15.0 & 20.0 \end{pmatrix} \quad \text{Determinant} = .9999999e+00$$

The above matrix, being a finite segment of Pascal's triangle, has determinant equal to 1.000000000.

$$A = \begin{pmatrix} 0.0 & 0.0 & 0.0 \\ 5.0 & 9.0 & 2.0 \\ 7.0 & 5.0 & 4.0 \end{pmatrix} \quad \text{Determinant} = .0000000e+00$$

This is, of course, exactly correct.

Finally, one major change can be made which does away with several instructions and reduces variable storage requirements by n^2 . This change is the complete removal of matrix C from the program. It is extraneous.

The revised Algorithm was translated into SCALP and run on the LGP-30 with exactly the same results as above.

The revised Algorithm 41 follows.

ALGORITHM 41, REVISION

EVALUATION OF DETERMINANT [Josef G. Solomon, RCA Digital Computation and Simulation Group, Moorestown, N. J.]

BRUCE H. FREED

Dartmouth College, Hanover, N. H.

```

real procedure determinant (a,n);
real array a; integer n; value a,n;
comment This procedure evaluates a determinant by triangulation;
begin real product, factor, temp;
array b[1:n,1:n];
integer count, ssign, i, j, r, y;
ssign := product := 1;
for i := 1 step 1 until n do
for j := 1 step 1 until n do
b[i,j] := a[i,j];
for r := 1 step 1 until n-1 do
begin count := r-1;
zerocheck: if b[r,r] ≠ 0 then go to resume;
if count < n-1 then count := count + 1 else go to zero;
for y := r step 1 until n do
begin temp := b[count+1,y];
b[count+1,y] := b[count,y];
b[count,y] := temp end;
ssign := -ssign;
go to zerocheck;
zero: determinant := 0; go to return;
resume: for i := r+1 step 1 until n do
begin factor := b[i,r]/b[r,r];
for j := r+1 step 1 until n do
b[i,j] := b[i,j] - factor × b[r,j] end end;
for i := 1 step 1 until n do
product := product × b[i,i];
determinant := ssign × product;
return: end

```

REMARK ON REVISION OF ALGORITHM 41

EVALUATION OF DETERMINANT [Josef G. Solomon,

Comm. ACM 4 (Apr. 1961), 176; Bruce H. Freed,

Comm. ACM 6 (Sept. 1963); 520]

LEO J. ROTENBERG (Recd 7 Oct. 63)

Box 2400, 362 Memorial Dr., Cambridge, Mass.

While desk-checking the program an error was found. For example, the algorithm as published would have calculated the value zero as the determinant of the matrix

$$\begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}$$

The error lies in the search for a nonzero element in the r th column of the matrix b .

Editor's Note. Apparently the best general determinant evaluators in this section are imbedded in the linear equation solvers Algorithm 43 [Comm. ACM 4 (Apr. 1961), 176, 182; and 6 (Aug. 1963), 445] and Algorithm 135 [Comm. ACM 5 (Nov. 1962), 553, 557]. They search each column for the largest pivot in absolute value. Algorithm 41 searches only for a nonzero pivot in each column, and will therefore fail for the matrix

$$\begin{bmatrix} 2^{-t} & 1 & 1 \\ 1 & 1 & 2 \\ 1 & 1 & 1 \end{bmatrix}$$

if $t \gg s$, for a machine with s -bit floating point.

It is hoped that soon a good determinant evaluator will be published to take the place of Algorithm 41.—G. E. F.

ALGORITHM 42

INVERT

T. C. Wood

RCA Digital Computation and Simulation Group,
Moorestown, New Jersey

```

procedure Invert (A) order: (n) Singular: (s) Inverse: (A1);
    array A, A1; integer n,s,value n;
comment This procedure inverts the square matrix A of order
n by applying a series of elementary row operation to the matrix
to reduce it to the identity matrix. These operations when
applied to the identity matrix yield the inverse A1. The case
of a singular matrix is indicated by the value s := 1;
begin    comment augment matrix A with identity matrix;
    array a[1:n, 1:2 × n]; integer i,j;
    for i := 1 step 1 until n do
    for j := 1 step 1 until 2 × n do
    if j ≤ n then a[i,j] := A[i,j] else
    if j = n+1 then a[i,j] := 1.0 else a[i,j] := 0.0;
    comment begin inversion;
    for i := 1 step 1 until n do
    integer k, l, ind; j := l := i; ind := s := 0;
begin    L1: if a[l,j] = 0 then
    begin ind := 1; if l < n then begin l := l + 1;
    go to L1 end
    else begin s := 1; go to L2 end
    end;
    if ind = 1 then for k := 1 step 1 until 2 × n do
    begin real temp;
    temp := a[l,k];
    a[l,k] := a[i,k];
    a[i,k] := temp end k loop;
    for k := j step 1 until 2 × n do
    a[i,k] := a[i,k] / a[i,j];
    for l := 1 step 1 until n do
    if l ≠ i then for k := 1 step 1 until 2 × n do
    a[l,k] := a[l,k] - a[i,k] × a[l,j];
    end l loop;
    for i := 1 step 1 until n do
    for j := 1 step 1 until n do
    A1[i,j] := a[i,n+j];
    L2: end of procedure

```

CERTIFICATION OF ALGORITHM 42
INVERT (T. C. Wood, *Comm. ACM*, Apr., 1961)
ANTHONY W. KNAPP AND PAUL SHAMAN
Dartmouth College, Hanover, N. H.

INVERT was hand-coded for the LGP-30 using machine language and the 24.0 floating-point interpretive system, which carries 24 bits of significance for the fractional part of a number and five bits for the exponent. The following changes were found necessary:

- (a) **if** j = n+1 **then** a[i, j] := 1.0 **else** a[i, j] := 0.0;
should be
if j = n+i **then** a[i, j] := 1.0 **else** a[i, j] := 0.0;
- (b) **for** k := j **step** 1 **until** 2 × n **do**
a[i, k] := a[i, k] / a[i, j];
should be
for k := 2 × n **step** -1 **until** i **do**
a[i, k] := a[i, k] / a[i, j];
- (c) **if** l ≠ i **then** **for** k := 1 **step** 1 **until** 2 × n **do**
a[l, k] := a[l, k] - a[i, k] × a[l, j];
should be
if l ≠ i **then** **for** k := 2 × n **step** -1 **until** i **do**
a[l, k] := a[l, k] - a[i, k] × a[l, j];

Given these changes, j becomes superfluous in the second i loop, and the other references to j may be changed to references to i.

INVERT obtained the following results:

The computer inverted a 17-by-17 matrix whose elements were integers less than ten in absolute value. When the matrix and its inverse were multiplied together, the largest nondiagonal element in the product was -.00003. Most nondiagonal elements were less than .00001 in absolute value.

INVERT was tested using finite segments of the Hilbert matrix.

The following results were obtained in the 4 × 4 case:

16.005	-120.052	240.125	-140.082
-120.052	1200.584	-2701.407	1680.917
240.126	-2701.411	6483.401	-4202.217
-140.082	1680.920	-4202.219	2801.446

The exact inverse is:

16	-120	240	-140
-120	1200	-2700	1680
240	-2700	6480	-4200
-140	1680	-4200	2800

INVERT was also coded for the LGP-30 in machine language and the 24.1 extended range interpretive system. This system, which uses 30 significant bits for the fraction, obtained the following as the inverse of the 4 × 4 Hilbert matrix:

16.000	-120.001	240.001	-140.001
-120.001	1200.006	-2700.015	1680.010
240.001	-2700.016	6480.037	-4200.024
-140.001	1680.010	-4200.024	2800.016

The program coded in the 24.0 interpretive system successfully inverted a matrix consisting of ones on the minor diagonal and zeros everywhere else.

REMARKS ON ALGORITHM 42

INVERT [T. C. Wood, *Comm. ACM*, Apr. 1961]

P. NAUR

Regnecentralen, Copenhagen, Denmark

INVERT cannot be recommended since it does not search for pivot and therefore will give poor accuracy. This is confirmed by the figures quoted by Knapp and Shaman in their certification [Comm. ACM 4 (Nov. 1961), 498]. The results obtained by them

using 30 significant bits for the fraction may be compared directly with those obtained using INVERSION II (Algorithm 120) and gjr with the GIER ALGOL system (see certification below). Inverting the 4×4 segment of the Hilbert matrix, the largest error in any element is found to be:

	Subscripts	Error
INVERT (Knapp and Shaman)	3,3	0.037
INVERSION II (see certification of	3,3	0.0306
gjr	4,3	0.00010

In view of this basic shortcoming of Algorithm 42, it is unnecessary to report on other features of it.

CORRECTION TO EARLIER REMARKS ON ALGORITHM 42 INVERT, ALG. 107 GAUSS'S METHOD, ALG. 120 INVERSION II, AND gjr [P. Naur, *Comm. ACM*, Jan. 1963, 38-40.]

P. NAUR

Regnecentralen, Copenhagen, Denmark

George Forsythe, Stanford University, in a private communication has informed me of two major weaknesses in my remarks on the above algorithms:

1) The computed inverses of rounded Hilbert matrices are compared with the exact inverses of unrounded Hilbert matrices, instead of with very accurate inverses of the rounded Hilbert matrices.

2) In criticizing matrix inversion procedures for not searching for pivot, the errors in inverting positive definite matrices cannot be used since pivot searching seems to make little difference with such matrices.

It is therefore clear that although the figures quoted in the earlier certification are correct as they stand, they do not substantiate the claims I have made for them.

To obtain a more valid criterion, without going into the considerable trouble of obtaining the very accurate inverses of the rounded Hilbert matrices, I have multiplied the calculated inverses by the original rounded matrices and compared the results with the unit matrix. The largest deviation was found as follows:

Order	Maximum deviation from elements of the unit matrix		
	INVERSION II	gjr	Ratio
2	-1.49 ₁₀ -8	-1.49 ₁₀ -8	1.0
3	-4.77 ₁₀ -7	-8.34 ₁₀ -7	0.57
4	-9.54 ₁₀ -6	-3.43 ₁₀ -5	0.28
5	-7.32 ₁₀ -4	-4.58 ₁₀ -4	1.6
6	-1.61 ₁₀ -2	-1.42 ₁₀ -2	1.1
7	-5.78 ₁₀ -1	-5.47 ₁₀ -1	1.1
8	-1.20 ₁₀ -2	-1.38 ₁₀ 1	8.7
9	-4.91 ₁₀ 1	-2.22 ₁₀ 1	2.2

This criterion supports Forsythe's criticism. In fact, on the basis of this criterion no preference of INVERSION II or gjr can be made.

The calculations were made in the GIER ALGOL system, which has floating numbers of 29 significant bits.

ALGORITHM 43 CROUT WITH PIVOTING II

HENRY C. THACHER, JR.*

Argonne National Laboratory, Argonne, Illinois

real procedure INNERPRODUCT (u,v) index : (k) start : (s)
finish : (f);

value s, f; **integer** k, s, f; **real** u, v;

comment INNERPRODUCT forms the sum of $u(k) \times v(k)$ for $k = s, s+1, \dots, f$. If $s > f$, the value of INNERPRODUCT is zero. The substitution of a very accurate inner product procedure would make CROUT more accurate;

comment INNERPRODUCT may be declared in the head of any block which includes the block in which CROUT is declared. It may be used independently for forming the inner product of vectors;

begin

real h;

h := 0; **for** k := s **step** 1 **until** f **do** h := h + u × v;

INNERPRODUCT := h

end INNERPRODUCT;

procedure CROUT II (A, b, n, y, pivot, det, repeat)

comment This procedure is a revision of Algorithm 16, Crout With Pivoting by George E. Forsythe, *Comm. ACM* 3, (1960) 507-8. In addition to modifications to improve the running of the program, and to conform to proper usage, it provides for the computation of the determinant, det, of the matrix A. The solution is obtained by Crout's method with row interchanges, as formulated in reference [1], for solving $Ay = b$ and transforming the augmented matrix $[A \ b]$ into its triangular decomposition LU with all $L(k,k) = 1$. If A is singular we exit to 'singular,' a nonlocal label. pivot (k) becomes the current row index of the pivot element in the k-th column. Thus enough information is preserved for the procedure to process a new right-hand side without repeating the triangularization, if the boolean parameter repeat is true. The accuracy obtainable from CROUT would be much increased by calling CROUT with a more accurate inner product procedure than INNERPRODUCT.

The contributions of Michael F. Lipp and George E. Forsythe by prepublication review and pointing out several errors are gratefully acknowledged;

comment Nonlocal identifiers appearing in this procedure are: (1) The nonlocal label 'singular', to which the procedure exits if $\det A = 0$, and (2) the real procedure 'INNERPRODUCT' given above;

value n; **array** A, b, y; **integer** n; **integer array** pivot; **real** det; **Boolean** repeat;

begin

integer k, i, j, imax, p; **real** TEMP, quot;

det := 1; **if** repeat **then go to** 6;

for k := 1 **step** 1 **until** n **do**

1: **begin**

TEMP := 0;

for i := k **step** 1 **until** n **do**

2: **begin**

A[i,k] := A[i,k] - INNERPRODUCT (A[i,p], A[p,k],
p, 1, k-1);

if abs(A[i,k]) > TEMP **then**

3: **begin**

TEMP := abs(A[i, k]); imax := i

end 3

end 2;

pivot [k] := imax;

comment We have found that A[imax, k] is the largest pivot in column k. Now we interchange rows k and imax;


```

if imax  $\neq$  k then
4: begin det := - det; for j := 1 step 1 until n do
5: begin
    TEMP := A[k,j]; A[k,j] := A[imax, j]; A[imax, j]
    := TEMP
end 5;
TEMP := b[k]; b[k] := b[imax]; b[imax] := TEMP
end 4;
comment The row interchange is done. We proceed
to the elimination;
if A[k,k] = 0 then go to singular;
quot := 1.0/A[k,k];
for i := k+1 step 1 until n do
    A[i,k] := quot  $\times$  A[i,k];
for j := k+1 step 1 until n do
    A[k,j] := A[k,j] - INNERPRODUCT (A[k,p],
    A[p,j], p, 1, k-1);
    b[k] := b[k] - INNERPRODUCT (A[k,p], b[p],
    p; i, k-1)
end j; go to 7;
comment The triangular decomposition is now finished,
and we skip to the back substitution;
6: begin comment This section is used when the formal
parameter repeat is true, indicating that the matrix A
has previously been decomposed into triangular form by
CROUT II, with row interchanges specified by pivot,
and that it is desired to solve the linear system with a
new vector b, without repeating the triangularization;
for k := 1 step 1 until n do
begin
    TEMP := b[pivot[k]]; b[pivot[k]] := b[k]; b[k] :=
    TEMP; b[k] := b[k] - INNERPRODUCT
    (A[k, p], b[p], p, 1, k-1) end;
end 6;
7: for k := n step - 1 until 1 do
8: begin if  $\neg$  repeat then det := A[k,k]  $\times$  det;
    y[k] := (b[k] - INNERPRODUCT (A[k,p], y[p], p,
    k+1, n)/A[k,k]
end 8;
end CROUT II;

```

REFERENCE:

- (1) J. H. WILKINSON, Theory and practice in linear systems. In John W. Carr III (editor), Application of Advanced Numerical Analysis to Digital Computers, pp. 43-100 (Lectures given at the University of Michigan, Summer 1958, College of Engineering, Engineering Summer Conferences, Ann Arbor, Michigan [1959]).

CERTIFICATION OF ALGORITHM 43 CROUT II (Henry C. Thacher, Jr., *Comm. ACM*, 1960) HENRY C. THACHER, JR.*

Argonne National Laboratory, Argonne, Illinois

CROUT II was coded by hand for the Royal Precision LGP-30 computer, using a 28-bit mantissa floating point interpretive system (24.2 modified).

The program was tested against the linear system:

$$A = \begin{bmatrix} 12.1719 & 27.3941 & 1.9827 & 7.3757 \\ 8.1163 & 23.3385 & 9.8397 & 4.9474 \\ 3.0706 & 13.5434 & 15.5973 & 7.5172 \\ 3.0581 & 3.1510 & 6.9841 & 13.1984 \end{bmatrix} \quad b = \begin{bmatrix} 6.0355 \\ 6.1304 \\ 4.6921 \\ 2.5393 \end{bmatrix}$$

with the following results:

$$A' = \begin{bmatrix} 12.171900 & 27.394100 & 1.9827000 & 7.3756999 \\ 0.25226957 & 6.6327021 & 15.097125 & 5.6565352 \\ 0.25124262 & -0.56260107 & 14.979620 & 14.527683 \\ 0.66680633 & 0.76468695 & -0.20207132 & -1.3606142 \end{bmatrix}$$

$$b' = \begin{bmatrix} 6.6354999 \\ 3.0181653 \\ 2.5702026 \\ -0.082780734 \end{bmatrix} \quad \text{pivot} = \begin{bmatrix} 1 \\ 3 \\ 4 \\ 4 \end{bmatrix} \quad y = \begin{bmatrix} 0.15929120 \\ 0.14691771 \\ 0.11257482 \\ 0.060840712 \end{bmatrix}$$

det = -1645.4499. All elements of $Ab - y$ were less than 10^{-7} in magnitude. Identical results were obtained with the same b, and repeat true. With the same b and the last row vector of A replaced by (19.1927, 33.4409, 25.1298, 5.2811), i.e. $A_4, j = A_1 j$, + $2A_2, j - 3A_3, j$, the results were:

$$\begin{aligned} \text{det} &= 0.10924352 \times 10^{-3}, \\ y &= (0.29214425 \times 10^8, -0.12131172 \times 10^8, 0.72411923 \times 10^7, \\ &\quad -0.51018392 \times 10^7) \end{aligned}$$

Failure to recognize this singular matrix is due to roundoff, either in the data input or in the calculation.

CERTIFICATION OF ALGORITHM 43 CROUT II (Henry Thacher, Jr., *Comm. ACM* (1960), 176]

C. DOMINGO AND F. RODRIGUEZ-GIL
Universidad Central, Caracas, Venezuela

CROUT II was coded in PUC-R2 and tested in the IBM-1620. Two types of INNERPRODUCT subroutines were used. The first one finds the scalar product in fixed-point arithmetic to increase accuracy, using an accumulator of 32 digits. The second one uses ordinary floating-point with eight significant figures.

Using a unit matrix as right-hand side, a 6×6 segment of Hilbert matrix was inverted. The inverse was inverted again.

The maximum difference between this result and the original segment of Hilbert matrix was:

$$\begin{aligned} \text{Using fixed-point INNERPRODUC} &\dots\dots\dots 8.2426 \times 10^{-4} \\ (\text{Value of determinant} &\dots\dots\dots 4.7737088 \times 10^{-18}) \\ \text{Using floating-point INNERPRODUC} &\dots\dots\dots 3.014016 \times 10^{-2} \\ (\text{Value of determinant} &\dots\dots\dots 4.4950721 \times 10^{-18}) \end{aligned}$$

Two typographical errors were observed in the algorithm:

The statement:

$$b[k] := g[k] - \text{INNERPRODUCT} (A[k,p], b[p], p, i, k-1)$$

should be:

$$b[k] := b[k] - \text{INNERPRODUCT} (A[k,p], b[p], 1, k-1)$$

The statement:

$$y[k] := (b[k] - \text{INNERPRODUCT} (A[k,p], y[p], p, k+1, n)) / A[k,k]$$

should be:

$$y[k] := (b[k] - \text{INNERPRODUCT} (A[k,p], y[p], p, k+1, n)) / A[k,k]$$

Storage may be saved eliminating the array y and using instead the array b, in which the solution is formed.

A previous certification of this algorithm [*Comm. ACM* 4, 4 (Apr. 1961), 182] was tested again with the same results. Two errors were detected in the certification: The row that must replace the last row of A in order to obtain a singular matrix must be:
19.1927 33.4409 -25.1298 -5.2811

ALGORITHM 44

BESSEL FUNCTIONS COMPUTED RECURSIVELY

MARIA E. WOJCICKI

RCA Digital Computation and Simulation Group,
Moorestown, New Jersey

```

procedure Bessfr(N, FX, LX, Z) Result: (J, Y);
  value LX, FX, N;
  real FX, LX, Z; real array J, Y; integer N;
comment Bessel Functions of the first and second kind,  $J_P(X)$ 
  and  $Y_P(X)$ , integral order P, are computed by recursion for
  values of X,  $FX \leq X \leq LX$ , in steps of Z. The functions are
  computed for values of P,  $0 \leq P \leq N$ . M[SUB], the initial
  value of P being chosen according to formulae in Erdelyi's
  Asymptotic Expansions. The computed values of  $J_P(X)$  and
   $Y_P(X)$  are stored as column vectors for constant argument in
  matrices J, Y of dimension (N+1) by entier  $((LX - FX)/Z + 1)$ ;
begin real PI, X, GAMMA, PAR, LAMDA, SUM, SUM1;
  integer P, SUB, MAXSUB;
  PI := 3.14159265;
  GAMMA := .57721566;
  PAR := 63.0 = 1.5  $\times \ln(2 \times PI)$ ;
  MAXSUB := entier  $((LX - FX)/Z)$ ;
begin real array JHAT[0:N, 0:MAXSUB];
  integer array M[0:MAXSUB];
  SUB := 0;
  for X := FX step Z until LX do
begin if (X > 0)  $\wedge$  (X < 10) then M[SUB] := 2  $\times$  entier (X) + 9
  else
begin real ALOG;
    ALOG := (PAR - 1.5  $\times \ln(X))$ /X;
    M[SUB] := entier (X  $\times$  (exp (ALOG) + exp
      (-ALOG))/2) end;
    if N > M[SUB] then
begin for P := M[SUB] + 1 step 1 until N do
      J[P, SUB] := 0 end;
      JHAT[M[SUB], SUB] := 10  $\uparrow$  (-9);
comment Having set the uppermost  $J_P(X)$  to a very small
  number we are now going to compute all the  $J_P(X)$  down to
  P = 0;
  for P := M[SUB] step -1 until 1 do
    JHAT[P-1, SUB] := 2  $\times$  P/X  $\times$  JHAT[P, SUB] - JHAT
      [P+1, SUB];
    SUM := SUM1 := 0;
    for P := 2 step 2 until (M[SUB]  $\div$  2) do
      SUM := SUM + JHAT[P, SUB];
      LAMDA := JHAT[0, SUB] + 2  $\times$  SUM;
      for P := 0 step 1 until N do
        J[P, SUB] := JHAT[P, SUB]/LAMDA;
comment  $J_P(X)$  have been computed by use of  $J_P(X)$ ;
  for P := 2 step 2 until (M[SUB]  $\div$  2) do
    SUM1 := SUM1 + (-1)  $\times$  (-1)  $\uparrow$  P  $\div$  J[2  $\times$  P, SUB]
      /2/P;
    Y[0, SUB] := 2/PI  $\times$  (J[0, SUB]  $\times$  (GAMMA +  $\ln(X/2)$ )
      + 4  $\times$  SUM1);
    for P := 0 step 1 until (M[SUB]-1) do
      Y[P+1, SUB] := (-2/PI/P + J[P+1, SUB]  $\times$  Y[P,
        SUB])/J[P, SUB];
  SUB := SUB + 1 end end end

```

ALGORITHM 45

INTEREST

PETER Z. INGERMAN

University of Pennsylvania, Philadelphia, Pa.

```

procedure monpay(i, B, L, t, k, m, tol, goof)
comment This procedure calculates the periodic payment
  necessary to retire a loan when the interest rate on the loan
  varies (possibly from period to period) as a function of the as-
  yet-unpaid principal.
  The formal parameters are: i, array identifier for the vector
  of interest rates; -B, array identifier for the minimum amounts
  at which the corresponding i applies; -L, the amount to be
  borrowed; -t, the number of periods for which the loan is to
  be taken out; -k, the number of different interest rates (and
  upper limit for vectors i and B); -m, the desired periodic pay-
  ment; -tol, the allowable deviation of m from some ideal;
  and goof, the error exit to use if convergence fails. The only
  output parameter is m. For further discussion, see Comm.
  ACM 3 (Oct. 1960), 542;
begin array h, S[1:k, 1:t], M, X[1:k];
integer array T, a, b[1:k];
integer p, q, r, sa, sb, I, ib, mb, nb;
comment This section sets up the procedure;
for p := 1 step 1 until k do
begin for q := 1 step 1 until t do
  begin  $h_{p,q} := i_p^q$ ;
     $S_{p,q} := (h_{p,q} - 1)/(i_p - 1)$  end;
    if p = 1 then  $X_p := 0$  else  $X_p := B_p \times (i_{p-1} - i_p)$ ;
     $M_p := L \times (h_{p,t}/S_{p,t})$  end;
  sa := sb := ib := mb := 0; nb := t;
for p := 1 step 1 until k do
begin  $a_p :=$  entier  $(B_{p+1}/M_{p+1} + 0.5) - sa$ ;
  sa := sa +  $a_p$ ;
   $T_p := b_p :=$  entier  $(B_{p+1}/M_p - 0.5) - sb$ ;
  sb := sb +  $b_p$ ;
  if  $b_p > mb$  then
    begin  $ib := p$ ;  $nb := nb - mb$ ;  $mb := b_p$  end
  else  $nb := nb - b_p$  end;
   $T_{ib} := nb$ ;
  I := 1;
for p := 1 step 1 until k do
  I := I  $\times$  ( $a_p - b_p + 1$ );
comment Having counted the number of possible iterations
  and established a set of trial values for the  $T_n$ 's, a trial m is
  found;
  D := 1; E := F := 0;
  newm: for p := 1 step 1 until k do
    begin D := D  $\times$   $h_{p,T_p}$ ;
      u := 1;
      if p  $\neq$  1 then for q := 1 step 1 until p - 1
        do u := u  $\times$   $h_{q,T_q}$ ;
      E := E +  $S_{p,T_p} \times u$ ;
      v := 0;
      if p  $\neq$  1 then for r := 1 step 1 until p
        do v := v +  $X_r$ ;
      F := F + u  $\times$  v end;
      m :=  $(L \times D + F)/E$ ;
comment Now find out whether m is good enough;
      q := 1; F := D := 0;
      for p := 1 step 1 until t do
begin get F: F :=  $(D + m - E)/(1 + i_q)$ ;
        if  $B_{q+1} \geq F$  then D := F else q := q + 1;
        if D  $\neq$  F go to get F end;
        if abs(D - L)  $\leq$  tol then go to exit;
comment If not within tolerance, adjust  $T_n$ 's and try
      again;

```

```

p := 0;
redo: p := p + 1;
    if p ≠ ib then
        begin if  $T_p \geq a_p$  then
            begin  $T_{ib} := T_{ib} + T_p - b_p$ 
                 $T_p := b_p$  end end
        else begin
             $T_p := T_p + 1$ ;
             $T_{ib} := T_{ib} - 1$ ;
            p := k end;
        if p = k then I := I - 1 else go to redo;
        go to if I > 0 then newm else goof;
exit: end monpay;

```

CERTIFICATION OF ALGORITHM 45

INTEREST [Peter Z. Ingerman, *Comm. ACM* Apr. 1961 and Oct. 1960]

CARL B. WRIGHT

Dartmouth College, Hanover, N. H.

INTEREST was translated into Dartmouth College Computation Center's "Self Contained ALGOL Processor" for the Royal-McBee LGP-30. When using SCALP, memory capacity is severely limited and thus it was necessary to run this program in two blocks. Block I ended with the computation of I, and Block II started with the "newm" loop. After making the changes listed below, test problems using up to three interest rates and up to 18 time periods were used with the following results:

Loan	Periods	Interest Rates	Payments	Final Balance*	Tolerance
\$100.00	1	0.05	\$105.00	\$0.00	\$0.25
1800.00	10	0.03	211.01	0.05	4.50
875.65	8	0.08 to 500.00			
		0.05 over 500.00	139.78	-1.49	2.19
14750.00	18	0.06 to 5000.00			
		0.05 to 10,000.00			
		0.04 over 10,000.00	1201.70	10.35	36.88

* Hand calculation.

It is noted that in each case the final balance is within the prescribed tolerance (0.0025 of the loan).

In the following corrections bracketed subscripts replace ordinary subscripts and exponentiation is represented by ↑ rather than superscript.

The following corrections should be made in the Note on Interest in the October, 1960, issue of *Comm. ACM*:

1. Definition of $B[n]$: Replace "minimum" by "maximum". Replace " $j[n]$ " by " $j[n-1]$ ".
2. Define $B[k+1] = L$.
3. Definition of $K[n]$: Replace " $B[n]$ " by " $B[n+1]$ ".

The following corrections were found necessary in the procedure:

1. The upper limit of the vector B is $k+1$, not k . It is not necessary to change the upper limit of the I -vector. (See correction 4 below.)
2. D, E, F, u, v were not declared and must be declared as **real**.
3. In the **array** declaration replace " $M[1:k]$ " by " $M[1:k+1]$ ".
4. As j approaches 0, i approaches 1 and $\lim (h/S) = 1/t$. Thus for $j[k+1] = 0$, $i[k+1] = 1$, and $M[k+1] = L/t$. Thus after $M[p] := L \times (h[p,t]/S[p,t])$ end; insert
 $M[k+1] := L/t$; $B[k+1] := L$;
5. In the conditional statement following computation of $b[p]$, replace ">" by "≥".
6. In same conditional statement, next line, " $mb := b[p]$ " should read " $mb := b[p]$ ".

```

7.  $D := 1$ ;  $E := F := 0$ ;
    newm: for p := 1 step 1 until k do
        should be changed to
        newm:  $D := 1$ ;  $E := F := 0$ ;
        for p := 1 step 1 until k do
8. begin get F:  $F := (D+m-E)/(1+i[q])$ ;
    if  $B[q+1] \geq F$  then  $D := F$  else  $q := q + 1$ ;
    if  $D \neq F$  go to get F end;
should be changed to read as follows:
begin get F:  $F := (D+m)/i[q]$ ;
    if  $B[q+1] \geq F$  then  $D := F$  else
        begin if  $q < k$  then  $q := q + 1$  else  $D := F$  end;
        if  $D \neq F$  then go to get F end;

```

Note that the "then" in the last line was omitted from the original procedure.

9. In the "redo" loop insert a semicolon after the statement

$T[ib] := T[ib] + T[p] - b[p]$;

10. In the "redo" loop, next line, omit the second "end".

11. In the "redo" loop,

$p := k$ end;

should be changed to

$p := k$ end end;

ALGORITHM 46

EXPONENTIAL OF A COMPLEX NUMBER

JOHN R. HERNDON

Stanford Research Institute, Menlo Park, California

```

procedure EXPC (a, b, c, d); value a, b; real a, b, c, d;
comment This procedure computes the number,  $c+di$ , which
    is equal to  $e^{(a+bi)}$ ;
begin c := exp (a);
        d := c × sin (b);
        c := c × cos (b)
end EXPC;

```

CERTIFICATION OF ALGORITHM 46

EXPONENTIAL OF A COMPLEX NUMBER (J. R.

Herndon, *Comm. ACM* 4 (Apr., 1961), 178)

A. P. RELPH

Atomic Power Div., The English Electric Co., Whetstone, England

Algorithm 46 was translated using the DEUCE ALGOL compiler, no corrections being required, and gave satisfactory results.

ALGORITHM 47

ASSOCIATED LEGENDRE FUNCTIONS OF THE FIRST KIND FOR REAL OR IMAGINARY ARGUMENTS

JOHN R. HERNDON

Stanford Research Institute, Menlo Park, California

```

procedure LEGENDREA (m, n, x, r); value m, n, x, r;
integer m, n; real x, r;

```

comment This procedure computes any $P_n^m(x)$ or $P_n^m(ix)$ for n an integer less than 20 and m an integer no larger than n . The upper limit of 20 was taken because $(42)!$ is larger than 10^{40} . Using a modification of this procedure values up to $n=35$ have been calculated. If $P_n^m(x)$ is desired, r is set to zero. If r is nonzero, $P_n^m(ix)$ is computed;

begin

```

integer i, j; array Gamma [1:41];
real p, z, w, y;
if n = 0 then
  begin p := 1;
  go to gate end;
if n < m then
  begin p := 0;
  go to gate end;
z := 1; w := z;
if n=m then go to main;
for i := 1 step 1 until n-m do
  z := x × z;
main: Gamma [1] := 1;
for i := 2 step 1 until n+1 do
  begin Gamma [i] := w × Gamma [i-1];
  w := w + 1 end;
w := 1; y := w/(x × x);
if r=0 then
  begin y := -y;
  w := -w end;
if x=0 then
  begin i := (n-m)/2;
  if (i+i) ≠ (n-m) then
    begin p := 0;
    go to gate end;
  p := Gamma [m+n+1]/(Gamma [i+1] × Gamma [m+i+1]);
  go to last end;
j := 3; p := 0;
for i := 1 step 1 until 12 do
  begin if (n-m+2)/2 < i then go to last end;
  p := p + Gamma [n+n-i-i+3] × z/(Gamma [i] × Gamma [n-i+2] × Gamma [n-i-i-m+j]);
  z := z × y end;
last: z := 1;
for i := step 1 until n do
  z := z + z;
p := p/z;
if r ≠ 0 then
  begin i := n-n/4;
  if 1 < i then
    p := -p end;
if m = 0 then go to gate;
j := m/2; z := abs(w+x × x);
if m ≠ (j+j) then
  begin z := sqrt (z);
  j := m end;
for i := step 1 until j do
  p := p × z;
gate: LEGENDREA := p
end LEGENDREA;
```

CERTIFICATION OF ALGORITHM 47

ASSOCIATED LEGENDRE FUNCTIONS OF THE FIRST KIND FOR REAL OR IMAGINARY ARGUMENTS [John R. Herndon, *Comm. ACM*, Apr. 1961] RICHARD GEORGE*

Argonne National Laboratory, Argonne, Ill.

* Work supported by United States Atomic Energy Commission.

This procedure was programmed in FORTRAN for the IBM 1620 and was tested with a number of real arguments. A few errors were detected:

1. In the following sequence the *end* must be removed:

begin if $(n - m + 2)/2 < i$ **then go to last end;**

2. In these, the lower bound of 1 is needed:

for i := step 1 until n do
for i := step 1 until j do

3. There are four places where integer arithmetic is clearly intended and we must substitute the symbol $\div$ for the symbol $/$.

In addition, it might be mentioned that the statement

if n = m then go to main;

could be omitted from the ALGOL program without harm, though the FORTRAN version requires it. Here, and elsewhere in the procedure, one might make an equivalent but more succinct statement. With change in style, the variable j could be eliminated.

ALGORITHM 48

LOGARITHM OF A COMPLEX NUMBER

JOHN R. HERNDON

Stanford Research Institute, Menlo Park, California

procedure LOGC(a, b, c, d); **value** a, b; **real** a, b, c, d;
comment This procedure computes the number, $c+di$, which is equal to $\log_e(a+bi)$;

```

begin c := sqrt (a × a + b × b);
      d := arctan (b/a);
      c := log (c);
      if a < 0 then d := d+3.1415927
end LOGC;
```

CERTIFICATION OF ALGORITHM 48

LOGARITHM OF A COMPLEX NUMBER (J. R.

Herndon, *Comm. ACM* 4 (Apr., 1961), 179)

A. P. RELPH

Atomic Power Div., The English Electric Co., Whetstone, England

Algorithm 48 was translated using the DEUCE ALGOL compiler, after certain modifications had been incorporated, and then gave satisfactory results.

The original version will fail if $a = 0$ when the procedure for arctan is entered. It also assumes that $-\pi/2 < d < 3\pi/2$, whereas the principal value for logarithm of a complex number assumes $-\pi < d \leq \pi$.

Incidentally, the ALGOL 60 identifier for natural logarithm is *ln*, not *log*.

The modified procedure is as follows:

```

procedure LOGC (a,b,c,d); value a,b; real a,b,c,d;
comment This procedure computes the number  $c + di$  which is
equal to the principal value of  $\log_e (a + bi)$ . If  $a = 0$  then  $c$  is
put equal to  $-1047$  which is used to represent " $-\infty$ ";
begin integer m,n
  m := sign (a); n := sign (b);
  if a = 0 then begin c := -1047;
    d := 1.5707963  $\times$  n;
    go to k
  end;
  c := sqrt(a  $\times$  a + b  $\times$  b);
  c := ln (c);
  d := 1.5707963  $\times$  (1-m)  $\times$  (1+n-n $\times$ n) + arctan (b/a);
k: end LOGC;

```

REMARK ON ALGORITHM 48

LOGARITHM OF A COMPLEX NUMBER [John R. Herndon, *Comm. ACM* 4 (Apr. 1961)]

MARGARET L. JOHNSON AND WARD SANGREN
Computer Applications, Inc., San Diego, Calif.

Considerable care must be taken in using the arctan function. In Algorithm 48 two such difficulties are ignored. First, it is necessary, because of a resulting division by zero, to deal separately with the case where the real part of the complex number is zero. Second, if the real part of the complex number is negative and the argument of the logarithm is to have a value between $-\pi$ and π then the action depends upon the sign of the imaginary part of the complex number. For clarity the following procedure exhibits in sequence the alternatives:

```

procedure LOGC (a, b, c, d); value a, b; real a, b, c, d;
comment This procedure computes the number  $c + di$  which is
equal to  $\log_e (a + bi)$ . It is assumed that the arctan has a value
between  $-\pi/2$  and  $\pi/2$ .
begin if a > 0 then begin THETA := 0; go to SOL end;
  if a < 0  $\wedge$  b  $\geq$  0 then begin THETA := 3.1415927;
    go to SOL end;
  if a < 0  $\wedge$  b < 0 then begin THETA := -3.1415927;
    go to SOL end;
  if a = 0  $\wedge$  b = 0 then begin c := d := 0;
    go to RETURN end;
  if a = 0  $\wedge$  b > 0 then begin c := ln(b); d := 1.570963;
    go to RETURN end;
  if a = 0  $\wedge$  b < 0 then begin c := ln(abs(b));
    d := 1.570963; go to RETURN end;
  SOL: d := arctan (b/a) + THETA;
  c := sqrt(a $\times$ a + b $\times$ b);
  c := ln(c);
  RETURN: end LOGC

```

REMARK ON REMARKS ON ALGORITHM 48 [B3]
LOGARITHM OF A COMPLEX NUMBER [John R. Herndon, *Comm. ACM* 4 (Apr. 1961), 179; 5 (Jun. 62), 347; 5 (Jul. 62), 391]

DAVID S. COLLENS (Recd. 24 Jan. 1964 and 1 Jun. 1964)
Computer Laboratory, The University, Liverpool 3, England

This procedure was designed to compute $\log_e(a + bi)$, namely $c + di$, and although some very necessary precautions about its use have already been stated, some points seem to have escaped notice. In particular, A. P. Relph [*Comm. ACM*, June 1962, 347] remarked that if $a = 0$, then c becomes " $-\infty$ ", but this is only the case if $b = 0$ also. Margaret L. Johnson and Ward Sangren [*Comm. ACM*, July 1962, 391] conceded that $a = b = 0$ was a special case, but wrongly gave zero as the result. The only reasonable way

of dealing with this case is to exit to some nonlocal label and to let the user decide whether to terminate his program or to assign particular values to c and d . The obvious values to use here are, for c , a negative number, larger than the largest which would be given by the procedure, and possibly zero for d . (In an implementation where 2^{-120} is the smallest representable nonzero number, the largest negative value of c possible is -89.416 .) Finally, in the Johnson-Sangren version of the procedure, the last conditional statement should read

```

if a = 0  $\wedge$  b < 0 then begin c := ln(abs(b));
  d := -1.570963; go to RETURN end;

```

the omission of the minus sign in the original being probably typographical in origin.

ALGORITHM 49

SPHERICAL NEUMANN FUNCTION

JOHN R. HERNDON

Stanford Research Institute, Menlo Park, California

```

real procedure SPHBEN (r,x); value r,x; real r,x;
comment This procedure computes the spherical Neumann
function  $(\pi/2x)^{1/2} N_{r+1/2}(x)$ . Infinity is represented by  $10^{47}$ ;
begin real z, g, t;
  if x = 0 then
    begin s := 10  $\uparrow$  47;
      go to gate
    end;
  s := -cos (x)/x;
  if r = 0 then
    go to gate;
  t := sin (x)/x;
  for g := 1 step 1 until r do
    begin z := s;
      s := s  $\times$  (g+g-1)/(x-t);
      t := z
    end;
  gate: SPHBEN := s
end SPHBEN;

```

ALGORITHM 50

INVERSE OF A FINITE SEGMENT OF THE HILBERT MATRIX

JOHN R. HERNDON

Stanford Research Institute, Menlo Park, California

```

procedure INVHILBERT (n,S); value n; real n;
  real array S;
comment This procedure computes the elements of the inverse
of an  $n \times n$  finite segment of the Hilbert matrix and stores them
in the array S;
begin real i, j, k;
  S[1, 1] = n  $\times$  n;
  for i := 2 step 1 until n do
    begin
      S[i, i] := (n+i-1)  $\times$  (n-i+1)/((i-1)  $\times$  (i-1));
      S[i, i] := S[i-1, i-1]  $\times$  S[i, i]
    end;

```

```

for i := 1 step 1 until n-1 do
  begin
    for j := i+1 step 1 until n do
      begin
        k := j-1;
        S[i,j] := -S[i,k] × (n+k) × (n-k)/(k × k)
      end
    end;
    for i := 2 step 1 until n do
      begin S[i,i] := S[i,i]/(i+1-1);
        for j := 1 step 1 until i-1 do
          begin S[j,i] := S[j,i]/(i+j-1);
            S[i,j] := S[j,i]
          end
        end
      end
    end
  end
end INVHILBERT;

```

CERTIFICATION OF ALGORITHM 50 INVERSE OF A FINITE SEGMENT OF THE HILBERT MATRIX [J. R. Herndon, *Comm. ACM* 4 (Apr. 1961)]

B. RANDELL

Atomic Power Division, The English Electric Co., Whetstone, England

INVHILBERT was translated using the DEUCE ALGOL compiler and the following corrections being needed.

1. $S[1,1] = n \times n$, replaced by $S[1,1] := n \times n$;

2. $S[j,i] := S(j,1)/(i+j-1)$

replaced by $S[j,i] := S[j,i]/(i+j-1)$

The compiled program, which used a 20 bit mantissa floating point notation then produced the following 4×4 segment

16.0	-120.0	240.0002	-140.0
-120.0	1200.0	-2700.0	1680.0019
240.0	-2700.0	6480.0	-4200.0
-140.0	1680.0019	-4200.0	2800.0039

REMARKS ON AND CERTIFICATION OF ALGORITHM 50

INVERSE OF A FINITE SEGMENT OF THE HILBERT MATRIX [J. R. Herndon, *Comm. ACM*, Apr. 1961]

P. NAUR

Regnecentralen, Copenhagen, Denmark

In addition to inserting the corrections indicated by B. Randell [*Comm. ACM* 5 (Jan. 1962), 50], we have modified and simplified the algorithm as follows:

1. The types of n, i, j and k have been changed to integer. This saves roundoff operations in subscripts.

2. Explicit multiplications have been replaced by squaring. This saves code length and execution time, at least in a compiler like ours for the GIER.

3. Repeated references to subscripted variables have been eliminated, partly with the aid of an additional simple working variable, w , partly by using simultaneous assignments.

4. An unnecessary **begin end** pair has been removed.

In total, these changes, in addition to reducing the code length, have increased speed by a factor of 1.6.

The resulting algorithm is as follows:

procedure INVHILBERT(n, S);

value n ; **integer** n ; **real array** S ;

comment ALG. 50: This procedure computes the elements of the inverse of an $n \times n$ finite segment of the Hilbert matrix and stores them in the array S . The Hilbert matrix has the elements $HILBERT[i,j] = 1/(i+j-1)$. The segments of this are known to be increasingly ill-conditioned with increasing size;

```

begin integer  $i, j, k$ ; real  $w$ ;
 $w := S[1,1] := n^2$ ;
for  $i := 2$  step 1 until  $n$  do  $w := S[i,i] := w \times ((n+i-1) \times (n-i+1)/(i-1)^2)^2$ ;
for  $i := 1$  step 1 until  $n-1$  do for  $j := i+1$  step 1 until  $n$  do
  begin
     $k := j-1$ ;
     $S[i,j] := -S[i,k] \times (n+k) \times (n-k)/k^2$ ;
  end;
for  $i := 2$  step 1 until  $n$  do for  $j := 1$  step 1 until  $i$  do
   $S[i,j] := S[j,i] := S[j,i]/(i+j-1)$ 
end INVHILBERT;

```

Both the original version and the above improved one have been run successfully on the GIER ALGOL system (30-bit mantissa). The test program included:

(a) Output of the 4×4 matrix, to be compared with the results of Randell [loc. cit.]. Results:

16.000000	-120.000000	240.000000	-140.000000
-120.000000	1200.000000	-2700.000000	1680.000000
240.000000	-2700.000000	6480.000000	-4200.000000
-140.000000	1680.000000	-4200.000000	2799.999977

(b) For $n := 1$ **step 1 until** 15; the inverse of the segment was calculated by INVHILBERT and multiplied by the segment of the Hilbert matrix, and the result was compared with the unit matrix. The maximum error was divided by the largest element of the inverse to form a relative error. Some of the results, which were entirely satisfactory throughout, are given below:

Order	Element of max error	abs (max error)	Largest element of INVHILBERT	Relative error
3	$S[3,3]$	$2.38_{10}-7$	$1.92_{10}2$	$1.24_{10}-9$
6	$S[2,4]$	$4.39_{10}-3$	$4.41_{10}6$	$9.96_{10}-10$
9	$S[2,8]$	$1.24_{10}2$	$1.22_{10}11$	$1.01_{10}-9$
12	$S[5,9]$	$1.54_{10}6$	$3.66_{10}15$	$4.21_{10}-10$
15	$S[1,12]$	$1.06_{10}11$	$1.15_{10}20$	$9.22_{10}-10$

(c) The time for a call of the revised INVHILBERT was found as follows:

n	
5	0.2 seconds
10	0.6 "
15	1.3 "

ALGORITHM 51

ADJUST INVERSE OF A MATRIX WHEN AN ELEMENT IS PERTURBED

JOHN R. HERNDON

Stanford Research Institute, Menlo Park, California

procedure ADJUST(n, d, i, j, A, B); **value** i, j, n, d ;

integer i, j, n ; **real** d ; **real array** A, B ;

comment If the $n \times n$ matrix $A = M^{-1}$ and a change, d , is made in the i, j -th element of M this procedure will calculate the corrected matrix for M^{-1} by adjusting matrix A . The adjusted matrix is stored in B ;

begin integer r, s ;

real t ;

$t := d/(A[j,i] \times d+1)$;

for $r := 1$ **step 1 until** n **do**

begin for $s := 1$ **step 1 until** n **do**

$B[r,s] = A[r,s] - t \times A[r,i] \times A[j,s]$ **end**

end ADJUST

CERTIFICATION OF ALGORITHM 51
ADJUST INVERSE OF A MATRIX WHEN AN
ELEMENT IS PERTURBED [John R. Herndon,
Comm. ACM 4 (Apr. 1961)]

RICHARD GEORGE*

Argonne National Laboratory, Argonne, Ill.

This procedure was programmed in FORTRAN and reduced to machine code mechanically. It was run on the Argonne-built computing machine, GEORGE. A floating-point routine was used which allows maximum accuracy to 31 bits.

The procedure was tested for matrices with n ranging from 2 to 10. For each value of n , there were 20 successive trials; each trial consisted of a random perturbation of a randomly selected element of the matrix M , followed by a use of ADJUST, followed by the matrix multiplication $N := B \cdot M$. For each trial, the adjustment was evaluated by computing

$$\text{sum} := \left\{ \sum_{i=1}^n \sum_{j=1}^n N[i,j] \right\} - n.$$

For random perturbations between -1.0 and $+1.0$, the value of sum never exceeded $2.0_{10}-8$.

There are two typographical errors present:

$B[r,s] = A[r,s] - t \times A[r,i] \times A[j,s]$ end

should be

$B[r,s] := A[r,s] - t \times A[r,i] \times A[j,s]$ end

ALGORITHM 52
A SET OF TEST MATRICES

JOHN R. HERNDON

Stanford Research Institute, Menlo Park, California

procedure TESTMATRIX (n,A); **value** n ; **integer** n ;
real array A ;

comment This procedure places in A an $n \times n$ matrix whose inverse and eigenvalues are known. The n -th row and the n -th column of the inverse are the set: 1, 2, 3, ..., n . The matrix formed by deleting the n -th row and the n -th column of the inverse is the identity matrix of order $n-1$;

begin **integer** i, j ;
real t, c, d, f ;
 $c := t \times (t+1) \times (t+t-5)/6$;
 $d := 1/c$;
 $A[n, n] := -d$;
for $i := 1$ **step** 1 **until** $n-1$ **do**
 begin $f := i$;
 $A[i, n] := d \times f$;
 $A[n, i] := A[i, n]$;
 $A[i, i] := d \times (c - f \times f)$;
 for $j := 1$ **step** 1 **until** $i-1$ **do**
 begin $t := j$;
 $A[i, j] := -d \times f \times t$;
 $A[j, i] := A[i, j]$
 end
 end
end
end TESTMATRIX;

CERTIFICATION OF ALGORITHM 52
A SET OF TEST MATRICES [J. R. Herndon, *Comm.*
ACM, Apr. 1961]

J. S. HILLMORE

Elliott Bros. (London) Ltd., Borehamwood, Herts.,
 England

The algorithm was corrected as recommended by H. E. Gilbert in his certification [*Comm. ACM*, Aug. 1961] and then successfully run using the Elliott ALGOL translator on the National-Elliott 803. The matrices so generated were used to test the matrix inversion procedure GJR given by H. R. Schwarz in his article "An Introduction to ALGOL" [*Comm. ACM*, Feb. 1962].

CERTIFICATION OF ALGORITHM 52
A SET OF TEST MATRICES (J. R. Herndon, *Comm.*
ACM, Apr. 1961)

H. E. GILBERT

University of California at San Diego, La Jolla, Calif.

The statement

$c := t \times (t+1) \times (t+t-5)/6$;

was changed to

$c := n \times (n+1) \times (n+n-5)/6$;

to make the inverse have the form described in the algorithm. The algorithm was translated to FORTRAN and tested with a matrix eigenvalue program on the CDC 1604 computer at UCSD.

The eigenvalues for the 20×20 test matrix are:

1. 1.000000
2. 1.000000
- ...
19. .01636693
20. -.02493833

REMARKS ON AND CERTIFICATION OF
ALGORITHM 52

A SET OF TEST MATRICES [J. R. Herndon, *Comm.*
ACM, Apr. 1961]

P. NAUR

Regnecentralen, Copenhagen, Denmark

In addition to inserting the correction indicated by H. E. Gilbert [*Comm. ACM* (Aug. 1961), 339] the algorithm was simplified by using the simultaneous assignment and by eliminating the local variables t and f . The resulting algorithm is as follows:

procedure TESTMATRIX (n,A);
value n ; **integer** n ; **real array** A ;
comment ALG. 52: This procedure places in A an $n \times n$ matrix whose inverse and eigenvalues are known. The n th row and the n th column of the inverse are the set: 1, 2, 3, ..., n . The matrix formed by deleting the n th row and the n th column of the inverse is the identity matrix of order $n-1$;
begin **integer** i, j ; **real** c, d ;
 $c := n \times (n+1) \times (n+n-5)/6$;
 $d := 1/c$;
 $A[n, n] := -d$;
for $i := 1$ **step** 1 **until** $n-1$ **do**
 begin
 $A[i, n] := A[n, i] := d \times i$;
 $A[n, i] := d \times (c - i^2)$;
 for $j := 1$ **step** 1 **until** $i-1$ **do** $A[i, j] := A[j, i] := -d \times i \times j$
 end
end TESTMATRIX;

This version of the algorithm was successfully run in the GIER ALGOL system together with the inversion procedures INVERSION II and gjr (see Certification of Algorithm 120 below). From the figures produced by INVERSION II it looks as if the determinant of these matrices is given by $6/(n(n+1)(5-2n))$, which is also the value of the element $A[n,n]$. For $n > 3$ the absolutely greatest element is $A[1,1] = 1 + A[n,n]$.

REMARK ON ALGORITHM 52

A SET OF TEST MATRICES (John R. Herndon, *Comm. ACM*, Apr. 1961)

G. H. DUBAY

University of St. Thomas, Houston, Tex.

In the assignment statement

$c := t \times (t + 1) \times (t + 5) / 6$; (a)

the t is undefined. A suitable definition would be provided by preceding (a) with $t := n$;

ADDITIONAL REMARKS ON ALGORITHM 52
A SET OF TEST MATRICES [J. R. Herndon, *Comm. ACM* (Apr. 1961), 180]

P. NAUR

Regnecentralen, Copenhagen, Denmark

From an inspection of the results of eigenvalue-finding algorithms I conclude that all but two of the eigenvalues of TEST-MATRIX are unity while the two remaining are given by the expressions $6/(p \times (n+1))$ and $p/(n \times (5-2 \times n))$ where

$$p = 3 + \sqrt{(4 \times n - 3) \times (n-1) \times 3/(n+1)}.$$

These expressions have been used for the determination of absolute errors of the eigenvalues calculated by JACOBI, Algorithm 85, and Householder Tridiagonalisation, etc. as reported below. They were also used to calculate the following table (using GIER ALGOL, with 29 significant bits):

n	Determinant	Eigenvalues Differing from unity	
3	-.500 000 00	.224 744 87	-2.224 744 9
4	-.100 000 00	.153 112 89	-.653 112 89
5	-.040 000 000	.113 238 08	-.353 238 08
6	-.020 408 163	.088 290 570	-.231 147 71
7	-.011 904 762	.071 428 571	-.166 666 67
8	-.007 575 757 6	.059 386 081	-.127 567 90
9	-.005 128 205 2	.050 422 549	-.101 704 60
10	-.003 636 363 6	.043 532 383	-.083 532 383
11	-.002 673 796 8	.038 097 478	-.070 183 039
12	-.002 024 291 5	.033 718 770	-.060 034 559
13	-.001 569 858 7	.030 128 103	-.052 106 125
14	-.001 242 236 0	.027 139 206	-.045 772 747
15	-.001 000 000 0	.024 619 013	-.040 619 013
16	-.000 816 993 47	.022 470 157	-.036 359 046
17	-.000 676 132 52	.020 619 902	-.032 790 288
18	-.000 565 930 96	.019 012 916	-.029 765 605
19	-.000 478 468 90	.017 606 429	-.027 175 807
20	-.000 408 163 27	.016 366 903	-.024 938 332

The figures for $n = 20$ agree very well with the results quoted by H. E. Gilbert in his certification [*Comm. ACM* 4 (Aug. 1961), 339].

ALGORITHM 53

NTH ROOTS OF A COMPLEX NUMBER

JOHN R. HERNDON

Stanford Research Institute, Menlo Park, California

```

procedure NTHROOT (n, r, u, REAL, UNREAL); value
    n, r, u; integer n;
    real r, u; real array REAL, UNREAL;
comment This procedure computes the n roots of the equation
     $x^n = r + ui$ . The real parts of the roots are stored in the vector
    REAL [ ]. The imaginary parts are stored in the corresponding
    locations in the vector UNREAL [ ];
begin
    integer n1, n2; real en, th, s, th1;
    REAL [n] := 0;
    en := 1/n;
    if u=0 then
        begin s := (abs(r)) ↑ en;
            th := 0;
        go to main end;
    if r=0 then
        begin s := (abs(u)) ↑ en;
            th := 1.5707963;
        if u < 0 then
            th := -th;
        go to main end;
    s := (r × r + u × u) ↑ (en/2);
    th := arctan (u/r);
main:
    if r < 0 then
        th := th + 3.1415926;
    th := en × th;
    th1 := 6.2831853 × en;
    for n2 := 1 step 1 until n do
        begin REAL [n2] := s × cos (th);
            UNREAL [n2] := s × sin (th);
            th = th + th1 end
end NTHROOT;

```

REMARK ON ALGORITHM 53

Nth ROOTS OF A COMPLEX NUMBER (John R. Herndon, *Comm. ACM* 4, Apr. 1961)

C. W. NESTOR, JR.

Oak Ridge National Laboratory, Oak Ridge, Tennessee

A considerable saving of machine time for $N \geq 3$ would result from the use of the recursion formulas for the sine and cosine in place of an entry into a sine-cosine subroutine in the do loop associated with the Nth roots of a complex number. That is, one could use

$$\begin{aligned}\sin (n+1) \theta &= \sin n \theta \cos \theta + \cos n \theta \sin \theta \\ \cos (n+1) \theta &= \cos n \theta \cos \theta - \sin n \theta \sin \theta,\end{aligned}$$

at the cost of some additional storage.

We have found this procedure to be very efficient in problems dealing with Fourier analysis, as suggested by G. Goerzel in chapter 24 of *Mathematical Methods for Digital Computers*.

ALGORITHM 54

GAMMA FUNCTION FOR RANGE 1 TO 2

JOHN R. HERNDON

Stanford Research Institute, Menlo Park, California

```

real procedure Q(x); value x; real x;
comment This procedure computes  $\Gamma(x)$  for  $1 \leq x \leq 2$ . This is
    a reference procedure for the more general gamma function
    procedure.  $\Gamma(x) = Q(x-1)$ ;

```



```

begin      Q := (((((((0.035868343 × x - 0.19352782) × x
              + 0.48219939) × x - 0.75670408) × x
              + 0.91820686) × x - 0.89705694) × x
              + 0.98820589) × x - 0.57719165) × x + 1.0
end        Q;

```

ALGORITHM 55 COMPLETE ELLIPTIC INTEGRAL OF THE FIRST KIND

JOHN R. HERNDON

Stanford Research Institute, Menlo Park, California

```

real procedure ELLIPTIC 1(k); value k; real k;
comment This procedure computes the elliptic integral of the
first kind K(k, π/2);
begin      real t;
              t := 1 - k × k;
              ELLIPTIC 1 := (((0.032024666 × t +
                0.054555509) × t
                + 0.097932891) × t + 1.3862944)
                - (((0.010944912 × t + 0.060118519) × t
                + 0.12475074) × t + 0.5) × log (t)
end        ELLIPTIC 1;

```

CERTIFICATION OF ALGORITHM 55
COMPLETE ELLIPTIC INTEGRAL OF THE FIRST
KIND [John R. Herndon, *Comm. ACM*, Apr. 1961]
and

CERTIFICATION OF ALGORITHM 149
COMPLETE ELLIPTIC INTEGRAL [J. N. Merner,
Comm. ACM, Dec. 1962]

HENRY C. THACHER, JR.*

Reactor Eng. Div., Argonne National Laboratory,
Argonne, Ill.

* Work supported by the U.S. Atomic Energy Commission.

The bodies of Algorithm 55 and of the second procedure of Algorithm 149 were tested on the LIG-30 computer using SCALP, the Dartmouth "LOAD-AND-GO" translator for a substantial subset of ALGOL 60. The floating-point arithmetic for this translator carries 7+ significant digits.

In addition to modifications required because of the limitations of the SCALP subset, the following need correction:

In Algorithm 55:

1. The constant 0.054555509 should be 0.054544409.
2. The function *log* should be *ln*.

In procedure ELIP 2 of Algorithm 149, the statement $a := c$ should be $a := C$.

The parameters of Algorithm 149 are related to the complete elliptic integral of the first kind by: $K = a \times ELIP(a, b)$ where the parameter $m = k^2 = 1 - b/a$.

The maximum approximation error in Algorithm 55 is given by Hastings as about 0.6n-6. In addition there is the possibility of serious cancellation error in forming the complementary parameter $t = 1 - k \times k$. For k near 1, errors as great as 4 significant digits were sustained. In these regions, the complementary parameter itself is a far more satisfactory parameter.

The accuracy obtainable with Algorithm 149 is limited only by the arithmetic accuracy and the amount of effort which it is desired to expend. Six-figure accuracy was obtained with 5 applications of the arithmetic-geometric mean for $a = 1000$, $b = 2$, and with one application for $a = 500$, $b = 500$.

Neither algorithm is satisfactory for $k = 1$. The behavior for Algorithm 55 will be governed by the error exit from the logarithm procedure. Under these circumstances, Algorithm 149 goes into an endless loop. Algorithm 149 may also go into an endless loop of the terminating constant (10^{-8} in the published algorithm) is too small for the arithmetic being used. For the SCALP arithmetic it was found necessary to increase this tolerance to 5.0×10^{-7} . The resulting values of the elliptic integrals were, however, accurate to within 2 in the 7th significant digit (6th decimal).

The relative efficiency of the two algorithms will depend strongly on the efficiency of the square-root and logarithm subroutines. With most systems, Algorithm 55 will provide sufficient accuracy, and will be more efficient. If a square-root operation or a highly efficient square-root subroutine is available, Algorithm 149 may well be the better method.

ALGORITHM 56 COMPLETE ELLIPTIC INTEGRAL OF THE SECOND KIND

JOHN R. HERNDON

Stanford Research Institute, Menlo Park, California

```

real procedure ELLIPTIC 2(k); value k; real k;
comment This procedure computes the elliptic integral of the
second kind E(k, π/2);
begin      real t;
              t := 1 - k × k;
              ELLIPTIC 2 := (((0.040905094 × t +
                0.085099193) × t
                + 0.44479204) × t + 1.0 - (((0.01382999 × t
                + 0.08150224) × t + 0.24969795) × t) × log (t)
end        ELLIPTIC 2;

```

ALGORITHM 57 BER OR BEI FUNCTION

JOHN R. HERNDON

Stanford Research Institute, Menlo Park, California

```

real procedure BERBEI (r, z); value r, z; real r, z;
comment This procedure computes ber(z) if r is set equal to
zero. bei(z) is produced if r equals 1.0;
begin

```

```

      real s, k, c, f, t;
      if r = 0 then
        s := 1
      else
        s := (z × z)/4;
        k := s;
        f := z × z;
        f := f × f;
        for c = 2 step 2 until 100 do
          begin
            if s = s + k then
              go to gate;
            t := (c+r) × (c+r-1);
            k := -0.0625 × k × f/(t × t);
            s := s+k end;

```

```

gate: BERBEI := s
end BERBEI;

```

CERTIFICATION OF ALGORITHM 57
BER OR BEI FUNCTION [J. R. Herndon, *Comm. ACM*
4 (Apr. 1961)]

A. P. RELPH
The English Electric Co. Whetstone, England

Algorithm 57 was translated using the DEUCE ALGOL compiler.
No corrections were required, and the results were satisfactory.

CERTIFICATION OF ALGORITHM 57
BER OR BEI FUNCTION [John R. Herndon, *Comm.*
ACM, Apr. 1961]

HENRY C. THACHER, JR.*
Reactor Engineering Div., Argonne National Lab.,
Argonne, Ill.

* Work supported by the U. S. Atomic Energy Commission.

The body of Algorithm 57 was tested on the LGP-30 using the
ALGOL 60 translator developed by the Dartmouth College Com-
puter Center. No syntactical errors were found. For $z = 0.1(0.1)1.0$,
with a 7+ significant decimal arithmetic routine, the program
gave results with errors less than 5 (and for $z = 1(1)5$ less than 12)
in the seventh digit. For large values of z , serious cancellation
errors may occur. For example, for $z = 20$, more than 2 decimals
of significance can be lost in this way.

ALGORITHM 58
MATRIX INVERSION

DONALD COHEN
Burroughs Corporation, Pasadena, Calif.

```

procedure invert (n) array: (a);
comment matrix inversion by Gauss-Jordan elimination;
  value n;
  array a; integer n;
begin
  array b, c [1:n]; integer i, j, k, l, p;
  integer array z [1:n];
    for j := 1 step 1 until n do z[j] := j;
    for i := 1 step 1 until n do begin
      k := i; y := a[i, i]; l := i - 1; p := i + 1;
      for j := p step 1 until n do begin
        w := a[i, j]; if abs(w) > abs(y) then begin
          k := j; y := w end end;
      for j := 1 step 1 until n do begin
        c[j] := a[j, k]; a[j, k] := a[j, i];
        a[j, i] := -c[j]/y; b[j] := a[i, j]/y end ;
        a[i, i] := 1/y; j := z[i]; z[i] := z[k]; z[k] := j ;
      for k := 1 step 1 until l, p step 1 until n do
        for j := 1 step 1 until l, p step 1 until n do
          a[k, j] := a[k, i] - b[j] × c[k] end; l := 0 ;
    back: l := l + 1; k := z[l]; if l ≤ n then begin
      for j := l while k ≠ j do begin
        for i := 1 step 1 until n do begin
          w := a[j, i]; a[j, i] := a[k, i]; a[k, i] := w end ;
        go to back end
      end invert.

```

CERTIFICATION OF ALGORITHM 58
MATRIX INVERSION (Donald Cohen, *Comm. ACM* 4,
May 1961)

RICHARD A. CONGER
Yale Computer Center, St. Louis University, St.
Louis, Mo.

Invert was hand-coded in FORTRAN for the IBM 1620. The
following corrections were found necessary:

The statement $a_{k,j} := a_{k,i} - b_j \times c_k$ should be

$$a_{k,j} := a_{k,j} - b_j \times c_k$$

The statement **go to** back should be changed to

$i := z_k$; $z_k := z_j$; $z_j := i$; **go to** back

After these corrections were made, the program was checked by
inverting a 6×6 matrix and then inverting the result. The second
result was equal to the original matrix within round-off.

CERTIFICATION OF ALGORITHM 58
MATRIX INVERSION [Donald Cohen, *Comm. ACM*,
May, 1961]

RICHARD GEORGE*
Particle Accelerator Div., Argonne National Lab.,
Argonne, Ill.

This procedure was programmed in FORTRAN and reduced to
machine code mechanically. It was run on the Argonne-built com-
puting machine, GEORGE. A floating-point routine was used which
allows maximum accuracy to 31 bits.

There are a number of errors of various types:

- (1) There are eight **begin**'s and only seven **end**'s.
- (2) The line

$a[k, j] := a[k, i] - b[j] \times c[k]$ **end**;

should be

$a[k, j] := a[k, j] - b[j] \times c[k]$ **end**;

- (3) The permutation of rows of the inverted matrix and permu-
tation of elements of the integer array z must be carried out simul-
taneously. This algorithm fails to do this, and consequently the
matrix at the time of exit from the procedure is left in a permuted
condition.
- (4) The algorithm permits the statement

$k := z[l]$;

to be executed even though the declarations place an upper limit
of n on the integer array z , and the test for $l \leq n$ has not yet been
made. Obviously, Mr. Cohen's compiling system would allow an
out-of-bounds array look-up. One could easily incorporate into an
ALGOL compiler a guard against such illicit array references, and
therefore the published algorithm might be considered machine
dependent.

- (5) This algorithm requires $3n^2$ divisions, most of which are un-
necessary. By inserting the statement

$y := 1.0/y$;

at the proper place, one may accomplish the obvious economy
of reducing this to only n divisions plus $2n^2$ multiplications.

- (6) If a matrix should be singular (or nearly so), some pivot
element will be zero (or very small), and a test should be made,
with provision for a jump to *ALARM*, a non-local label.
- (7) The identifiers w and y should be declared within this pro-
cedure, to avoid trouble.
- (8) This algorithm omits calculation of the determinant of the
matrix. This could be computed with very little extra effort.

The revised algorithm was then tested on the LGP-30 computer, using ALGOL-30, a small subset of ALGOL. Within the restrictions of this subset, the program worked satisfactorily on test matrices.

REMARK ON ALGORITHM 58

MATRIX INVERSION [D. Cohen, *Comm. ACM*,

May 61]

PETER G. BEHRENS

Matematikmaskinnmäanden, Box 6131, Stockholm 6, Sweden

invert was run on FACIT EDB using FACIT-ALGOL 1. Some changes in the procedure had to be made:

1. *y* and *w* had to be declared in the procedure-body as *real y, w*;

2. The last part of the procedure starting with $l := 0$; which should interchange the matrix rows did not work correctly, even with the corrections proposed by R. A. Conger [*Comm. ACM*, June 62]. We propose the following code:

```
for l := 1 step 1 until n do begin
  k := z[l]; for j := l while k ≠ j do begin
    for i := 1 step 1 until n do begin
      w := a[j, i]; a[j, i] := a[k, i]; a[k, i] := w end;
      i := z[k]; z[k] := z[j]; k := z[j] := i end end end invert
```

If the matrix *a* is singular, the value of the pivot element *y* will once be zero or very nearly zero and division by zero would occur in the course of the calculation. It would therefore be advantageous to introduce an empirical tolerance parameter *epsilon* into the procedure.

To calculate the determinant of the matrix *a* it is only necessary to put three more statements into the code. With these augmentations *invert* should read:

```
procedure invert (n, a, epsilon, determinant);
value n, epsilon; real epsilon, determinant;
array a; integer n;
begin real y, w; integer i, j, k, l, p;
array b, c[1:n]; integer array z[1:n];
determinant := 1;
```

followed by the same code as before until:

```
y := w end end;
determinant := y × determinant;
if k ≠ i then determinant := -determinant;
if abs(y) < epsilon then go to singular;
```

followed by the same code as before with the changes mentioned in the certification by R. A. Conger [*Comm. ACM*, June 62] and the changes given above. *singular* should be a nonlocal label in the main program.

REMARK ON ALGORITHM 58

MATRIX INVERSION [Donald Cohen, *Comm. ACM*,

May, 1961]

GEORGE STRUBLE

University of Oregon, Eugene, Oregon

For the last seven lines, beginning with $a[k, j] := a[k, i]$, substitute:

```
a[k, j] := a[k, j] - b[j] × c[k] end;
l := 0;
```

back: $l := l + 1$;

again: $k := z[l]$;

if $k \neq l$ then

```
begin for i := 1 step 1 until n do
  begin w := a[l, i];
    a[l, i] := a[k, i];
    a[k, i] := w end;
```

```
z[l] := z[k];
z[k] := l;
go to again end;
else if l ≠ n go to back
end invert
```

ALGORITHM 59

ZEROS OF A REAL POLYNOMIAL BY RESULTANT PROCEDURE

E. H. BAREISS and M. A. FISHERKELLER

Argonne National Laboratory, Argonne, Ill.

```
procedure RES (n, c, alpha, mu, re, im, rt, gc) ; value n,
c, alpha ; integer n, alpha ; integer array
mu ; array c, re, im, rt, gc ;
```

comment RES finds simultaneously all zeros of a polynomial of degree *n* with real coefficients, c_j ($j = 0, \dots, n$), where c_n is the constant term. The real part, re_i , and imaginary part, im_i , of each zero, with corresponding multiplicity, mu_i , and remainder term, rt_i , ($i = 1, \dots, n$), are found and a polynomial with coefficients gc_j ($j = 0, \dots, n$), is generated from these zeros. Alpha provides an option for local or nonlocal selection of *M*, the number of root-squaring iterations, and delta and epsilon, acceptance criteria. If $\alpha = 1$, these parameters are assigned locally. If $\alpha = 2$, *M*, delta and epsilon are set equal to the global parameters *Mp*, *deltap*, and *epsilonp*, respectively. In cases where zeros may be found more than once, the superfluous ones are eliminated by factorization. The method has been described by E. H. Bareiss (*J. ACM* 7, Oct. 1960, pp. 346-386).

```
begin integer M ; real delta, epsilon ; switch U :=
U1, U2 ;
go to U [alpha];
```

U1: $M := 10$; $\delta := 0.2$; $\epsilon := 10^{-8}$;
go to START ;

U2: $M := Mp$; $\delta := \text{deltap}$; $\epsilon := \text{epsilonp}$;

START: begin integer CT, nu, nuc, beta, m, j, jc, k, i, p ; Boolean ROOT ;
real X, Y, GX, rp ; array a, ac [0:n, 0:M], R, Rc, t [0:n];

$s [-1:n]$, $ag [-2:n]$, $rh, q, G, F [1:2 \times n]$;

switch S := S1, S2 ; switch T := T1, T2 ;

switch V := V1, V2 ;

real procedure min (u, v) ; real u, v ;

min := if $u \leq v$ then u else v ;

real procedure SYND (W, Q, I, T) ;

integer I ; real W, Q ;

array T ;

begin s [-1] := 0 ; s [0] := T [0] ; for
m := 1 step 1 until I do

$s [m] := T [m] - W \cdot s [m - 1] - Q \times s [m - 2]$;

if $Q = 0$ then SYND := abs (s[I]) else

SYND := abs ($W/2 \times s [I - 1] + s [I]$)
end SYND ;

CT := beta := 1 ; for j := 0 step 1 until
n do a [j, 0] := c[j] ;

SQUARING
OPERATION: begin integer el ; real h ; for m :=
1 step 1 until M do

begin for j := 1 step 1 until n do

```

begin h := 0 ; for el := 1 step 1 until
min (n - j, j) do
  h := h + (-1) ↑ el × a [j - el, m - 1] × a
  (j + el, m - 1) ;
  a [j, m] := (-1) ↑ j × (a [j, m - 1] ↑
  2 + 2 × h) end end end ;
for j := 0 step 1 until n do R [j] := (-1) ↑
j × a [j, M - 1] ↑ 2/a [j, M] ;
  j := 0 ; nu := 1 ;
RD: if (1 - delta ≤ R [j]) ∧ (R [j] ≤ 1 + delta)
then
  begin rp := (a [j, M]/a [j - nu, M]) ↑ (1/(2 ↑
  M × nu)) ;
  go to T [beta] end ;
1: nu := nu + 1 ;
2: j := j + 1 ; if j = n then go to S [beta]
else go to RD ;
3: nu := 1 ; go to 2 ;
T1: rh [CT] := rp ; X := rp + epsilon × rp ;
Y := X + epsilon × rp ;
for k := 0 step 1 until n do t [k] := abs (c [k]) ;
  F [CT] := SYND (Y, 0, n, t) - SYND
  (X, 0, n, t) ;
  G [CT] := SYND (rh [CT], 0, n, c) ; if
  F [CT] > G [CT] then
    begin ROOT := true ; q [CT] := 0 ;
    CT := CT + 1 ; F [CT] := F [CT - 1] end ;
    rh [CT] := -rp ; G [CT] := SYND (rh
    [CT], 0, n, c) ;
    if F [CT] > G [CT] then begin ROOT :=
    true ; q [CT] := 0 ; CT := CT + 1 ;
    F [CT] := F [CT - 1] end ; if nu = 1 then
    go to 2 ;
    q [CT] := rp ↑ 2 ; nuc := nu ; jc := j ;
    for j := 0 step 1 until n do
      begin R [j] := R [j] ; ac [j, M] := a [j, M]
      end ;
RESULTANT: begin real h ; array b [-1:n + 1,
-1:n + 1], A [1:n],
  r [0:n, 0:n], CB [-1:n + 1] ;
  b [-1, 0] := CB [-1] := CB [n + 1] := 0 ;
  for j := 0 step 1 until n do
    CB [j] := c [j] ; b [0, 0] := 1 ; for k :=
    1 step 1 until n do
      begin b [k, -1] := 0 ; for j := 0 step 1
      until k do
        b [k + 1, j] := b [k, j - 1] - q [CT] × b
        [k - 1, j] ;
        b [k + 1, k + 1] := h := 0 ; for j :=
        n - k step -1 until 0 do
          h := h + (CB [j] × CB [k + j] - CB [j - 1]
          × CB [k + j + 1]) × q [CT] ↑ (n - k - j) ;
          A [k] := (-1) ↑ k × h ; for j := 0 step
          1 until k - 1 do
            begin r [0, j] := 0 ; r [k, j] := r [k - 1, j] +
            A [k] × b [k, j] end ;
            r [k, k] := A [k] end ; beta := 2 ; for
            j := 0 step 1 until n do
              a [j, 0] := r [n, j] end ; go to SQUAR-
              ING OPERATION ;
T2: if (rp/2) ↑ 2 ≥ q [CT] then go to 3 ; rh
[CT] := rp ;
  G [CT] := SYND (rh [CT], q [CT], n, c) ;
  if F [CT] > G [CT] then
    begin CT := CT + 1 ; F [CT] := F
    [CT - 1] ; q [CT] := q [CT - 1] end ;
    rh [CT] := -rp ; G [CT] := SYND (rh [CT],
    q [CT], n, c) ;
    if F [CT] > G [CT] then begin CT := CT
    + 1 ; F [CT] := F [CT - 1] ; q [CT] := q
    [CT - 1] ; go to 3 else
      nu := nuc ; go to 1 ;
S1: ag [-2] := ag [-1] := 0 ; ag [0] := 1 ;
  for j := 1 step 1 until n do
    ag [j] := 0 ; k := 1 ; i := n ; m := 1 ;
    for j := 0 step 1 until n do
      t [j] := c [j] ;
MULT: mu [m] := 0 ; p := if q [k] = 0 then 1
else 2 ;
IT: GX := SYND (rh [k], q [k], i, t) ; if F [k]
> GX then
  begin for j := 1 step 1 until n do
    ag [j] := ag [j] - rh [k] × ag [j - 1] + q
    [k] × ag [j - 2] ;
    mu [m] := mu [m] + p ; i := i - p ;
    for j := 0 step 1 until i do
      t [j] := s [j] ; go to IT end else if
      mu [m] ≠ 0 then begin
        rt [m] := G [k] ; go to V [p] end else
        go to D ;
V1: re [m] := rh [k] ; im [m] := 0 ; go to E ;
V2: re [m] := rh [k]/2 ; im [m] := sqrt (q [k] -
re [m] ↑ 2) ;
E: m := m + 1 ;
D: k := k + 1 ; if k ≤ CT ∧ m ≤ n then go to
MULT ;
  for j := 0 step 1 until n do go [j] := ag [j] end
end RES

```

ALGORITHM 60

ROMBERG INTEGRATION

F. L. BAUER

Gutenberg University, Mainz, Germany

```

real procedure rombergintegr (fct, lgr, rgr, ord) ;
  value lgr, rgr, ord ;
  real lgr, rgr; integer ord ; real procedure fct ;
  comment rombergintegr is the value of the integral of the
  function fct between the limits lgr and rgr, calculated by the
  algorithm of Romberg with an error term of the order
  2 × ord + 2, ord ≥ 0. Computation time will roughly be doubled
  when ord is increased by 1;
begin
  real array t [1 : ord + 1];
  real l, u, m ;
  integer f, h, j, n ;
  l := rgr - lgr ;
  t [1] := (fct (lgr) + fct (rgr)) / 2 ;
  n := 1 ;
  for h := 1 step 1 until ord do
    begin u := 0 ;
      m := l / (2 × n) ;

```

```

for j := 1 step 2 until 2Xn-1 do
  u := u+fct(ℓgr+jXm) ;
  t[h+1] := (u/n+t[h])/2 ;
  f := 1 ;
for j := h step -1 until 1 do
  begin f := 4Xf ;
    t[j] := t[j+1]+(t[j+1]-t[j])/(f-1)
  end ;
  n := 2Xn
end ;
rombergintegr := t[1]Xℓ
end

```

CERTIFICATION OF ALGORITHM 60
ROMBERG INTEGRATION (F. L. Bauer, *Comm.*
ACM, June 1961)
 KARL HEINZ BUCHNER
 Lurgi Gesellschaft für Mineraloltechnik m.b.H., Frank-
 furt, Germany

Since August 1961, the Romberg Integration has been success-
 fully applied in FORTRAN language to various problems on an
 IBM 1620. Due to its elegant method and the memory saving
 features, the Romberg Integration has succeeded other methods
 in our program library, e.g., the Newton-Cotes integration of
 order 10.

Reference is made to Stiefel, *Numerische Mathematik* (Teubner
 Verlag, Stuttgart). Stiefel discusses in his book various methods
 of numerical integration including the Romberg algorithm.

CERTIFICATION OF ALGORITHM 60
ROMBERG INTEGRATION (F. L. Bauer, *Comm.*
ACM, June, 1961)
 HENRY C. THACHER, JR.*
 Argonne National Laboratory, Argonne, Ill.

* Work supported by the U. S. Atomic Energy Commission.

This procedure was translated to the ACT III compiler lan-
 guage for the Royal Precision LGP-30 computer. This system pro-
 vides 7+ significant decimal digits. The program was used to
 integrate x^n between the limits 0.01 and 1.1, and between the
 limits 1.1 and 0.01. The results in Table I were obtained. The
 pole at 0 for negative n affords a test of the reliability of the
 method when the higher derivatives of the integrand are large.
 The agreement between integrations in the forward and backward
 directions is an indication of the effects of round-off error.

It is apparent that the procedure gives results well within the
 noise level for the positive powers, and that even the effect of a
 closely adjacent singularity for the negative powers can be over-
 come.

The flexibility of the algorithm would be improved by adding
 to the formal parameters a procedure, check, to decide if sufficient
 accuracy had been obtained without carrying through the entire
 iteration. A possible form for this procedure would be:

```

procedure check (t1, t2, f, exit);
  real t1, t2;
  label exit;
  integer f;
begin if abs ((t2 - t1) X f) / t1 < tolerance ^ f > minimum order
  then go to exit end.

```

The global variables tolerance, which is the maximum relative
 difference between approximations of increasing order, and the
 minimum acceptable order should be selected by the programmer
 for the exigencies of the problem. A check of this sort is clearly
 not as sound as an a priori estimate of the necessary order, but is
 frequently an acceptable expedient.

The Romberg quadrature algorithm is analyzed in the follow-
 ing references:

- Romberg, W. Vereinfachte numerische Integration. *Det Kongelige Norske Videnskaber Selskab Forhandlinger* 28, (1955), 30-36.
 Stiefel, E., and Rutishauser, H. Remarques concernant l'integration numerique. *Comptes Rendus Acad. Sci. (Paris)* 252, (1961), 1899-1900.

TABLE I. INTEGRATION OF $\int_{0.01}^{1.1} x^n dx$ AND $\int_{1.1}^{0.01} x^n dx$

n	0	+12	+12	-1
True Value	1.0900000	.26555932	-.26555932	4.7004831
Order 1	1.0899997	.57076812	-.57076842	19.641113
Order 2	1.0899997	.30614608	-.30614626	10.656923
Order 5	1.0899991	.26555693	-.26555818	4.9017590
Order 10				4.7002345

n	-1	-5	-5
True Value	-4.7004831	.25000000X10 ⁸	-18.166667 X10 ⁸
Order 1	-19.641125	18.166655 X10 ⁸	-.25000000X10 ⁸
Order 2	-10.656929	8.4777719 X10 ⁸	-8.4777766 X10 ⁸
Order 5	-4.9017805	1.0408634 X10 ⁸	-1.0408640 X10 ⁸
Order 10	-4.7004402	.25000715X10 ⁸	-.25000727X10 ⁸
Order 12		.24999291X10 ⁸	-.25001311X10 ⁸

REMARK ON ALGORITHM 60 [D1]
ROMBERG INTEGRATION [F. L. Bauer, *Comm.*
ACM 4 (June 1961) 255; 5 (Mar. 1962), 168; 5 (May
 1962), 281]
 HENRY C. THACHER, JR.* (Recd. 20 Feb. 1964 and 23 Mar.
 1964)

Argonne National Laboratory, Argonne, Ill.

* Work supported by the U. S. Atomic Energy Commission.

The Romberg integration algorithm has been used with great
 success by many groups [1, 2], and appears to be among the most
 generally reliable quadrature methods available. It is, therefore,
 worth pointing out that it is not entirely foolproof, and that a sig-
 nificant class of integrands exists for which the extrapolated values
 are poorer estimates of the integral than the corresponding
 trapezoidal sums.

The validity of the Romberg procedure depends upon the possi-
 bility of expanding the error of the trapezoidal rule in powers of
 h^2 , where h is the stepsize. One expansion of this type is the Euler-
 Maclaurin sum formula. An alternative expression may be ob-
 tained from the Fourier series expansion. The coefficients of h^{2r} in
 the Euler Maclaurin formula are proportional to the difference of
 the values of the $(2r+1)$ -th derivative at the two ends of the range.
 Thus, any integral for which the odd derivatives of the integrand
 either vanish or are equal at the limits will not be improved by
 Romberg extrapolation. Among the common examples of such
 integrals are integrals of periodic functions over a period and
 integrals for which the derivatives vanish at both limits. An exam-
 ple of the last type is the integral approximation to the modified
 Hankel function [3], $e^x K_p(x) = \int_0^L e^{x(1-\cosh t)} \cosh(pt) dt$, where L
 is taken so large that the contribution of the integral from L to ∞
 may be neglected. Several other examples are given under the
 heading "Exceptional cases" by Bauer, Rutishauser and Stie-
 fele [7]. This paper is among the most extensive discussions of
 the Romberg method in English.

The algorithm also fails when the expansion of the error term
 contains other powers of h along with the even ones. Rutishauser
 [4] discusses estimating integrals of the form $\int_0^1 f(x) dx =$
 $\int_0^1 (\varphi(x)/\sqrt{x}) dx$. If such integrals are estimated by the trapezoidal

rule, assigning the value 0 to $f(0)$, the error may be expressed in the form $\sum c_h h^{2k} + \sqrt{h} \sum d_h h^k$. Although the standard Romberg extrapolation fails when applied to this sequence of estimates, Rutishauser presents a modified procedure which is effective.

The extrapolation is also invalid when the integrand is discontinuous, although this exception is trivial from the computational standpoint.

It has also been pointed out [5, 6] that the Romberg procedure may amplify round-off errors. The losses, while significant, do not appear prohibitive for most applications.

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1. THACHER, H. C., JR. Certification of algorithm 60. *Comm. ACM* 5 (Mar. 1962), 168.
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ALGORITHM 61

PROCEDURES FOR RANGE ARITHMETIC

ALLAN GIBB*

University of Alberta, Calgary, Alberta, Canada

begin

procedure RANGESUM (a, b, c, d, e, f);

real a, b, c, d, e, f;

comment The term "range number" was used by P. S. Dwyer, *Linear Computations* (Wiley, 1951). Machine procedures for range arithmetic were developed about 1958 by Ramon Moore, "Automatic Error Analysis in Digital Computation," LMSD Report 48421, 28 Jan. 1959, Lockheed Missiles and Space Division, Palo Alto, California, 59 pp. If $a \leq x \leq b$ and $c \leq y \leq d$, then RANGESUM yields an interval $[e, f]$ such that $e \leq (x + y) \leq f$. Because of machine operation (truncation or rounding) the machine sums $a + c$ and $b + d$ may not provide safe end-points of the output interval. Thus RANGESUM requires a non-local real procedure ADJUSTSUM which will compensate for the machine arithmetic. The body of ADJUSTSUM will be dependent upon the type of machine for which it is written and so is not given here. (An example, however, appears below.) It is assumed that ADJUSTSUM has as parameters real v and w, and integer i, and is accompanied by a non-local real procedure CORRECTION which gives an upper bound to the magnitude of the error involved in the machine representation of a number. The output ADJUSTSUM provides the left end-point of the output interval of RANGESUM when ADJUSTSUM is called with $i = -1$, and the right end-point when called with $i = 1$. The procedures RANGESUB, RANGEMPY, and RANGEDVD provide for the remaining fundamental operations in range arithmetic. RANGESQR gives an interval within which the square of a range number must lie. RNGSUMC, RNGSUBC, RNGMPYC and RNGDVDC provide for range arithmetic with complex range arguments, i.e. the real and imaginary parts are range numbers;

begin

e := ADJUSTSUM (a, c, -1);

f := ADJUSTSUM (b, d, 1)

end RANGESUM;

procedure RANGESUB (a, b, c, d, e, f);

real a, b, c, d, e, f;

comment RANGESUM is a non-local procedure;

begin

RANGESUM (a, b, -d, -c, e, f)

end RANGESUB;

procedure RANGEMPY (a, b, c, d, e, f);

real a, b, c, d, e, f;

comment ADJUSTPROD, which appears at the end of this procedure, is analogous to ADJUSTSUM above and is a non-local real procedure. MAX and MIN find the maximum and minimum of a set of real numbers and are non-local;

begin

real v, w;

if $a < 0 \wedge c \geq 0$ then

1: begin

v := c; c := a; a := v; w := d; d := b; b := w

end 1;

if $a \geq 0$ then

2: begin

if $c \geq 0$ then

3: begin

e := a × c; f := b × d; go to 8

end 3;

e := b × c;

if $d \geq 0$ then

4: begin

f := b × d; go to 8

end 4;

f := a × d; go to 8

5: end 2;

if $b > 0$ then

6: begin

if $d > 0$ then

begin

e := MIN(a × d, b × c);

f := MAX(a × c, b × d); go to 8

end 6;

e := b × c; f := a × c; go to 8

end 5;

f := a × c;

if $d \leq 0$ then

7: begin

e := b × d; go to 8

end 7;

e := a × d;

8: e := ADJUSTPROD (e, -1);

f := ADJUSTPROD (f, 1)

end RANGEMPY;

procedure RANGEDVD (a, b, c, d, e, f);

real a, b, c, d, e, f;

comment If the range divisor includes zero the program exists to a non-local label "zerodvsv". RANGEDVD assumes a non-local real procedure ADJUSTQUOT which is analogous (possibly identical) to ADJUSTPROD;

begin

if $c \leq 0 \wedge d \geq 0$ then go to zerodvsv;

if $c < 0$ then

1: begin

if $b > 0$ then

2: begin

e := b/d; go to 3

end 2;

e := b/c;

3: if $a \geq 0$ then

4: begin

f := a/c; go to 8

end 4;

f := a/d; go to 8

end 1;

```

    if a < 0 then
5:  begin
        e := a/c; go to 6
    end 5;
    e := a/d;
6:  if b > 0 then
7:  begin
        f := b/c; go to 8
    end 7;
    f := b/d;
8:  e := ADJUSTQUOT (e, -1); f := ADJUSTQUOT (f, 1)
end RANGEDVD;
procedure RANGESQR (a, b, e, f);
    real a, b, e, f;
comment ADJUSTPROD is a non-local procedure;
begin
    if a < 0 then
1:  begin
        if b < 0 then
2:  begin
            e := b × b; f := a × a; go to 3
        end 2;
        e := 0; m := MAX (-a, b); f := m × m; go to 3
    end 1;
    e := a × a; f := b × b;
3:  ADJUSTPROD (e, -1);
    ADJUSTPROD (f, 1)
end RANGESQR;
procedure RANGSUMC (aL, aR, bL, bU, cL, cR, dL, dU, eL,
eR, fL, fU);
    real aL, aR, bL, bU, cL, cR, dL, dU, eL, eR, fL, fU;
comment Rangesum is a non-local procedure;
begin
    RANGESUM (aL, aR, cL, cR, eL, eR);
    RANGESUM (bL, bU, dL, dU, fL, fU)
end RANGSUMC;
procedure RANGSUBC (aL, aR, bL, bU, cL, cR, dL, dU, eL,
eR, fL, fU);
    real aL, aR, bL, bU, cL, cR, dL, dU, eL, eR, fL, fU;
comment RANGSUMC is a non-local procedure;
begin
    RANGSUMC (aL, aR, bL, bR, -cR, -cL, -dU, -dL, eL, eR,
fL, fU)
end RANGSUBC;
procedure RANGMPYC (aL, aR, bL, bU, cL, cR, dL, dU, eL,
eR, fL, fU);
    real aL, aR, bL, bU, cL, cR, dL, dU, eL, eR, fL, fU;
comment RANGEMPY, RANGESUB, and RANGESUM are
non-local procedures;
begin
    real L1, R1, L2, R2, L3, R3, L4, R4;
    RANGEMPY (aL, aR, cL, cR, L1, R1);
    RANGEMPY (bL, bU, dL, dU, L2, R2);
    RANGESUB (L1, R1, L2, R2, eL, eR);
    RANGEMPY (aL, aR, dL, dU, L3, R3);
    RANGEMPY (bL, bU, cL, cR, L4, R4);
    RANGESUM (L3, R3, L4, R4, fL, fU);
end RANGMPYC;
procedure RNGDVDC (aL, aR, bL, bU, cL, cR, dL, dU, eL,
eR, fL, fU);
    real aL, aR, bL, bU, cL, cR, dL, dU, eL, eR, fL, fU;
comment RANGMPYC, RANGESQR, RANGESUM, and
RANGEDVD are non-local procedures;
begin
    real L1, R1, L2, R2, L3, R3, L4, R4, L5, R5;
    RANGMPYC (aL, aR, bL, bU, cL, cR, -dU, -dL, L1, R1, L2,
R2);
    RANGESQR (cL, cR, L3, R3);
    RANGESQR (dL, dU, L4, R4);
    RANGESUM (L3, R3, L4, R4, L5, R5);

```

```

    RANGEDVD (L1, R1, L5, R5, eL, eR);
    RANGEDVD (L2, R2, L5, R5, fL, fU)
end RNGDVDC
end

```

EXAMPLE

real procedure CORRECTION (p); **real** p;
comment CORRECTION and the procedures below are intended for use with single-precision normalized floating-point arithmetic for machines in which the mantissa of a floating-point number is expressible to s significant figures, base b . Limitations of the machine or requirements of the user will limit the range of p to $b^m \leq |p| < b^{n+1}$ for some integers m and n . Appropriate integers must replace s , b , m and n below. Signal is a non-local label. The procedures of the example would be included in the same block as the range procedures above;

```

begin
    integer w;
    for w := m step 1 until n do
1:  begin
        if (b ↑ w ≤ abs (p)) ∧ (abs (p) < b ↑ (w + 1)) then
2:  begin
            CORRECTION := b ↑ (w+1-s); go to exit
        end 2
    end 1;
    go to signal;
exit: end CORRECTION;
real procedure ADJUSTSUM (w, v, i); integer i;
    real w, v;
comment ADJUSTSUM exemplifies a possible procedure for use with machines which, when operating in floating point addition, simply shift out any lower order digits that may not be used. No attempt is made here to examine the possibility that every digit that is dropped is zero. CORRECTION is a non-local real procedure which gives an upper bound to the magnitude of the error involved in the machine representation of a number;
begin
    real r, cw, cv, cr;
    r := w + v;
    if w = 0 ∨ v = 0 then go to 1;
    cw := CORRECTION (w);
    cv := CORRECTION (v);
    cr := CORRECTION (r);
    if cw = cv ∧ cr ≤ cw then go to 1;
    if sign (i × sign (w) × sign (v) × sign (r)) = -1 then go to 1;
    ADJUSTSUM := r + i × MAX (cw, cv, cr); go to exit;
1:  ADJUSTSUM := r;
exit: end ADJUSTSUM;
real procedure ADJUSTPROD (p, i); real p; integer i;
comment ADJUSTPROD is for machines which truncate when lower order digits are dropped. CORRECTION is a non-local real procedure;
begin
    if p × i ≤ 0 then
1:  begin
        ADJUSTPROD := p; go to out
    end 1;
    ADJUSTPROD := p + i × CORRECTION (p);
out: end ADJUSTPROD;
comment Although ordinarily rounded arithmetic is preferable to truncated (chopped) arithmetic, for these range procedures truncated arithmetic leads to closer bounds than rounding does.

```

* These procedures were written and tested in the Burroughs 220 version of the ALGOL language in the summer of 1960 at Stanford University. The typing and editorial work were done under Office of Naval Research Contract Nonr-225(37). The author wishes to thank Professor George E. Forsythe for encouraging this work and for assistance with the syntax of ALGOL 60.

ALGORITHM 62

A SET OF ASSOCIATE LEGENDRE POLYNOMIALS OF THE SECOND KIND*

JOHN R. HERNDON

Stanford Research Institute, Menlo Park, California

comment This procedure places a set of values of $Q_n^m(x)$ in the array $Q[]$ for values of n from 0 to $n_{\max}$ for a particular value of m and a value of x which is real if ri is 0 and is purely imaginary, ix , otherwise. $R[]$ will contain the set of ratios of successive values of Q . These ratios may be especially valuable when the $Q_n^m(x)$ of the smallest size is so small as to underflow the machine representation (e.g. 10^{-60} if 10^{-51} were the smallest representable number). 9.9×10^{46} is used to represent infinity. Imaginary values of x may not be negative and real values of x may not be smaller than 1.

Values of $Q_n^m(x)$ may be calculated easily by hypergeometric series if x is not too small nor $(n - m)$ too large. $Q_n^m(x)$ can be computed from an appropriate set of values of $P_n^m(x)$ if x is near 1.0 or ix is near 0. Loss of significant digits occurs for x as small as 1.1 if n is larger than 10. Loss of significant digits is a major difficulty in using finite polynomial representations also if n is larger than m . However, QLEG has been tested in regions of x and n both large and small;

```

procedure QLEG(m, nmax, x, ri, R, Q); value m, nmax, x, ri;
    real m, nmax, x, ri; real array R, Q;
begin real t, i, n, q0, s;
    n := 20;
    if nmax > 13 then
        n := nmax + 7;
    if ri = 0 then
        begin if m = 0 then
            Q[0] := 0.5 × log((x + 1)/(x - 1));
            else
                begin t := -1.0/sqrt(x × x - 1);
                    q0 := 0;
                    Q[0] := t;
                    for i := 1 step 1 until m do
                        begin s := (x + x) × (i - 1) × t
                            × Q[0] + (3i - i × i - 2) × q0;
                            q0 := Q[0];
                            Q[i] := s end end;
                if x = 1 then
                    Q[0] := 9.9 ↑ 45;
                R[n + 1] := x - sqrt(x × x - 1);
                for i := n step -1 until 1 do
                    R[i] := (i + m)/((i + i + 1) × x
                        + (m - i - 1) × R[i + 1]);
                go to the end;
            if m = 0 then
                begin if x < 0.5 then
                    Q[0] := arctan(x) - 1.5707963 else
                        Q[0] := - arctan(1/x) end else
                    begin t := 1/sqrt(x × x + 1);
                        q0 := 0;
                        Q[0] := t;
                        for i := 2 step 1 until m do
                            begin s := (x + x) × (i - 1) × t × Q[0]
                                + (3i + i × i - 2) × q0;
                                q0 := Q[0];
                                Q[i] := s end end;
                    R[n + 1] := x - sqrt(x × x + 1);
                    for i := n step -1 until 1 do
                        R[i] := (i + m)/((i - m + 1) × R[i + 1]
                            - (i + i + 1) × x);
                    for i := 1 step 2 until nmax do
                        R[i] := - R[i];

```

```

the: for i := 1 step 1 until nmax do
    Q[i] := Q[i - 1] × R[i]
end QLEG;

```

* This procedure was developed in part under the sponsorship of the Air Force Cambridge Research Center.

REMARK ON ALGORITHM 62

A SET OF ASSOCIATE LEGENDRE POLYNOMIALS OF THE SECOND KIND (John R. Herndon, *Comm. ACM* 4 (July, 1961))

JOHN R. HERNDON

Stanford Research Institute, Menlo Park, California

In regard to Algorithm 62 in *Communications of the ACM*, two errors were found:

The 14th line of the procedure

```

for i := 1 step 1 until m do
    should read
        for i := 2 step 1 until m do

```

The 35th line

```

    + (3i - iXi - 2)Xq0
should read
    + (3i - i × i - 2) × q0

```

The procedure QLEG was developed from the standard recurrence formula

$(n + m - 1)Q_{n-2}^m = (2n - 1) \cdot x \cdot Q_{n-1}^m - (n - m)Q_n^m$.
Invert and multiply by $(n + m - 1)Q_{n-1}^m$.

$$\frac{Q_{n-1}^m}{Q_{n-2}^m} = \frac{(n + m - 1)}{(2n - 1) \cdot x - (n - m)Q_n^m/Q_{n-1}^m},$$

or

$$R_{n-1}^m = \frac{(n + m - 1)}{(2n - 1) \cdot x - (n - m)R_n^m}.$$

Analysis (and testing) shows that, for n large, this infinite continued fraction need only be carried to about eight terms for eight-digit accuracy if the final term is evaluated with the asymptotic value derived by setting

$$R_{n-1}^m = R_n^m, \quad \lim_{n \rightarrow \infty} R_n^m = x \pm \sqrt{x^2 - 1},$$

the minus sign being chosen since in general $Q_n^m < Q_{n-1}^m$. The formulas pertaining to purely imaginary parameters follow readily. The value of

$$Q_0^0(x) = \frac{1}{2} \log_e \frac{x + 1}{x - 1},$$

while

$$Q_1^0(x) = x \cdot Q_0^0(x) - 1,$$

and

$$Q_0^1(x) = \frac{-1}{\sqrt{x^2 - 1}}.$$

Other values are derived using the ratios $R_n^m(x)$ and/or the recurrence formula

$$Q_n^m = -\frac{2(m - 1)x}{\sqrt{x^2 - 1}} Q_{n-1}^{m-1} + (n - m + 2)(n + m - 2)Q_{n-2}^{m-2}.$$

The derivation of the expression for $Q_0^0(ix)$ is not trivial and proceeds as follows:

$$i \cdot Q_0^0(ix) = \frac{1}{2} \log_e \frac{ix+1}{ix-1} = \frac{1}{2} \log_e \left[-\frac{x^2-1}{x^2+1} + \frac{2x}{x^2+1} \right]$$

$$e^{a+ib} = e^a \cdot e^{ib} = e^a \cos b + i \sin b.$$

Thus

$$\tan b = \frac{-2x}{1-x^2}$$

and

$$Q_0^0(ix) = (\arctan x - \pi/2)i.$$

ALGORITHM 63

PARTITION

C. A. R. HOARE

Elliott Brothers Ltd., Borehamwood, Hertfordshire, Eng.

procedure partition (A,M,N,I,J); **value** M,N;
array A; **integer** M,N,I,J;

comment I and J are output variables, and A is the array (with subscript bounds M:N) which is operated upon by this procedure. Partition takes the value X of a random element of the array A, and rearranges the values of the elements of the array in such a way that there exist integers I and J with the following properties:

$$M \leq J < I \leq N \text{ provided } M < N$$

$$A[R] \leq X \text{ for } M \leq R \leq J$$

$$A[R] = X \text{ for } J < R < I$$

$$A[R] \geq X \text{ for } I \leq R \leq N$$

The procedure uses an integer procedure random (M,N) which chooses equiprobably a random integer F between M and N, and also a procedure exchange, which exchanges the values of its two parameters;

```
begin   real X; integer F;
        F := random (M,N); X := A[F];
        I := M; J := N;
up:     for I := I step 1 until N do
        if X < A [I] then go to down;
        I := N;
down:   for J := J step -1 until M do
        if A[J] < X then go to change;
        J := M;
change: if I < J then begin exchange (A[I], A[J]);
        I := I + 1; J := J - 1;
        go to up
        end
else   if I < F then begin exchange (A[I], A[F]);
        I := I + 1
        end
else   if F < J then begin exchange (A[F], A[J]);
        J := J - 1
        end;
end   partition
```

CERTIFICATION OF ALGORITHMS 63, 64, 65
 PARTITION, QUICKSORT, FIND [C. A. R. Hoare,
Comm. ACM, July 1961]

J. S. HILLMORE

Elliott Bros. (London) Ltd., Borehamwood, Herts.,
 England

The body of the procedure find was corrected to read:

```
begin integer I, J;
if M < N then begin partition (A, M, N, I, J);
        if K ≤ I then find (A, M, J, K)
        else if J ≤ K then find (A, I, N, K)
        end
end find
```

and the trio of procedures was then successfully run using the Elliott ALGOL translator on the National-Elliott 803.

The author's estimate of $\frac{1}{2}(N-M)\ln(N-M)$ for the number of exchanges required to sort a random set was found to be correct. However, the number of comparisons was generally less than $2(N-M)\ln(N-M)$ even without the modification mentioned below.

The efficiency of the procedure quicksort was increased by changing its body to read:

```
begin integer I, J;
if M < N-1 then begin partition (A, M, N, I, J);
        quicksort (A, M, J);
        quicksort (A, I, N)
        end
else if N-M = 1 then begin if A[N] < A[M] then
        exchange (A[M], A[N])
        end
```

end quicksort

This alteration reduced the number of comparisons involved in sorting a set of random numbers by 4-5 percent, and the number of entries to the procedure partition by 25-30 percent.

CERTIFICATION OF ALGORITHMS 63, 64 AND 65,
 PARTITION, QUICKSORT, AND FIND, [Comm. ACM,
 July 1961]

B. RANDELL AND L. J. RUSSELL

The English Electric Company Ltd., Whetstone, England

Algorithms 63, 64, and 65 have been tested using the Pegasus ALGOL 60 Compiler developed at the De Havilland Aircraft Company Ltd., Hatfield, England.

No changes were necessary to Algorithms 63 and 64 (Partition and Quicksort) which worked satisfactorily. However, the comment that Quicksort will sort an array without the need for any extra storage space is incorrect, as space is needed for the organization of the sequence of recursive procedure activations, or, if implemented without using recursive procedures, for storing information which records the progress of the partitioning and sorting.

A misprint ('if' for 'if' on the line starting 'else if J ≤ K then ...') was corrected in Algorithm 65 (Find), but it was found that in certain cases the sequence of recursive activations of Find would not terminate successfully. Since Partition produces as output two integers J and I such that elements of the array A[M:N] which lie between A[J] and A[I] are in the positions that they will occupy when the sorting of the array is completed, Find should cease to make further recursive activations of itself if K fulfills the condition J < K < I.

Therefore the conditional statement in the body of Find was changed to read

```
if K ≤ J then find (A, M, J, K)
else if I ≤ K then find (A, I, N, K)
```

With this change the procedure worked satisfactorily.

ALGORITHM 64

QUICKSORT

C. A. R. HOARE

Elliott Brothers Ltd., Borehamwood, Hertfordshire, Eng.

```

procedure quicksort (A,M,N); value M,N;
    array A; integer M,N;
comment Quicksort is a very fast and convenient method of
    sorting an array in the random-access store of a computer. The
    entire contents of the store may be sorted, since no extra space is
    required. The average number of comparisons made is  $2(M-N) \ln$ 
     $(N-M)$ , and the average number of exchanges is one sixth this
    amount. Suitable refinements of this method will be desirable for
    its implementation on any actual computer;
begin    integer I,J;
        if M < N then begin partition (A,M,N,I,J);
            quicksort (A,M,J);
            quicksort (A, I, N)
        end
    end    quicksort

```

SEE ALGORITHM 63

ALGORITHM 65

FIND

C. A. R. HOARE

Elliott Brothers Ltd., Borehamwood, Hertfordshire, Eng.

```

procedure find (A,M,N,K); value M,N,K;
    array A; integer M,N,K;
comment Find will assign to A [K] the value which it would
    have if the array A [M:N] had been sorted. The array A will be
    partly sorted, and subsequent entries will be faster than the first;
begin    integer I,J;
        if M < N then begin partition (A, M, N, I, J);
            if K ≤ I then find (A,M,I,K)
            else if J ≤ K then find (A,J,N,K)
        end
    end    find

```

SEE ALGORITHM 63

ALGORITHM 66

INVRS

JOHN CAFFREY

Director of Research, Palo Alto Unified School District,
Palo Alto, California

```

procedure InvrS (t) size : (n); value n; real array t; inte-
ger n;
comment Inverts a positive definite symmetric matrix t, of
    order n, by a simplified variant of the square root method. Re-
    places the  $n(n+1)/2$  diagonal and superdiagonal elements of t
    with elements of  $t^{-1}$ , leaving subdiagonal elements unchanged.
    Advantages: only n temporary storage registers are required, no
    identity matrix is used, no square roots are computed, only n
    divisions are performed, and, as n becomes large, the number of
    multiplications approaches  $n^3/2$ ;

```

```

begin integer i, j, s; real array vll:n-1; real y, pivot;
for s := 0 step 1 until n-1 do
    begin pivot := 1.0/t[1,1];
        comment If  $t[1,1] \leq 0$ , t is not positive defi-
        nite;
        for i := 2 step 1 until n do v[i-1] := t[1, i];
        for i := 1 step 1 until n-1 do
            begin t[i,n] := y := -v[i] × pivot;
                for j := i step 1 until n-1 do
                    t[i, j] := t[i + 1, j + 1] + v[j] × y
                end;
            t[n,n] := -pivot
        end;
        comment At this point, elements of  $t^{-1}$  occupy
        the original array space but with signs reversed,
        and the following statements effect a simple re-
        flection;
        for i := 1 step 1 until n do
            for j := i step 1 until n do t[i,j] := -t[i,j]
    end InvrS

```

CERTIFICATION OF ALGORITHM 66

INVRS (J. Caffrey, Comm. ACM. July 1961)

B. RANDELL, C. G. BROYDEN.

Atomic Power Division, The English Electric Company,
Whetstone, England.

INVRS was translated using the DEUCE ALGOL Compiler, and
needed the following correction.

The repeat of the line,

begin pivot := 1.0/t[1, 1];

was deleted.

The compiled program, which used a 20 bit mantissa floating
point notation, was tested using Wilson's matrix

5	7	6	5
7	10	8	7
6	8	10	9
5	7	9	10

and gave results

67.9982	-40.9991	-16.9995	9.9997
-40.9991	24.9995	9.9997	-5.9998
-16.9995	9.9997	4.9998	-2.9999
9.9997	-5.9998	-2.9999	1.9999

(The output routine completed the symmetric matrix)

INVRS will in fact invert non-positive symmetric matrices, the
only restriction appearing to be that the leading minors of the
matrix must be non-zero. The variable T[1, 1] takes as its succe-
ssive values ratios of the (r + 1)th to the r th leading minors of the
matrix, and if it becomes zero the variable 'pivot' cannot be com-
puted.

The following matrix, for which the successive values of T[1, 1]
were +2, -2, -1, -0.6, +5 gave results correct to one unit in the
fifth significant figure.

2	-3	1	-1	4
-3	2	-4	3	-2
1	-4	-3	2	4
-1	3	2	-2	-3
4	-2	4	-3	2

CERTIFICATION OF ALGORITHM 66 INVRS (J. Caffrey, *Comm. ACM*, July 1961)

JOHN CAFFREY

Palo Alto Unified School District, Palo Alto, California

INVRS was translated using the Burroughs 220 Algebraic Computer (BALCOM) at Stanford University, using 8-digit floating-point arithmetic. The misprint noted by Randell and Broyden (*Comm. ACM*, Jan. 1962, p. 50) was corrected, and the same example (Wilson's 4×4 matrix) was used as a test case. The resulting inverse was:

68.0000	-41.0000	-17.0000	10.0000
	25.0000	10.0000	-6.0000
		5.0000	-3.0000
			2.0000

It may also be useful to note that the determinant of the matrix may be obtained as the successive product of the pivots. That is, if $t_i (=T(1, 1))$ is the i th pivot of a matrix of order n ,

$$\text{determinant} = \prod_{i=1}^n t_i.$$

For the above input example,

$$\text{determinant} = 1.0$$

Randell and Broyden's observation concerning the apparent limitation of INVRS to positive definite cases is correct: That is, any nonsingular real symmetric matrix (positive, indefinite, or negative) may be inverted using this algorithm. The original INVRS should therefore be modified as follows:

if pivot = 0 then go to singular;

Randell and Broyden's second example (of order 5) was also used as a test case, with the resulting inverse:

-.0000	.9999	.0000	.0000	.9999
1.5333	-.7333	-.1333	.7999	
	-.8666	-1.0666	-.5999	
		-1.4666	-.1999	
			.2000	

$$\text{determinant} = -14.999999$$

An attempt to invert the inverse of the 4×4 segment of the Hilbert matrix, as presented by Randell (*Comm. ACM*, Jan. 1962, p. 50), yielded the following results:

.9999	.4999	.3333	.2499
	.3333	.2499	.1999
		.1999	.1666
			.1428

$$\text{determinant} = 6048020.6$$

ALGORITHM 67

CRAM

JOHN CAFFREY

Director of Research, Palo Alto Unified School District,
Palo Alto, California

procedure CRAM (n, r, a) Result: (f); **value** n, r; **integer** n, r; **real array** a, f;

comment CRAM stores, via an unspecified input procedure READ, the diagonal and superdiagonal elements of a square symmetric matrix e, of order n, as a pseudo-array of dimension $1:n(n+1)/2$. READ (u) puts one number into u. Elements $e[i, j]$ are addressable as $a[c + j]$, where $c = (2n - i)(i - 1)/2$ and $c[i + 1]$ may be found as $c[i] + n - i$. Since $c[1] = 0$, it is simpler to develop a table of the $c[i]$ by recursion, as shown in the sequence labelled "table". Further manipulation of the elements so stored is illustrated by premultiplying a rectangular matrix f, of order n, r, by the matrix e, replacing the elements of f with the new values, requiring a temporary storage array v of dimension $1:n$;

```
begin integer i, j, k, m; real array v[1:n]; real s;
integer array c[1:n];
table: j := -n; k := n + 1; for i := 1 step 1 until n do
begin
j := j + k - i; c[i] := j end;
load: for i := 1 step 1 until n do
begin for j := i step 1 until n do READ (v[j]); m :=
c[i];
for k := i step 1 until n do a[m + k] := v[k] end;
premult: for j := 1 step 1 until r do
begin for i := 1 step 1 until n do
begin s := 0.0;
for k := 1 step 1 until i do
begin m := c[k]; s := s + a[m + i]
× f[k, j] end;
for k := i + 1 step 1 until n do
s := s + a[m + k] × f[k, j]; v[i] = s
end;
for k := 1 step 1 until n do f[k, j] = v[k]
end
end
end CRAM
```

CERTIFICATION OF ALGORITHM 67

CRAM (J. Caffrey, *Comm. ACM* 4 (July 1961), 322)

A. P. RELPH

Atomic Power Div., The English Electric Co., Whetstone,
England

CRAM was translated using the DEUCE ALGOL compiler with the following corrections:

V[i] = S was changed to V[i] := S

f[k, j] = V[k] was changed to f[k, j] := V[k]

It is quicker not to use the table of the C[i] in the "load" sequence and instead use the following sequence:

load: m := n × (n+1)/2;

for i := 1 step 1 until m do READ (a[i]);

ALGORITHM 68

AUGMENTATION

H. G. RICE

Computer Sciences Corp., Palos Verdes, Calif.

real procedure Aug(x, y); **value** x, y; **integer** x, y;

comment This algorithm makes use of the implicitly defined recursive properties of ALGOL procedures to compute the augment of x by y, using the basic technique of incrementation by unit step size;

begin Aug := if x = 0 then (if y > x then (Aug(y - 1, x) + 1) else y)

else Aug(x - 1, y + 1) **end** Aug

CERTIFICATION OF ALGORITHM 68

AUGMENTATION (H. G. Rice, *Comm. ACM*, Aug. 1961)

L. M. BREED

Stanford University, Stanford, Calif.

AUGMENTATION was transliterated into BALGOL for the Burroughs 220, and proved successful in a number of test cases. However, the following algorithm has exactly the same effect and is considerably simpler:

real procedure Aug(x, y); **value** x, y; **integer** x, y;

begin if x < 0 then L : go to L **else** Aug := x + y **end** Aug

ALGORITHM 69 CHAIN TRACING

BRIAN H. MAYOH
Regnecentralen, Gl. Carlsbergvet. 2, Copenhagen.

```

procedure CHAIN tracing (iteration counter, number of
  identifiers, number of identifier links, final linkage
  matrix, couples);
  Boolean array final linkage matrix;
  integer array couples;
  integer iteration counter, number of identifiers, number of
  identifier links;
begin comment This procedure is given a list of pairs of inte-
  gers, the second being related to the first in some way. It finds
  those pairs of integers which are related to each other if the
  relation is transitive. It is supplied with,
  couples a matrix whose bound pairlist is [1:2, 1:number of
  identifier links] where couples [2, i] is related to couples
  [1, i] in some way.
  final linkage matrix a matrix whose bound pair list is
  [1:number of identifiers, 1:number of identifiers] and into
  which the procedure puts true if the second subscript
  expression is an integer which is related to the integer
  corresponding to the first subscript expression, if the
  relation is irreflexive then the diagonal entries of this
  matrix are false.
  iteration counter a place for the procedure to put the
  length of the longest chain it finds. CHAIN tracing can be
  applied to any system which can be represented by a Turing
  machine by letting the integers in couples correspond to
  the Turing machine states. Two integers j, k are related if
  there is an input symbol which causes state j to change to
  state k. If the Turing machine always stops whatever the
  sequence of input symbols, then its final linkage matrix
  will have false for all leading diagonal entries;
  integer i, j;
  Boolean array working linkage matrix [1:number of identi-
  fiers, 1:number of identifiers];
  Boolean procedure PROGRESS;
  begin PROGRESS := false;
    for i := 1 step 1 until number of identifiers
      do for j := 1 step 1 until number of identifiers
        do begin if Working linkage matrix [i, j] = ¬ Final
          linkage matrix [i, j] then PROGRESS := true;
          Final linkage matrix [i, j] := Working linkage
          matrix [i, j]
        end of comparison
      end of PROGRESS;
  BEGIN OF PROGRAM:
    for iteration counter := -1, 0, iteration counter + 1 while
    PROGRESS
      do for i := 1 step 1 until number of identifier links
        do for j := 1 step 1 until number of identifiers
          do begin if iteration number = -1
            then Final linkage Matrix [couples [1, i], j]
              := Working linkage Matrix [couples [1, i], j]
              := couples [2, i] = j
          else Working linkage Matrix [couples [1, i], j]
            := Working linkage Matrix [couples [1, i], j]
            ∨ Working linkage Matrix [couples [2, i], j];
          end of setting one linkage
        end of CHAIN tracing;

```

ALGORITHM 70 INTERPOLATION BY AITKEN

CHARLES J. MIFSUD
General Electric Co., Bethesda, Md.

```

procedure AITKEN (x, f, n, X, F); real array x, f;
  integer n; real X, F;

comment If given  $x_0, x_1, \dots, x_n$ ,  $n+1$  abscissas and also given
   $f(x_0), f(x_1), \dots, f(x_n)$ ,  $n+1$  functional values, this procedure
  generates a Lagrange polynomial,  $F(X)$  of the  $n$ th degree so that
   $F(x_i) = f(x_i)$ . Hence, for any given value  $X$ , a functional value
   $F(X)$  is generated. The procedure is good for either equal or
  unequal intervals of the  $x_i$ . Aitken's iterative scheme is used
  in the generation of  $F(X)$ . Since the  $f$  array is used for tem-
  porary storage, as the calculation proceeds its original values
  are destroyed;

  begin integer i, j, t;
    for j := 0 step 1 until n-1 do
      begin t := j+1
        for i := t step 1 until n do
           $f[i] := ((X - x[j]) \times f[i] - (X - x[i]) \times f[j]) /$ 
             $(x[i] - x[j])$  end
           $F := f[n]$ 

```

end

CERTIFICATION OF ALGORITHM 70 INTERPOLATION BY AITKEN [C. J. Mifsud, *Comm.* *ACM* 4 (Nov. 1961)]

A. P. RELPH

The English Electric Co., Whetstone, England

Algorithm 70 was translated using the DEUCE ALGOL compiler
and gave satisfactory results after semicolons had been added to

$t := j+1$ to make it $t := j+1$;

and $(x[i] - x[j])$ **end** to make it $(x[i] - x[j])$ **end**;

The identifier t can be eliminated and the algorithm shortened
by the following changes:

Replace **begin** **integer** i, j, t; **by** **begin** **integer** i, j;
Replace $t := j+1$; **by** **for** i := j+1 **step** 1 **until**
for i := t **step** 1 **until** n **do**
n do

ALGORITHM 71 PERMUTATION

R. R. COVEYOU AND J. G. SULLIVAN

Oak Ridge National Laboratory, Oak Ridge, Tenn.

```

procedure PERMUTATION (I, P, N);
  value I, N; integer N; integer array P; boolean I;
  comment This procedure produces all permutations of the
  integers from 0 thru N. Upon entry with I = false the pro-
  cedure initializes itself producing no permutation. Upon each
  successive entry into the procedure with I = true a new
  permutation is stored in P[0] thru P[N]. When the process has
  been exhausted a sentinel is set:

```

```

P[0] := -1,
N ≥ 0;
begin
  integer i; own integer array x[0:N];
  if ¬ 1 then
    begin for i := 0 step 1 until N-1 do x[i] := 0; x[N] := -1;
      go to E end;
    for i := N step -1 until 0 do begin if x[i] ≠ i then go to A;
      x[i] := 0 end;
    P[0] := -1; go to E;
  A: x[i] := x[i]+1; P[0] := 0;
    for i := 1 step 1 until N do
      begin P[i] := P[i-x[i]]; P[i-x[i]] := i end;
  E: end PERMUTATION

```

CERTIFICATION OF ALGORITHM 71

PERMUTATION (R. R. Coveyou and J. G. Sullivan,
Comm. ACM, Nov. 1961)

P. J. BROWN

University of North Carolina, Chapel Hill, N. C.

PERMUTATION was transliterated into GAT for the UNIVAC 1105 and successfully run for a number of cases.

CERTIFICATION OF ALGORITHM 71

PERMUTATION [R. R. Coveyou and J. G. Sullivan,
Comm. ACM, Nov. 1961]

J. S. HILLMORE

Elliott Bros. (London) Ltd., Borehamwood, Herts.,
England

The algorithm was successfully run using the Elliott ALGOL translator on the National-Elliott 803. The integer array x was made a parameter of the procedure in order to avoid having an own array with variable bounds.

CERTIFICATION OF ALGORITHM 71

PERMUTATION (R. R. Coveyou and J. G. Sullivan,
Comm. ACM, Nov. 1961)

J. E. L. PECK AND G. F. SCHRACK

University of Alberta, Calgary, Alberta, Canada

PERMUTATION was translated into FORTRAN for the IBM 1620 and it performed satisfactorily. The own integer array $x[0:n]$ may be shortened to $x[1:n]$, provided corresponding corrections are made in the first two for statements.

However, PERMUTE (Algorithm 86) is superior to PERMUTATION in two respects.

(1) PERMUTATION, using storage of order $2n$, is designed to permute the specific vector $0, 1, 2, \dots, n-1$ rather than an arbitrary vector. Thus storage of order $3n$ is required to permute an arbitrary vector. PERMUTE, in contrast, only needs storage of order $2n$ to permute an arbitrary vector.

(2) PERMUTE is built up from cyclic permutations. The number of permutations actually executed internally (the redundant ones are suppressed) by PERMUTE is asymptotic to $(e-1)n!$ rather than $n!$. In spite of this, PERMUTE is distinctly faster (1316 against 2823 seconds for $n=8$) than PERMUTATION. If t_n is the time taken for all permutations of a vector with n components, and if $r_n = t_n/nt_{n-1}$, then one would expect r_n to be close to 1. Experiment with small values of n gave the following results for r_n .

	n	6	7	8
PERMUTE		0.96	0.99	1.00
PERMUTATION		1.10	1.13	1.12

Is there yet a faster way to do it?

See also: C. Tompkins, "Machine Attacks on Problems whose Variables are Permutations", *Proceedings of Symposia in Applied Mathematics*, Vol. VI: *Numerical Analysis* (N. Y., McGraw-Hill, 1956).

ALGORITHM 72

COMPOSITION GENERATOR

L. HELLERMAN AND S. OGDEN

IBM-Product Development Laboratory, Poughkeepsie,
N. Y.

```

procedure comp (c, k); value k; integer array c;
integer k;
comment Given a k-part composition c of the positive integer n,
comp generates a consequent composition if there is one. If
comp operates on each consequent composition after it is found,
all compositions will be generated, provided that 1, 1, ..., 1,
n-k+1 is the initial c. If c is of the form n-k+1, 1, ..., 1,
there is no consequent, and c will be replaced by a k vector of
0's. Reference: John Riordan, An Introduction to Combinatorial Analysis, John Wiley and Sons, Inc., New York, 1958,
Chapter 6;
begin integer j; integer array d [1:k];
  if k = 1 then go to last;
  for j := 1 step 1 until k do d[j] := c[j] - 1;
test: if d[j] > 0 then go to set;
  j := j-1;
  go to if j = 1 then last else test;
set: d[j] := 0;
  d[j-1] := d[j-1] + 1;
  d[k] := c[j] - 2;
  for j := 1 step 1 until k do c[j] := d[j] + 1;
  go to exit;
last: for j := 1 step 1 until k do c[j] := 0;
exit: end comp

```

CERTIFICATION OF ALGORITHM 72

COMPOSITION GENERATOR [L. Hellerman and S.
Ogden, *Comm. ACM*, Nov. 1961]

D. M. COLLISON

Elliott Bros. (London) Ltd., Borehamwood, Herts.,
England

After

for j := 1 step 1 until k do d[j] := c[j]-1;

the statement

j := k;

should be inserted (see ALGOL 60 report, para 4.6.5). With this alteration, the algorithm was successfully run using the Elliott ALGOL translator on the National-Elliott 803.

ALGORITHM 73

INCOMPLETE ELLIPTIC INTEGRALS

DAVID K. JEFFERSON

U. S. Naval Weapons Laboratory, Dahlgren, Virginia

```

procedure ellint (k, phi, E, F);
value k, phi;
real phi, F, k, E;
comment ellint computes the value of the incomplete elliptic
integrals of the first and second kinds, F(phi, k) and E(phi, k),
where phi is in radians. If |k| > 1 or |phi| > pi/2, E and F
will be set equal to 100,000,000, otherwise they will contain the
computed integrals. For the formulation of this procedure, see
DiDonato, A. R., and Hershey, A. V., "New Formulae for
Computing Incomplete Elliptic Integrals of the First and
Second Kind", J. ACM 6, 4 (Oct. 1959);

```

```

begin real kp, sinphi, n, cosphi;
  real array H [1:2], A [1:2], sigma [1:4], L [1:2], M [1:2],
    N [1:2], T [1:2], del [1:4];
  sigma [1] := sigma [2] := sigma [3] := sigma [4] := 0;
  H [1] := 1;
  n := 0;
  sinphi := sin(phi);
if abs (k × sinphi) ≤ tanh (1) then go to small else if abs (k) ≤
  1 ∧ abs(phi) ≤ π/2 then go to large;
  E := F := 100000000;
  go to stop;
small: A [1] := phi;
step 1: n := n + 1;
  cosphi := cos (phi);
  E := (2 × n - 1) / (2 × N);
  H [2] := E × k ↑ 2 × H [1];
  A [2] := E × A [1] - sinphi ↑ (2 × n - 1) × cosphi / (2 × n);
  del [1] := H [2] × A [2];
  del [2] := -k ↑ 2 × H [1] × A [2] / (2 × n);
  sigma [1] := sigma [1] + del [1];
  sigma [2] := sigma [2] + del [2];
  H [1] := H [2];
  A [1] := A [2];
if abs ((sigma [1] + del [1]) - sigma [1]) > 0 ∧ phi × sinphi
  ↑ (2 × n) ≥ A [2] then go to step 1;
  F := phi + sigma [1];
  E := phi + sigma [2];
  go to stop;
large: kp := sqrt (1 - k ↑ 2);
  A [1] := 1;
  L [1] := M [1] := N [1] := 0;
step 2: n := n + 1;
  E := (2 × n - 1) / (2 × n);
  F := abs (k) × sqrt (1 - sinphi ↑ 2) × (1 - k ↑ 2 × sinphi
    ↑ 2) ↑ ((2 × n - 1) / (2 × n));
  H [2] := E × H [1];
  A [2] := E ↑ 2 × kp ↑ 2 × A [1];
  L [2] := L [1] + 1 / (n × 2 × n - 1);
  M [2] := (M [1] - F × H [2]) × ((2 × n + 1) / (2 × n + 2)) ↑ 2 ×
    kp ↑ 2;
  N [2] := (N [1] - F × H [1]) × E × (2 × n + 1) × kp ↑ 2 / (2 ×
    n + 2);
  del [1] := M [2] - A [2] × L [2];
  del [2] := N [2] - E × kp ↑ 2 × A [1] × L [2] + kp ↑ 2 × A [1]
    / ((2 × n) ↑ 2);
  del [3] := A [2];
  del [4] := (2 × n + 1) × A [2] / (2 × n + 2);
  sigma [1] := sigma [1] + del [1];
  sigma [2] := sigma [2] + del [2];
  sigma [3] := sigma [3] + del [3];
  sigma [4] := sigma [4] + del [4];
  H [1] := H [2];
  A [1] := A [2];
  L [1] := L [2];
  M [1] := M [2];
  N [1] := N [2];
if abs ((sigma [1] + del [1]) - sigma [1]) > 0 then go to step 2;
  T [1] := ln (4 / (sqrt (1 - k ↑ 2 × sinphi ↑ 2) + abs (k) × sqrt (1 -
    sinphi ↑ 2)));
  T [2] := abs (k) × sqrt ((1 - sinphi ↑ 2) / (1 - k ↑ 2 × sinphi ↑ 2));
  F := T [1] × (1 + sigma [3]) + T [2] × ln (.5 + .5 × abs (k ×
    sinphi)) + sigma [1];
  E := (.5 + sigma [4]) × kp ↑ 2 × T [1] + 1 - T [2] × (1 - abs
    (k × sinphi)) + sigma [2];
stop: end

```

CERTIFICATION OF ALGORITHM 73
INCOMPLETE ELLIPTIC INTEGRALS (David K.
 Jefferson, *Comm. ACM*, Dec. 1961)
 DEAN C. KRIEBEL
 U. S. Naval Weapons Laboratory, Dahlgren, Virginia

This algorithm was originally coded in Norac machine language and K. Pearson's incomplete elliptic integral tables of the first and second kind generated. (See DiDonato, A. R., and Hershey, A. V., "New Formulae for Computing Incomplete Elliptic Integrals of the First and Second Kind", *J. ACM* 6, 4 (Oct. 1959)).

The algorithm was coded for the MAD Compiler exactly as written in ALGOL and run on an IBM 7090. Forty cases were computed with K ranging from 0° to 90° and PHI ranging from 0° to 90°. The results contained eight significant digits which agreed with the DiDonato and Hershey tables to within 0 to 2 units in the 8th digit. (This may be attributed to the decimal to binary, binary to decimal input-output conversion used with a binary computer as compared to straight decimal computation on the Norac.)

CERTIFICATION OF ALGORITHM 73
INCOMPLETE ELLIPTIC INTEGRALS [David K.
 Jefferson, *Comm. ACM* Dec. 1961]
 R. P. VAN DE RIET
 Mathematical Centre, Amsterdam

The algorithm contained three misprints:

The 26th line of the procedure

$$E := (2 \times n - 1) / (2 \times N);$$

should read

$$E := (2 \times n - 1) / (2 \times n);$$

The 46th line of the procedure

$$\uparrow 2) \uparrow ((2 \times n - 1) / (2 \times n));$$

should read

$$\uparrow 2) \uparrow ((2 \times n - 1) / 2) / (2 \times n);$$

The 49th line of the procedure

$$L [2] := L [4] + 1 / (n \times 2 \times n - 1);$$

should read

$$L [2] := L [1] + 1 / (n \times (2 \times n - 1));$$

The program was run on the X1 computer of the Mathematical Centre. For $\phi = 45^\circ$, $k = \sin(10^\circ(10^\circ)180^\circ)$, E and F were calculated. The result contained 12 significant digits.

Comparison with a 12-decimal table of Legendre-Emde (1931) showed that the 12th digit was affected with an error, at most 4 units large. After about 10 minutes of calculation (i.e. more than 100 cycles) no results were obtained for $k = \sin 89^\circ$, $\phi = 1^\circ$ and the calculation was discontinued.

REMARKS. As ϕ is unchanged during the calculation, we placed the statement $\cos \phi := \cos (\phi)$ in the beginning of the program, to be certain that the cosine was not calculated 30 or more times. Moreover, in the expression for $T[1]$ and $T[2]$, $\sqrt{1 - \sin \phi \uparrow 2}$ was replaced by $\cos \phi$, so that loss of significant figures does not occur.

The expression $2 \times n$ was changed in a new variable, to obtain a more rapid program.

CERTIFICATION OF ALGORITHM 73
INCOMPLETE ELLIPTIC INTEGRALS [David K.
 Jefferson, *Comm. ACM* 4, Dec. 1961]
 NOELLE A. MEYER
 E. I. du Pont de Nemours & Co., Wilmington, Del.

Ellint was hand-coded in FORTRAN for the IBM 7070. The following corrections were made:

The statement

$$E := (2 \times n - 1) / (2 \times N);$$

should be

$$E := (2 \times n - 1) / (2 \times n);$$

The statement

$$F := \text{abs}(k) \times \text{sqrt}(1 - \sin^2 \phi) \times (1 - k \uparrow 2 \times \sin^2 \phi \uparrow 2) \uparrow ((2 \times n - 1)/(2 \times n));$$

should be

$$F := (\text{abs}(k) \times \text{sqrt}(1 - \sin^2 \phi) \times (1 - k \uparrow 2 \times \sin^2 \phi \uparrow 2) \uparrow (n - .5))/(2 \times n)$$

The statement

$$L[2] := L[1] + 1/(n \times 2 \times n - 1);$$

should be

$$L[2] := L[1] + (1/(n \times (2 \times n - 1)));$$

In order to accommodate negative ϕ the following changes were made:

The statement
if $\text{abs}((\text{sigma}[1] + \text{del}[1]) - \text{sigma}[1]) > 0 \wedge \phi \times \sin^2 \phi \uparrow (2 \times n) \geq A[2]$ **then go to step 1;**

was changed to
if $\text{abs}((\text{sigma}[1] + \text{del}[1]) - \text{sigma}[1]) > 0 \wedge \text{abs}(\phi \times \sin^2 \phi \uparrow (2 \times n)) \geq \text{abs}(A[2])$ **then go to step 1;**

Also the following was inserted before the last statement (stop: end)

if $\phi < 0$ **then go to wait else go to stop;**
wait: $F := -F;$
 $E := -E;$

The revised algorithm yielded satisfactory answers when compared with the DiDonato and Hershey tables. Differences occurred in the eighth significant digit as shown in the following difference tables.

DIFFERENCE TABLES

F-TABLE

θ (in degrees)

(in degrees)	0	30	60	90
0	0.	0.	0.	0.
30	-1×10^{-8}	-1×10^{-8}	-1×10^{-8}	-3×10^{-8}
60	1×10^{-8}	1×10^{-8}	2×10^{-8}	-3×10^{-8}
90	0.	2×10^{-8}	6×10^{-8}	0.

E-TABLE

	0	30	60	90
0	0.	0.	0.	0.
30	-1×10^{-8}	-1×10^{-8}	-1×10^{-8}	-1×10^{-8}
60	1×10^{-8}	1×10^{-8}	-7×10^{-8}	3×10^{-8}
90	0.	0.	1×10^{-8}	0.

REMARK ON ALGORITHM 73
 INCOMPLETE ELLIPTIC INTEGRALS [David K. Jefferson, *Comm. ACM* (Dec. 1961)]

DAVID K. JEFFERSON
 U. S. Naval Weapons Laboratory, Dahlgren, Virginia

In regard to Algorithm 73, two errors were found:
 The 34th line of the procedure

$$F := \text{abs}(k) \times \text{sqrt}(1 - \sin^2 \phi) \times (1 - k \uparrow 2 \times \sin^2 \phi \uparrow 2) \uparrow ((2 \times n - 1)/(2 \times n));$$

should read

$$F := \text{abs}(k) \times \text{sqrt}(1 - \sin^2 \phi) \times (1 - k \uparrow 2 \times \sin^2 \phi \uparrow 2) \uparrow ((2 \times n - 1)/2)/(2 \times n);$$

The 37th line

$$L[2] := L[1] + 1/(n \times 2 \times n - 1);$$

should read

$$L[2] := L[1] + 1/(n \times (2 \times n - 1));$$

In addition, efficiency is improved by interchanging lines 13 and 14:

Step 1: $n := n + 1;$
 $\cos \phi := \cos(\phi);$

can be replaced by

$\cos \phi := \cos(\phi);$
 Step 1: $n := n + 1;$

ALGORITHM 74 CURVE FITTING WITH CONSTRAINTS

J. E. L. PECK,
 University of Alberta, Calgary, Alberta, Canada

procedure Curve fitting ($k, a, b, m, x, y, w, n, \alpha, \beta, s, \text{sgmsq}, x_0, \gamma, c, z, r$);

comment This procedure finds, by the method of least squares, the polynomial of degree n , $k \leq n < k + m$, whose graph contains $(a_1, b_1), \dots, (a_k, b_k)$ and approximates $(x_1, y_1), \dots, (x_m, y_m)$, where w_i is the weight attached to the point (x_i, y_i) . The details will be found in the reference cited below, where a similar notation is used. A nonlocal label "error" is assumed;

value a, x, y, w ; **integer** k, m, n, r ; **real** x_0, γ ; **array** $a, b, x, y, w, \alpha, \beta, s, \text{sgmsq}; c, z$;

begin integer i, j ; **array** $w[1:k]$; **real** p, f, lambda ;

comment We shall first define several procedures to be used in the main program, which begins at the label START;

procedure Eval (x, nu);

comment This procedure evaluates $f = s_0 p_0 + s_1 p_1 + \dots + s_\nu p_\nu$, where $p_{-1}(x) = 0$, $p_0(x) = 1$, $\beta_0 = 0$ and $p_{i+1}(x) = (x - \alpha_i)p_i(x) - \beta_i p_{i-1}(x)$, $i = 0, 1, \dots, \nu - 1$. The value of $p_\nu(x)$ remains in p ;

real x ; **integer** nu ;

begin real p_0, temp ; **integer** i ; $p_0 := 0$; $p := 1$; $f := s[0]$;

for $i := 0$ **step 1 until** $nu - 1$ **do**

begin $\text{temp} := p$;

$p := (x - \alpha[i]) \times p - \beta[i] \times p_0$;

$p_0 := \text{temp}$; $f := f + p \times s[i + 1]$ **end i**

end Eval;

procedure Coda (n, c);

comment This procedure finds the c 's when $c_0 + c_1 x + \dots + c_n x^n = s_0 p_0(x) + \dots + s_n p_n(x)$;

integer n ; **array** c ;

begin integer i, r ; **real** t_1, t_2 ; **array** $\text{pm}, p[0:n]$;

for $r := 1$ **step 1 until** n **do**

$c[r] := \text{pm}[r] := p[r] := 0$;

$\text{pm}[0] := 0$; $p[0] := 1$; $c[0] := s[0]$;

for $i := 0$ **step 1 until** $n - 1$ **do**

begin $t_2 := 0$;

for $r := 0$ **step 1 until** $i + 1$ **do**

begin $t_1 := (t_2 - \alpha[i] \times p[r] - \beta[i] \times \text{pm}[r]) / \text{lambda}$;

$t_2 := \text{pm}[r] := p[r]$; $p[r] := t_1$;

$c[r] := c[r] + t_1 \times s[i + 1]$ **end r**

end i

end Coda;

procedure GEFYT (n, n_0, x, y, w, m);

comment This is the heart of the main program. It computes the $\alpha_i, \beta_i, s_i, \sigma_i^2$, using the method of orthogonal polynomials, as described in the reference;

integer n, n_0, m ; **array** x, y, w ;

begin real $\text{dsq}, \text{wpp}, \text{wpp0}, \text{wxpp}, \text{wyp}, \text{temp}$;

integer $i, j, \text{freedom}$; **array** $p, p_0[1:m]$; **boolean** exact ;

if $n - n_0 > m \vee n < n_0$ **then go to error**;

$\text{beta}[n_0] := \text{dsq} := \text{wpp} := 0$; $\text{exact} := n - n_0 \geq m - 1$;

for $j := 1$ **step 1 until** m **do**

begin $p[j] := 1$; $p_0[j] := 0$; $\text{wpp} := \text{wpp} + w[j]$;

if $\neg \text{exact}$ **then** $\text{dsq} := \text{dsq} + w[j] \times y[j] \times y[j]$ **end initialise**;

for $i := n_0$ **step 1 until** n **do**

begin $\text{freedom} := m - 1 - (i - n_0)$; $\text{wyp} := \text{wxpp} := 0$;

for $j := 1$ **step 1 until** m **do**

begin $\text{temp} := w[j] \times p[j]$;

if $i < n$ **then** $\text{wxpp} := \text{wxpp} + \text{temp} \times x[j] \times p[j]$;

if $\text{freedom} \geq 0$ **then** $\text{wyp} := \text{wyp} + \text{temp} \times y[j]$ **end j**;

if $\text{freedom} \geq 0$ **then** $s[i] := \text{wyp} / \text{wpp}$;

if $\neg \text{exact}$ **then** **begin** $\text{dsq} := \text{dsq} - s[i] \times s[i] \times \text{wpp}$;

$\text{sgmsq}[i] := \text{dsq} / \text{freedom}$ **end if**;

```

if i < n then begin alpha[i] := wxpp/wpp; wpp0 := wpp;
wpp := 0;
for j := 1 step 1 until m do
  begin temp := (x[j]-alpha[i]) × p[j] - beta[i] × p0[j];
  wpp := wpp + w[j] × temp × temp;
  p0[j] := p[j]; p[j] := temp end j;
beta[i+1] := wpp/wpp0 end if
end i
end GEFYT;

START: for j := 1 step 1 until k do
begin w1[j] := 1; a[j] := (a[j]-x0)/gamma end j;
GEFYT (k,0,a,b,w1,k);
comment This finds the polynomial of degree k-1 whose graph
contains (a1,b1), ..., (ak,bk) supplying the  $\alpha_i, \beta_i, s_i, 0 \leq i \leq k$ ;
begin real rho; rho := 0;
for j := 1 step 1 until m do
begin rho := rho + w[j];
x[j] := (x[j] - x0)/gamma end j; rho := m/rho;
comment The factor  $\rho$  is used to normalize the weights. We shall
now put  $s_k = 0$  in order to evaluate  $p_k(x)$  and the polynomial of
degree  $k-1$  simultaneously;
s[k] := 0;
for j := 1 step 1 until m do
begin Evalue (x[j],k);
if p = 0 then go to error;
y[j] := (y[j] - f)/p;
w[j] := w[j] × p × p × rho end j
end rho;
comment We have now normalized the weights and adjusted
the weights and ordinates ready for the least squares approxi-
mation;
GEFYT (n,k,x,y,w,m);
comment The coefficients  $\alpha_i, \beta_i, 0 \leq i < n$ , and  $s_i, 0 \leq i \leq n$ 
are now ready. The polynomial may be evaluated for  $x = z_1, z_2, \dots, z_r$ ,
but the variable must be adjusted first. Note that we
may evaluate the best polynomial of lower degree by decreas-
ing n;
begin real x;
for j := 1 step 1 until r do
begin x := (z[j]-x0)/gamma;
Evalue (x,n); comment the values of  $z_i$  and  $f$  should now be
printed; end j;
comment We may now adjust the coefficients for scale and then
find the coefficients of the power series  $c_0 + c_1x + \dots + c_nx^n = s_0p_0(x) + \dots + s_np_n(x)$ ;
for i := 0 step 1 until n-1 do
begin alpha[i] := alpha[i] × gamma + x0;
beta[i] := beta[i] × gamma end i; lambda := gamma;
Coda (n,c);
comment We may now re-evaluate the polynomial from the
power series;
for j := 1 step 1 until r do
begin x := z[j]; f := c[n];
for i := n-1 step -1 until 0 do
f := f × x + c[i];
comment the values of  $x$  and  $f$  should now be printed; end j
end x
end Curve fitting

```

REFERENCE: PECK, J. E. L. Polynomial curve fitting with constraint, *Soc. Indust. Appl. Math. Rev.* (1961).

CERTIFICATION OF ALGORITHM 74 CURVE FITTING WITH CONSTRAINTS [J. E.

Peck, *Comm. ACM*, Jan. 62]

KAZUO ISODA

Japan Atomic Energy Research Institute, Tokai, Ibaraki,
Japan

Algorithm 74 was hand-compiled into SOAP IIa for the IBM 650 and run successfully with no corrections except the case in which the origin (0, 0) are given as both a constraint and a sample.

ALGORITHM 75

FACTORS

J. E. L. PECK,

University of Alberta, Calgary, Alberta, Canada

```

procedure factors (n,a,u,v,r,c);
comment This procedure finds all the rational linear factors of
the polynomial  $a_0x^n + a_1x^{n-1} + \dots + a_{n-1}x + a_n$ , with integral
coefficients. An absolute value procedure abs is assumed;
value n,a; integer r,n,c; integer array a,u,v;
begin comment We find whether p divides  $a_0, 1 \leq p \leq |a_0|$  and
q divides  $a_n, 0 \leq q \leq |a_n|$ . If this is the case we try  $(px \pm q)$ ;
integer p,q,a0,a;
r := 0; c := 1; comment r will be the number of linear factors
and c the common constant factor;
TRY AGAIN: a0 := a[0]; an := a[n];
for p := 1 step 1 until abs(a0) do
begin if (a0 ÷ p) × p = a0 then
begin comment p divides  $a_0$ ;
for q := 0 step 1 until abs(an) do
begin if q = 0 ∨ (an ÷ q) × q = an then
begin comment q divides  $a_n$  (or q = 0). If p = q we
may have a common constant factor, therefore; if q
> 1 ∧ p = 1 then
begin integer j;
for j := 1 step 1 until n-1 do
if (a[j] ÷ q) × q ≠ a[j] then go to NO CONSTANT;
for j := 0 step 1 until n do
a[j] := a[j]/q;
c := c × q; go to TRY AGAIN
end the search for a common constant factor;
NO CONSTANT:
begin comment try  $(px - q)$  as a factor;
integer f,g,i; f := a0; g := 1;
comment we try  $x = q/p$ ;
for i := 1 step 1 until n do
begin g := g × p; f := f × q + a[i] × g
end evaluation;
if f = 0 then
begin comment we have found the factor  $(px - q)$ ;
r := r + 1; u[r] := p; v[r] := q;
comment there are now r linear factors;
begin comment we divide by  $(px - q)$ ;
integer i,t; t := 0;
for i := 0 step 1 until n do
begin a[i] := t := (a[i] + t)/p; t := t × q
end i;
n := n - 1
end reduction of polynomial. Therefore;
go to if n = 0 then REDUCED else TRY AGAIN
end discovery of  $px - q$  as a factor. But
if we got this far it was not a factor so try  $px + q$ ;
q := -q; if q < 0 then go to NO CONSTANT
end trial of  $px \pm q$ ,
end q divides  $a_n$  and
end of q loop.
end p divides  $a_0$ , also
end p loop, which means;
REDUCED: if n = 0 then
be_ < a0; a0 := 1
end it ..
end factors procedure. There are now r ( $r > 0$ ) rational linear
factors  $(u_i x - v_i), 1 \leq i \leq r$ , and the reduced polynomial of
reduced degree n replaces the original. The common constant
factor is c. Acknowledgments to Clay Perry.

```


CERTIFICATION OF ALGORITHM 75 FACTORS [J. E. L. Peck, *Comm. ACM*, Jan. 1962]

J. S. HILLMORE

Elliott Bros. (London) Ltd., Borehamwood, Herts.,
England

The following changes had to be made to the algorithm:

- (1) For if $q > 1 \wedge p = 1$ then
put if $q > 1 \wedge p = q$ then
- (2) For begin $c := c \times a_0$; $a_0 := 1$ end
put begin $c := c \times a[0]$; $a[0] := 1$ end
- (3) For if $q = 0 \vee (an \div q) \times q = an$ then
put if (if $q = 0$ then true else $(an \div q) \times q = an$) then

This change is necessary to ensure that the term $(an \div q)$ is not evaluated when $q = 0$.

The algorithm, thus modified, was successfully run using the Elliott ALGOL translator on the National-Elliott 803.

CERTIFICATION OF ALGORITHM 75 FACTORS [J. E. L. Peck, *Comm. ACM* 5 (Jan. 1962)]

A. P. RELPH

The English Electric Co., Whetstone, England

Algorithm 75 was translated using the DEUCE ALGOL compiler and gave satisfactory results after the following corrections had been made:

```
begin if  $q = 0 \vee (an \div q) \times q = an$  then
  begin if  $q > 1 \wedge p = 1$  then
```

was changed to

```
begin if  $q \leq 1$  then go to NO CONSTANT;
  if  $(an \div q) \times q = an$  then
    begin if  $p = q$  then
```

```
begin  $c := c \times a_0$ ;  $a_0 := 1$ 
end
```

was changed to

```
begin  $c := c \times a[0]$ ;  $a[0] := 1$ ;
end
```

There are now r ($r > 0$) rational linear factors $(u_i x - v_i)$,
 $1 \leq i \leq r$,

was changed to

If $r > 0$ there are now r rational linear factors $(u_i x - v_i)$, $1 \leq i \leq r$,

To return to the state ($p=1, q=0$) after every factor or constant is found is inefficient. This can be avoided by substituting $a[0]$ and $a[n]$ for the identifiers a_0 and an respectively. The procedure then becomes:

procedure factors (n, a, u, v, r, c); value n, a ;

integer array a, u, v ;

integer r, n, c ;

begin integer p, q ;

$r := 0$; $c := 1$;

ZERO: if $a[n] = 0$ then

```
begin  $r := r + 1$ ;  $u[r] := 1$ ;  $v[r] := 0$ ;  $n := n - 1$ ;
  go to ZERO
```

end;

```
for  $p := 1$  step 1 until abs ( $a[0]$ ) do
```

```
begin if ( $a[0] \div p$ )  $\times p = a[0]$  then
```

```
begin for  $q := 1$  step 1 until abs ( $a[n]$ ) do
```

```
begin if  $q = 1$  then go to NO CONSTANT;
```

```
TRY AGAIN: if ( $a[n] \div q$ )  $\times q = a[n]$  then
```

```
begin integer  $j$ ;
```

```
for  $j := 0$  step 1 until  $n - 1$  do
```

```
if ( $a[j] \div q$ )  $\times q \neq a[j]$  then go to
  NO CONSTANT;
```

```
for  $j := 0$  step 1 until  $n$  do
   $a[j] := a[j] / q$ ;
   $c := c \times q$ ; go to TRY AGAIN
end;
```

NO CONSTANT: begin integer f, g, i ; $f := a[0]$;

$g := 1$;

```
for  $i := 1$  step 1 until  $n$  do
```

```
begin  $g := g \times p$ ;
```

```
 $f := f \times q + a[i] \times g$ 
```

end;

if $f = 0$ then

```
begin  $r := r + 1$ ;  $u[r] := p$ ;
```

```
 $v[r] := q$ ;
```

```
begin integer  $i, t$ ;  $t := 0$ ;
```

```
for  $i := 0$  step 1 until  $n$  do
```

```
begin  $a[i] := t := (a[i] + t) / p$ ;
```

```
 $t := t \times q$ 
```

end;

$n := n - 1$

end

```
go to if  $n = 0$  then REDUCED
  else NO CONSTANT
```

end;

```
 $q := -q$ ; if  $q < 0$  then go to NO
  CONSTANT
```

end

end

end

end;

REDUCED: if $n = 0$ then

```
begin  $c := c \times a[0]$ ;  $a[0] := 1$ 
```

end

end

ALGORITHM 76 SORTING PROCEDURES

IVAN FLORES

Private Consultant, Norwalk, Connecticut

comment The following ALGOL 60 algorithms are procedures for the sorting of records stored within the memory of the computer. These procedures are described in detail, flow-charted, compared, and contrasted in "Analysis of Internal Computer Sorting" by Ivan Flores [*J. ACM* 8 (Jan. 1961)]. Although sorting is usually a business computer application, it can be described completely in ALGOL if we stretch our imagination a little. Sorting is ordering with respect to a key contained within the record. If the key is the active record, the sorting is trivial. A means is required to extract the key from the record. This is essentially string manipulation, for which no provision, as yet, has been made in ALGOL. We circumambulate this difficulty by defining an integer procedure $K(I)$ which "creates" a key from the record, I . ALGOL does provide for machine language code substitutions, which is one way to think of $K(I)$. This could be more accurately represented by using the string notation proposed by Julien Green ["Remarks on ALGOL and Symbol Manipulation," *Comm. ACM* 2 (Sept. 1959), 25-27]. The function $\text{sub} (\$, i, g)$ represents the procedure, $K(I)$. $\$$ corresponds to the record I , i corresponds to the starting position of the key and g corresponds to the length of the key. Both i and g are values which must be specified when the sort procedure is called for as a statement instead of a declaration.

Another factor, which might vex some, is that the key might be alphabetic instead of numeric. Then, of course, $K(I)$ would not be integer. It would, however, be string when such is defined eventually. Note, also, that keys are frequently compared. This is done using the ordering relations ">" for "greater than," etc. These are not really defined in the ALGOL statement [NAUR, PETER, ET AL. "Report on the Algorithmic Language ALGOL 60". *Comm. ACM* 3 (May 1960), 294-314]. They can simply be defined so that $Z > Y > \dots > A > 9 > \dots > 1 > 0$. Also the assignment $X[i] := z$ should be interpreted as "Assign the key 'z' which is larger than any other key." For any sort procedure (I, N, S) , "I" is the set of unsorted records, "N" is their number, and "S" the sorted set of records.

Caution, these algorithms were developed purely for the love of it: No one was available with the combined knowledge of sorting and ALGOL to check this work. Hence each algorithm should be carefully checked before use. I will be glad to answer any questions which may arise;

```
Sort insert (I,N,S); value N; array I[1:N], S[1:N];
integer procedure K(I); integer N;
begin integer i, j, k;
  S[1] := I[1];
  for i := 2 step 1 until N do begin
    for j := i - 1, j - 1 while K(I[i]) > K(S[j]) do
      for k := i step - 1 until j + 1 do
        S[k] := S[k - 1];
      S[j + 1] := I[i] end end
```

```
Sort count (I,N,S); value N; array I[1:N], S[1:N];
integer procedure K(I); integer N;
begin integer array C[1:N]; integer i, j;
  for i := 1 step 1 until N do C[i] := 0;
  for i := 2 step 1 until N do
    for j := 1 step 1 until i - 1 do
      if K(I[i]) > K(I[j]) then C[i] := C[i] + 1
      else C[j] := C[j] + 1;
    for i := 1 step 1 until N do
      S[C[i]] := I[i] end
```

```
Sort select (I,N,S); value N; array I[1:N], S[1:N];
integer procedure K(I); integer N;
begin integer i, j, A, h;
  for i := 1 step 1 until N do begin
    h := K(I[1]);
    for j := 2 step 1 until N do
      if h > K(I[j]) then begin h := K(I[j]); A := j end;
    S[i] := I[A];
    I[A] := z end end
```

```
Sort select exchange (I,N); value N; array I[1:N];
integer procedure K(I); integer N;
begin integer h, i, j, H; real T;
  for i := 1 step 1 until N do begin
    H := K(I[i]); h := i;
    for j := i + 1 step 1 until N do
      if K(I[j]) < H then begin
        H := K(I[j]); h := j end
    T := I[i]; I[i] := I[h]; I[h] := T end
  end
```

```
Sort binary insert (I,N,S); value N; array I[1:N], S[1:N];
integer procedure K(I); integer N;
begin integer i, k, j, l;
  if K(I[1]) < K(I[2]) then begin
    S[1] := I[1]; S[2] := I[2] end
  else begin S[1] := I[2]; S[2] := I[1] end;
  start: for i := 3 step 1 until N do begin
    j := (i + 1) ÷ 2;
    find spot: for k := (i + 1) ÷ 2, (k + 1) ÷ 2 while k > 1 do
```

```
    if K(I[i]) < K(S[j]) then j := j - k
    else j := j + k;
    if K(I[i]) ≥ K(S[j]) then j := j - 1;
  move items: for l := i step - 1 until j do
    S[l + 1] := S[l];
```

```
  enter this
  one: S[j] := I[i] end end
```

```
Sort address calculation (I,N,S,F); value N;
array S[1:M], I[1:N]; integer procedure F(K), K(I);
integer N, M;
```

```
begin integer i, j, G, H, F, M;
  M := entier(2.5 × N)
  for i := 1 step 1 until M do S[i] := 0;
  Address: for i := 1 step 1 until N do begin
    F := F(K(I[i]));
    if S[F] = 0 then begin S[F] := I[i];
      go to NEXT end
    else if K(S[F]) > K(I[i]) then go to SMALLER;
  LARGER: for H := F, H + 1 while K(S[H]) < K(I[i]) do
    for G := H, G + 1 while K(S[G]) ≠ 0 do
      for j := G step - 1 until H + 1 do
        S[j] := S[j - 1];
      S[H] := I[i]; go to NEXT;
  SMALLER: for H := F, H - 1 while K(S[H]) > K(I[i]) do
    for G := H, G - 1 while K(S[G]) ≠ 0 do
      for j := G step 1 until H - 1 do
        S[j] := S[j + 1];
      S[H] := I[i];
  NEXT: end end
```

```
Sort quadratic select (I,N,S); value N; array I[1:N], S[1:N];
integer procedure K(I); integer N;
```

```
begin integer i, j, k, C, D, J, M;
  integer array C[1:M], D[1:M];
  array I[1:M, 1:M];
  Divide inputs: M := entier(sqrt(N)) + 1; j := k := 1;
  for i := 1 step 1 until N do begin
    I[j, k] := I[i]; k := k + 1;
    if k > M then begin k := 1;
      j := j + 1 end end
```

```
  Fill up inputs: I[j, k] := z; k := k + 1;
  if k > M then begin k := 1; j := j + 1 end
  if j ≤ M then go to Fill up inputs;
```

```
  Set controls: for j := 1 step 1 until M do begin
    C[j] := K(I[j, 1]); D[j] := 1;
    for k = 2 step 1 until M do
      if C[j] > K(I[j, k]) then begin
        C[j] := K(I[j, k]); D[j] := k end end;
    i := 1;
```

```
  Find least: C := C[1]; D := D[1]; J := 1;
  for j := 2 step 1 until M do
    if C > C[j] then begin C := C[j];
      D := D[j]; J := j end;
```

```
  Fill file: S[i] := I[J, D]; i := i + 1; I[J, D] := z;
  if i = N + 1 go to STOP;
```

```
  Reset controls: for j := J do begin
    C[j] := K(I[j, 1]); D[j] := 1;
    for k = 2 step 1 until M do
      if C[j] > K(I[j, k]) then begin C[j] :=
        K(I[j, k]); D[j] := k end end;
    go to Find least;
  STOP: end
```

```
Presort quadratic selection (I,N,S); value N;
array I[1:N], S[1:N]; integer procedure K(I); integer N;
begin integer i, j, k, C, J, M;
  integer array C[1:M], D[1:M];
  array I[1:M, 1:M];
```

```

Divide inputs:  M := entier (sqrt(N)) + 1; j := k := 1;
                for i := 1 step 1 until N do begin
                    I[j,k] := I[i]; k := k + 1;
                    if k > M then begin k := 1;
                        j := j + 1 end end
Fill up inputs:  I[j,k] := z; k := k + 1;
                if k > M then begin k := 1; j := j + 1 end
                if j ≤ M then go to Fill up inputs;
First sort:      for j := 1 step 1 until M do
                    sort select exchange (I[j,k],M);
Set controls:    for j := 1 step 1 until M do begin
                    C[j] := K(I[j,1]); D[j] := 1 end
                    i := 1;
Find least:      C := C[1]; J := 1;
                for j := 1 step 1 until M do
                    if C > C[j] then begin C := C[j];
                        J := j end;
Fill file:        S[i] := I[J,D[J]]; i := i + 1;
                if i = N + 1 go to STOP
Reset control:    for j := J do begin
                    D[j] := D[j] + 1;
                    if D[j] > M then C[j] := z else C[j] :=
                        K(I[j, D[j]]) end
                    go to Find least;
STOP:            end

Sort binary merge (I,N,S); value N; array I[1:N];
integer procedure K(I); integer N;
begin real array S[1:N];
integer array A[0:1, 0:J[a]], B[0:1, 0:K[b]], Aloc[0:1, 0:J[a]],
        Bloc[0:1, 0:K[b]], J[0:1], K[0:1], j[0:1], k[0:1];
integer a,b,i,j,k;
distribute:      a := b := j[0] := j[1] := 1;
                for i := 1 step 1 until N do begin
                    if K(I[i]) < K(I[i-1]) then
                        if a = 1 then a := 0 else a := 1;
                        A[a, j[a]] := K(I[i]); Aloc[a, j[a]] := i;
                        j[a] := j[a] + 1 end;
                    J[0] := j[0]; J[1] := j[1];
next sort:        begin a := b := j[0] := j[1] := k[0] :=
                    k[1] := 1;
two inputs:       if A[1, j[1]] ≤ A[0, j[0]] then a := 1 else
                    a := 0;
                    B[b, k[b]] := A[a, j[a]];
                    Bloc[b, k[b]] := Aloc[a, j[a]];
                    j[a] := j[a] + 1; k[b] := k[b] + 1;
                    if A[a, j[a]] ≥ A[a, j[a] - 1] then go to two
                        inputs else
                    if a = 1 then a := 0 else a := 1;
single step:      B[b, k[b]] := A[a, j[a]];
                    Bloc[b, k[b]] := Aloc[a, j[a]];
                    j[a] := j[a] + 1; k[b] := k[b] + 1;
                    if A[a, j[a]] ≥ A[a, j[a] - 1] then go to
                        single step;
switch file:      if b = 1 then b := 0 else b := 1;
check rollout:    for a := 0, 1 do
                    if j[a] = J[a] then go to rollout;
                    go to two inputs;
rollout:          B[b, k[b]] := A[a, j[a]];
                    Bloc[b, k[b]] := Aloc[a, j[a]];
                    k[b] := k[b] + 1; j[a] := j[a] + 1;
                    if j[a] = J[a] then go to interchange files;
                    if A[a, j[a]] < A[a, j[a] - 1] then
                        if b = 1 then b := 0 else b := 1;
                    go to rollout;
interchange files: K[0] := k[0]; K[1] := k[1];
                    if K[0] = 1 then go to output end

```

```

                for b := 1, 0 do begin
                    for k[b] := 1 step 1 until K[b] do begin
                        A[b, k[b]] := B[b, k[b]];
                        Aloc[b, k[b]] := Bloc[b, k[b]];
                        J[b] := K[b] end end
                    go to next sort;
output:          for i := 1 step 1 until N do
                    S[i] := I[Bloc[0, i]];
                end

```

REMARK ON ALGORITHM 76 SORTING PROCEDURES (Ivan Flores, *Comm. ACM* 5, Jan. 1962)

B. RANDELL
Atomic Power Div., The English Electric Co., Whetstone,
England

The following types of errors have been found in the Sorting
Procedures:

1. Procedure declarations not starting with **procedure**.
 2. Bound pair list given with array specification.
 3. = used instead of :=, in assignment statements, and in a **for** clause.
 4. A large number of semicolons missing (usually after **end**).
 5. Expressions in bound pair lists in array declarations depending on local variables.
 6. Right parentheses missing in some procedure statements.
 7. Conditional statement following a **then**.
 8. No declarations for A, or z, which is presumably a misprint.
 9. In several procedures attempt is made to use the same identifier for two different quantities, and sometimes to declare an identifier twice in the same block head.
 10. In the Presort quadratic selection procedure an array, declared as having two dimensions, is used by a subscripted variable with only one subscript.
 11. At one point a subscripted variable is given as an actual parameter corresponding to a formal parameter specified as an array.
 12. In several of the procedures, identifiers used as formal parameters are redeclared, and still assumed to be available as parameters.
 13. In every procedure K is given in the specification part, with a parameter, whilst not given in the formal parameter list.
- No attempt has been made to translate, or even to understand the logic of these procedures. Indeed it is felt that such a grossly inaccurate attempt at ALGOL should never have appeared as an algorithm in the *Communications*.

ALGORITHM 77 INTERPOLATION, DIFFERENTIATION, AND IN- TEGRATION

PAUL E. HENNION
Grumman Aircraft Engineering Corporation, Bethpage,
L. I., New York

```

real procedure AVINT (nop, jt, xarg, xlo, xup, xa, ya);
value nop, jt, xarg, xlo, xup; real xarg, xlo, xup;
integer nop, jt; real array xa, ya;
comment This procedure will perform interpolation, differen-
tiation, or integration operating upon functions of one vari-
able which over part or all of the interval of interest are ade-
quately described by a di-parabolic fit.

```

The routine was originally programmed as an open subroutine for the IBM 704 in FORTRAN II and occupied 323 memory locations. It is based upon a Lagrange interpolation scheme specialized for averaged second order parabolas. The technique finds the slope of a function numerically defined at points 1, 2, 3 and 4 by fitting a parabola through the points 1, 2, 3, and another parabola through the points 2, 3, and 4. The slope then, at point 2, is the average analytical derivative of the two parabolas, i.e. the coefficients of the parabola through points 1, 2 and 3 ($a_1x_2^2 + b_1x_2 + c_1$) and the coefficients of the parabola through points 2, 3, and 4 ($a_2x_2^2 + b_2x_2 + c_2$) are determined by applying Lagrange's equations as shown below. The arithmetic mean of these coefficients $a = (a_1 + a_2)/2$, $b = (b_1 + b_2)/2$, $c = (c_1 + c_2)/2$ are used to supply the slope in the interval from 2 to 3, namely $(2ax + b)$.

The interpolation is calculated in similar fashion, except the final formula is that a parabola ($ax^2 + bx + c$).

The integration is performed likewise by a curve fitting process, e.g. the integral between any two points say 2 and 3 is the average integral of the two parabolas between the independent coordinate limits for points 2 and 3. The averaging process is done for each interval along the abscissa as the results obtained are accumulated to evaluate the definite integral.

Applying Lagrange's equations, the coefficients a , b , and c may be found by defining: $T_j = y_j / \prod_{i=1, i \neq j}^n (X_j - X_i)$ where $y = f(x)$, $n = 3$, $j = 1, 2, \dots, n$, then $a = \sum_{i=1}^n T_i$, $b = \sum_{i=1}^n T_i \sum_{j=1}^n X_j$, $c = \sum_{i=1}^n T_i \prod_{j=1, j \neq i}^n X_j$;

```
begin real  ca, cb, cc, a, b, c, syl, syu, term1, term2, term3, da,
            dif, sum;
integer    jm, js, jul, ia, ib;
start:    switch alpha := L1, L1, L12; switch beta := L9,
            L5, L6;
            switch gamma := L10, L11; switch delta := L8,
            L8, L13;
comment    For interpolation, differentiation or integration set
            jt = 1, 2, or 3 respectively;
            go to alpha [jt];
L1:        if xarg >= xa [nop] then go to L2;
            if xarg >= xa [nop-1] then go to L2;
            if xarg <= xa [1] then go to L3;
            if xarg <= xa [2] then go to L3; go to L4;
L2:        jm := nop-1; js := 1; go to term;
L3:        jm := 2; js := 1; go to term;
comment    Locate argument;
L4:        for ia := 2 step 1 until nop do begin
            if xa [ia] > xarg then go to L7; jm := ia end;
comment    Before loop is complete xarg <= xa [ia];
L5:        ca := a; cb := b; cc := c; js := 3; jm :=
            jm+1; go to term;
L6:        a := (ca+a)/2; b := (cb+b)/2; c := (cc+c)/2;
            go to L9;
L7:        js := 2; go to term;
L8:        go to beta [js];
L9:        go to gamma [jt];
comment    Interpolation, jt = 1;
L10:       da := a * xarg ↑ 2 + b * xarg + c; go to exit1;
comment    Differentiation, jt = 2;
L11:       dif := 2 * xarg + b; go to exit2;
comment    Integration, jt = 3;
L12:       sum := 0; syl := xlo; jul := nop - 1;
            ib := 2;
L16:       for jm := ib step 1 until jul do begin;
comment    Lagrange formulae;
            term1 := ya [jm - 1] / ((xa [jm - 1] - xa [jm]) *
            (xa [jm - 1] - xa [jm + 1]));
            term2 := ya [jm] / ((xa [jm] - xa [jm - 1]) *
            (xa [jm] - xa [jm + 1]));
```

```
term3 := ya [jm + 1] / ((xa [jm + 1] - xa [jm - 1]) *
            (xa [jm + 1] - xa [jm]));
a := term1 + term2 + term3;
b := -(xa [jm] + xa [jm + 1]) * term1 - (xa
            [jm - 1] + xa [jm + 1]) * term2 - (xa [jm - 1] +
            xa [jm]) * term3;
c := xa [jm] * xa [jm + 1] * term1 + xa [jm - 1] *
            xa [jm + 1] * term2 + xa [jm - 1] * xa [jm] *
            term3; go to delta [jt];
```

```
L13:       if jm ≠ 2 then go to L14;
            ca := a; cb := b; cc := c; go to L15;
L14:       ca := (a + ca)/2; cb := (b + cb)/2; cc :=
            (c + cc)/2;
L15:       syu := xa [jm];
```

```
sum := sum + ca * (syu ↑ 3 - syl ↑ 3)/3 + cb *
            (syu ↑ 2 - syl ↑ 2)/2 + cc * (syu - syl);
ca := a; cb := b; cc := c; syl := syu end;
comment    End of loop on [jm] index;
sum := sum + ca * (xup ↑ 3 - syl ↑ 3)/3 + cb *
            (xup ↑ 2 - syl ↑ 2)/2 + cc * (xup - syl); go
            to exit3;
```

```
term:      ib := jm; jul := ib; go to L16;
```

```
comment    The results for interpolation, differentiation, and
            integration are da, dif, and sum respectively;
```

```
exit1:     AVINT := da; go to exit;
```

```
exit2:     AVINT := dif; go to exit;
```

```
exit3:     AVINT := sum;
```

```
exit:      end
```

CERTIFICATION OF ALGORITHM 77

AVINT (Paul E. Hennion, *Comm. ACM* 5, Feb., 1962)

VICTOR E. WHITTIER

Computations Res. Lab., The Dow Chemical Co., Midland, Mich.

AVINT was transliterated into BAC-220 (a dialect of ALGOL-58) and was tested on the Burroughs 220 computer. The following minor errors were found:

1. The first statement following label L11 should read:
dif := 2 * a * xarg + b;
2. The semicolon (;) at the end of the line beginning with the label L16 should be deleted.
3. There appears to be a confusion between "1" (numeric) and "I" (alphabetic) following label L12. This portion of the program should read:

```
L12: sum := 0; syl := xlo; jul := nop - 1; ib := 2;
```

After making the above corrections the procedure was tested for interpolation, differentiation, and integration using e^x , $\log X$, and $\sin X$ in the range $(1.0 \leq X \leq 5.0)$. Twenty-one values of each of these functions, evenly spaced with respect to X and accurate to at least 7 significant digits, were tabulated in the above range. Then the procedure was tested. The following table indicates approximately the accuracy obtained:

Function	Number of Significant Digits		
	Interpolation	Differentiation	Integration
e^x	$\geq 4^*$	≥ 2	≥ 4
$\log X$	$\geq 4^*$	≥ 2	≥ 3
$\sin X$	$\geq 4^*$	≥ 2	≥ 4

* Except for interpolation between the first two points in the table.

The above results are quite reasonable in view of the relatively large increment in X . Tests using smaller increments in X and uneven spacing of X were also satisfactory.

It was also discovered that for integration the following restrictions must be observed:

1. $xlo \leq xa(1)$.
2. $xup \geq xa(nop)$.

REMARK ON ALGORITHM 77 INTERPOLATION, DIFFERENTIATION, AND IN- TEGRATION [P. E. Hennion, *Comm. ACM* 5, Feb. 1962]

P. E. HENNION

Giannini Controls Corp., Berwyn, Penn.

It was brought to my attention through the CERTIFICATION OF ALGORITHM 77 AVINT (V. E. Whittier, *Comm. ACM*, June, 1962) that restrictions on the upper and lower limits of integration existed, i.e., (1) $x_{lo} \leq x_a(1)$, (2) $x_{up} \geq x_a(nop)$. To remove these restrictions the following two changes should be made.

1. Replace the two lines starting at line L12: and ending after the statement $ib := 2$; with the following code:

```
L12: sum := 0; syl := xlo; ib := 2; jul := nop;
    for ia := 1 step 1 until nop do begin
        if xa [ia] ≥ xlo then go to L17; ib := ib + 1; end;
L17: for ia := 1 step 1 until nop do begin
        if xup ≥ xa [jul] then go to L18; jul := jul - 1; end;
L18: jul := jul - 1;
```

2. Change line L13: to read
L13: if $jm \neq ib$ then go to L14;

ALGORITHM 78 RATIONAL ROOTS OF POLYNOMIALS WITH IN- TEGER COEFFICIENTS

C. PERRY

University of California at San Diego, La Jolla, California

comment This ALGOL procedure, named ratfact, for finding rational roots of polynomials with integer coefficients is a pedagogical example illustrating the use of the **for** statement described in section 4.6.3. Also, an extension suggested by J. Peck of the well-known polynomial evaluation by nesting, i.e. Horner's method, is used. The polynomial $f(x) = a_0 + a_1x + \dots + a_nx^n$ with integer coefficients and with $a_0a_n \neq 0$ has a lowest term rational root p/q if and only if $a_0q^n + a_1q^{n-1}p + \dots + a_{n-1}q p^{n-1} + a_n p^n = 0$, also q must be a factor of a_n and p a factor of a_0 . Procedure RATFACT outputs the nonzero rational roots p/q by execution of the procedure whose formal name is print. The output procedure uses the string whose formal name is format for control of the output format;

```
procedure ratfact (a, n, print, format);
    integer array a[0:n]; integer n; procedure print; string
    format;
    begin integer i, p, q, r, t, f, g;
    p loop: for p := 1 step 1 until abs (a[0]) do
        begin comment if p is not a factor of a [0] or q is not a factor
        of a[n] then skip to the end of the loop for advance in the
        respective for list;
        if a[0] ≠ (a[0] ÷ p) × p then go to 1
        else q loop: for q := 1 step 1 until abs (a[n]) do
            begin if a[n] ≠ (a[n] ÷ q) × q then go to 2
            else
                begin comment root test and print;
                comment start polynomial evaluation;
                f := g := a[0]; t := p;
                for i := 1 step 1 until n do
                    begin r := a[i] × t;
                    f := f × q + r;
                    g := -g × q + r;
                    t := t × p;
                end polynomial evaluation;
```

```
comment computing r saves one subscript
evaluation;
if f=0 then print (format, p, q);
if g=0 then print (format, -p, q);
comment print is the formal name of the procedure
to be used to output the variables in the format
specified by the string whose formal name is format;
end root test and print;
2: end q loop;
1: end p loop;
end ratfact, without overflow test.
```

CERTIFICATION OF ALGORITHM 78 RATFACT (C. Perry, *Comm. ACM* 5, Feb. 1962)

M. H. HALSTEAD

Navy Electronics Laboratory, San Diego, Calif.

RATFACT was copied in the Navy Electronics Laboratory International ALGOL Compiler, NELIAC, and tested on the UNIVAC M-490 Countess and the CDC 1604. Polynomials of order 2 through 6 were tested. No corrections were found necessary. It was noted that a polynomial whose coefficients included a common factor would produce superfluous values of p/q , in which this fraction was indeed a root, but one in which p and q contained a common factor.

REMARK ON ALGORITHM 78 RATIONAL ROOTS OF POLYNOMIALS WITH INTEGER COEFFICIENTS [C. Perry, *Comm. ACM*, Feb. 1962]

D. M. COLLISON

Elliott Bros. (London) Ltd., Borehamwood, Herts.,
England

The algorithm was successfully run using the Elliott ALGOL translator on the National-Elliott 803. It was noticed that a multiple rational root will only be printed once by the procedure.

ALGORITHM 79 DIFFERENCE EXPRESSION COEFFICIENTS THOMAS P. GIAMMO

Space Technology Laboratories, Inc., Los Angeles, Cali-
fornia

```
procedure dicol (k, n, xp, xtab, coef);
    value k, n; integer k, n; real xp;
    array xtab, coef;
    comment dicol produces the coefficients for the n ordinates
    (corresponding to the abscissae, xtab) in the n-point finite
    difference expression for the k-th derivative evaluated at xp.
    The method used is to determine the analytic expression for
    the k-th derivative of each coefficient in the n-point Lagrangian
    interpolation formula and evaluate it at xp. Note that k=0
    will produce the Lagrangian interpolation coefficients them-
    selves;
    begin integer array xuse [1 : n-1]; real factk, sum, denom,
    part;
    integer i, terms, j, m, high;
    factk := 1.0; for i := 2 step 1 until k do factk := i × factk;
    terms := n - k - 1; if terms < 0 then go to Z;
    for j := 1 step 1 until n do
```

```

loop: begin sum := 0; denom := 1.0; part := 1.0;
      for i := 1 step 1 until n do
        if i ≠ j then denom := denom × (xtab [j] - xtab [i]);
        if terms = 0 then go to Y;
        m := 1; high := 1;
      A: if (high = j) ∨ (xtab [high] = xp) then
        A1: begin high := high + 1; go to A end A1;
        if high > n then A2: begin m := m - 1; if m > 0
          then
            A3: begin high := xuse [m] + 1; go to A end A3;
            go to X end A2;
            xuse [m] := high; m := m + 1;
            if m ≤ terms then begin high := high + 1; go to
              A end;
            for i := 1 step 1 until terms do
              part := part × (xp - xtab [xuse [i]]);
              sum := sum + part; m := terms; part := 1.0;
              high := xuse [terms] + 1; go to A;
        Y: sum := 1.0;
        X: coef [j] := sum × factk / denom end loop;
        go to EXIT;
        Z: for i := 1 step 1 until n do coef [i] := 0;
      EXIT: end dicol

```

CERTIFICATION OF ALGORITHM 79 DIFFERENCE EXPRESSION COEFFICIENTS

[Thomas Giamo, *Comm. ACM*, Feb. 1962]

EVA S. CLARK

University of California at San Diego, La Jolla, California

The procedure was translated into FORTRAN and run on the CDC 1604. Reasonable accuracy was obtained for $k = 0, 4 \leq n \leq 12$. For increasing n and increasing k , the accuracy diminished. It was found that the execution time increased rapidly as n was increased. For $k = 0$, the following results were obtained:

n	Approximate Number of Machine Operations
4	1.3×10^3
6	6.9×10^3
8	3.8×10^4
10	1.8×10^5
12	8.6×10^5

The author indicated in a letter that the procedure was developed for use with small n and small k .

ALGORITHM 80 RECIPROCAL GAMMA FUNCTION OF REAL ARGUMENT

WILLIAM HOLSTEN

University of California at San Diego, La Jolla, California

```

real procedure RGR(x); real x; real procedure RGAM;
comment Procedure RGAM computes the real reciprocal
Gamma function of real x for  $-1 < x < 1$ , utilizing Horner's
method for polynomial evaluation of the approximation poly-
nomial. RGR extends the range of RGAM by use of the formulae
(1)  $1/\Gamma(x-1) = (x-1)/\Gamma(x)$  for  $x < -1$ ,
(2)  $1/\Gamma(x+1) = 1/x \times \Gamma(x)$  for  $x < 1$ ;
begin real y;
  if x = 0 then begin RGR := 0; go to EXIT end
  if x = 1 then begin RGR := 1; go to EXIT end
  if x < 1 then go to BB;

```

```

y := 1;
AA: x := x - 1; y := y × x; if x > 1 then go to AA;
  if x = 1 then begin RGR := 1/y; go to EXIT end
  RGR := RGAM(x)/y; go to EXIT;
BB: if x = -1 then begin RGR := 0; go to EXIT end
  if x > -1 then begin RGR := RGAM(x);
    go to EXIT end
  y := x;
CC: x := x + 1; if x < -1 then begin y := y × x;
  go to CC end
  RGR := RGAM(x) × y;
EXIT: end RGR;
real procedure RGAM(x); real x; integer i;
  real array B[0:13];
comment The algorithm for this routine was adapted from
"University of Illinois Digital Computer, Auxiliary Library
Routine B-17-328", by John Ehrman. Reference may also be
made to Algorithm 34, dated February, 1961. Approximation
accuracy is  $\pm 2^{-36}$ ;
begin real z;
  B[0] := 1.00000 00000 00; B[1] := -.42278 43350 92;
  B[2] := -.23309 37363 65; B[3] := +.19109 11011 62;
  B[4] := -.02455 24908 87; B[5] := -.01764 52421 18;
  B[6] := +.00802 32781 13; B[7] := -.00080 43413 35;
  B[8] := -.00036 08514 96; B[9] := +.00014 56243 24;
  B[10] := -.00001 75279 17; B[11] := -.00000 26257 21;
  B[12] := +.00000 13285 54; B[13] := -.00000 01812 20;
  z := B[13];
  for i := 12 step -1 until 0 do z := z × x + B[i];
  RGAM := z × x × (x + 1)
end RGAM;

```

ALGORITHM 81 ECONOMISING A SEQUENCE 1

BRIAN H. MAYOH

Digital Computer Laboratory, University of Illinois,
Urbana, Ill.

```

procedure ECONOMISER 1 (desired property, costs, n, C);
  array costs; integer n;
  Boolean procedure desired property;
  Boolean array C;
begin comment Given a finite, monotonely increasing
sequence of positive numbers, looked upon as prices, ECONO-
MISER 1 selects the cheapest subsequence with a given prop-
erty. The formal parameters are: Desired property, a function
designator to answer the question: Does the subsequence held
in array C possess the required property?  $n$  is (number of ele-
ments in the sequence) + 1. Costs is an array of size  $[1:n]$ .
Costs[1] to costs[n-1] hold the numbers of the sequence and
costs[n] is any arbitrary number greater than the sum of all
other elements of costs. C is an array of the same size and indi-
cates a subsequence by the rule:  $C[i] = \text{element } i \text{ of the original}$ 
sequence is in the subsequence. At exit from ECONOMISER 1,
C indicates the cheapest subsequence. It is supposed that the
original sequence has the desired property.;
integer d, j, k, l; real i;
for j := 1 step 1 until n do C[j] := j = 1; d := 0;
reenter: d := d + 1;
INSIDE: begin own real array prices [1:d];
  own Boolean array alternatives [1:d, 1:n];
  procedure ENTER SUCCESSORS;

```

```

begin k := n-1;
A: if  $\neg C[k]$  then
  begin k := k-1; go to A end; i := 0;
  for j := 1 step 1 until n do
    begin alternatives[l,j]
      := j  $\neq$  k  $\wedge$  j  $\neq$  k-1  $\equiv C[j]$ ;
      if alternatives[l,j] then
        i := i + costs[j]
      end;
  B: k := k-1;
  go to if k = 0 then find cheapest
    else if C[k] then (if k=1 then
      find cheapest else B)
    else if k=1 then E
    else if C[k-1] then D
    else find cheapest;
  D: C[k-1] := false;
  E: C[k] := true; go to reenter
end of ENTER SUCCESSORS;
i := 0; for j := 1 step 1 until n do
  begin alternatives[d,j] := C[j]; if C[j] then
    i := i + costs[j]
  end; prices[d] := i;
find cheapest: i := 0; for j := 1 step 1 until d do
  begin if prices[j] < i then
    begin l := j; i := prices[l] end
  end;
  for j := 1 step 1 until n do
    C[j] := alternatives[l,j];
    if  $\neg$  desired property then
      ENTER SUCCESSORS
    end of INSIDE;
end of ECONOMISER 1;

```

ALGORITHM 82 ECONOMISING A SEQUENCE 2

BRIAN H. MAYOH

Digital Computer Laboratory, University of Illinois,
Urbana, Ill.

procedure ECONOMISER 2 (desired property, costs, n, C, r, Reject list); **Boolean procedure** desired property;
integer n, r; **array** costs; **Boolean array** Reject list;
begin comment In some applications of ECONOMISER 1, it is simple to establish that some subsequences are redundant in the sense that any sequence containing them is certainly not the cheapest subsequence with the desired property. For such applications ECONOMISER 2 avoids all unnecessary calls of *desired property*. The new formal parameters are: *r* a variable whose value is initially 0 and is increased by 1 every time that *desired property* discovers a new redundant subsequence. *Reject list* an array of size [1:r,1:n]. *Reject list* [a,b] carries the answer to: Is element b of the original sequence in the *a*th redundant subsequence found by *desired property*?;
real i; **integer** d, j, k, l; **Boolean** gapfilled, first time;
procedure INSIDE (entrymaker); **Boolean** entrymaker;
begin own **real array** prices[1:d];
 own Boolean array alternatives[1:d,1:n];
 procedure ENTER SUCCESSORS;
 begin integer c; **Boolean array** ssq[1:n];
 for j := 1 step 1 until n do ssq[j] := C[j];
 c := n-1;

```

A: if  $\neg$  ssq[c] then begin c := c-1; go to A end;
  C[c] := false; C[c+1] := true;
  INSIDE (true);
  gapfilled := true;
B: c := c-1;
  go to if c=0 then F else if ssq[c] then
    (if c=1 then F else B) else if c=1 then
      E else if ssq[c-1] then D else F;
D: ssq[c-1] := false;
E: for j := 1 step 1 until n do C[j] := ssq[j]  $\equiv$  j $\neq$ c;
  INSIDE (true);
F: end of ENTER SUCCESSORS;
if entrymaker then
  begin for j := 1 step 1 until r do
    begin for k := 1 step 1 until n do
      begin if  $\neg C[k] \wedge$  Reject list[j,k] then
        go to G end;
      ENTER SUCCESSORS; go to H;
    end;
    i := 0; if gapfilled then d := d+1;
    for j := 1 step 1 until n do
      begin alternatives[if gapfilled then
        d else l, j] := C[j];
        if C[j] then i := i + costs[j]
      end; prices[if gapfilled then d else l] := i
    end; if first time  $\vee$   $\neg$  entrymaker then
      begin i := 0; gapfilled := first time := false;
        for j := 1 step 1 until d do
          begin if prices[j] < i then
            begin l := j; i := prices[l] end
          end;
          for j := 1 step 1 until n do
            C[j] := alternatives[l,j];
            if desired property then go to found;
            ENTER SUCCESSORS; go to reenter
          end;
        H: end of INSIDE;
        for j := 1 step 1 until n do C[j] := j=1;
        d := 0; first time := gapfilled := true;
        reenter: INSIDE (first time);
        found:
        end of ECONOMISER 2;

```

ALGORITHM 83 OPTIMAL CLASSIFICATION OF OBJECTS

BRIAN H. MAYOH

Digital Computer Laboratory, University of Illinois,
Urbana, Ill.

procedure OPTIMUM COVERING FINDER (Pattern, population, set number, set prices, chosen sets, bounds, overflow);
Boolean array Pattern, chosen sets; **integer** population, set number, bounds; **array** set prices; **label** overflow;
begin comment The number of objects in some given set is given by *population*. The procedure is given a classification of these objects by a collection of overlapping subsets. A cost is assigned to each subset. Then OPTIMUM COVERING FINDER selects the cheapest subcollection such that every object is contained in at least one of the subsets of the subcollection. *set prices[i]* carries the cost of subset *i*. *Pattern* is an array of size [1:set number,1:population] such that *Pattern*[a,b] = does subset *a* include object *b*. *chosen sets*[i] finally

carries the answer to the question: Is set i in the cheapest subcollection? The programmer must restrict the amount of space available to the procedure by setting *bounds*. From experience $\text{bounds} = \text{set number} \uparrow 2$ suffices to avoid most alarm exits to *overflow*;

Boolean array C[1:population], D[1:bounds, 1:population],
R, S[1:bounds, 1:set number];

integer a, b, d, r, s;

Boolean procedure HAVE WE A COVERING;

begin procedure ADD to (Q,q,f); **integer** q;

real f; **Boolean array** Q;

begin if q=bounds **then go to overflow** **else** q := q+1;

for a := 1 **step** 1 **until** set number **do** Q[q,a] := f

end; **for** a := 1 **step** 1 **until** population **do**

C[a] := false;

for a := 1 **step** 1 **until** set number **do**

begin if chosen sets[a] **then**

for b := 1 **step** 1 **until** population **do**

C[b] := C[b] $\vee$ Pattern[a,b]

end; **for** a := 1 **step** 1 **until** population **do**

begin if $\neg$ C[a] **then go to E** **end**;

go to found;

E: **for** d := 1 **step** 1 **until** s **do**

begin for b := 1 **step** 1 **until** population **do**

begin if C[b] $\wedge$ $\neg$ D[d,b] **then go to try another** **end**;

ADD to (R, r, chosen sets[a]);

for b := 1 **step** 1 **until** set number **do**

begin if chosen sets[b] $\wedge$ $\neg$ S[d,b] **then**

ADD to (R, r, S[d,a] $\vee$ a=b)

end; **go to F**;

try another:

end of for statement labelled **E**;

ADD to (S, s, chosen sets[a]);

for a := 1 **step** 1 **until** population **do** D[s,a] := C[a];

F: HAVE WE A COVERING := false

end; r := s := 0;

ECONOMISER 2 (HAVE WE A COVERING, set prices,
set number, r, R, chosen sets);

found: **end**

ALGORITHM 84

SIMPSON'S INTEGRATION

PAUL E. HENNION

Giannini Controls Corporation

Astromechanics Research Division, Berwyn, Penn.

real procedure SIM (n, a, b, y);

value n, a, b; **real** a, b; **integer** n; **array** y;

comment This is a method for obtaining the approximate value of the definite integral of a continuous function when the integral cannot be evaluated in elementary functions. Given $y = f(x)$ and the $\int_a^b y \, dx$ to be evaluated. Plot the curve $f(x)$, and divide $[a, b]$ evenly into n equal parts, erecting the ordinates $y_0, y_1, \dots, y_n$. Then the approximate value of the definite integral by Simpson's rule states that:

$$\int_a^b f(x) \, dx = \frac{b-a}{3n} (y_0 + 4y_1 + 2y_2 + \dots + 4y_{n-1} + y_n);$$

begin **real** s; **integer** i;

s := (y[0] - y[n])/2;

for i := 1 **step** 2 **until** n - 1 **do** s := s + 2 $\times$ y[i] + y[i+1];

SIM := 2 $\times$ (b - a) $\times$ s/(3 $\times$ n)

end

CERTIFICATION OF ALGORITHM 84

SIMPSON'S INTEGRATION [P. E. Hennion, *Comm.*

ACM, Apr. 62]

PETER G. BEHRENS

Matematikmaskinnämnden, Stockholm, Sweden

SIM was successfully run on FACIT EDB using FACIT-ALGOL 1, which is a realization of ALGOL 60 for FACIT EDB. No changes in the program were necessary. To test SIM some polynomials were integrated.

CERTIFICATION OF ALGORITHM 84

SIMPSON'S INTEGRATION [P. E. Hennion, *Comm.*

ACM 5 (Apr. 1962)]

A. P. RELPH

The English Electric Co., Whetstone, England

Simpson's Integration was translated using the DEUCE ALGOL compiler and, with no corrections, gave satisfactory results.

It is not stated in the comment that integer n needs to be even.

REMARK ON ALGORITHM 84

SIMPSON'S INTEGRATION [Paul E. Hennion, *Comm.*

ACM, Apr. 1962]

RICHARD GEORGE*

Particle Accelerator Div., Argonne National Lab., Argonne, Ill.

* Work supported by the U. S. Atomic Energy Commission.

In performing integration by the use of Simpson's rule, it is well known that the interval $[a, b]$ must be divided evenly into n equal parts, and that it is essential for n to be an even number.

In the published algorithm, there is neither a comment on this important restriction, nor a programmed test for the parity of n . It is therefore a potential trap for the unwary programmer.

ALGORITHM 85

JACOBI

THOMAS G. EVANS

Bolt, Beranek, and Newman*, Cambridge, Mass.

* This work has been sponsored by the Air Force Cambridge Research Laboratories, OAR (USAF), Detection Physics Laboratory, under contract AF 19(628)-227.

procedure JACOBI (A, S, n, rho);

value n, rho; **integer** n; **real** rho; **real array** A, S;

comment This procedure finds all eigenvalues and eigenvectors of a given square symmetric matrix by a modified Jacobi (iterative) method (cf. J. Greenstadt, "The determination of the characteristic roots of a matrix by the Jacobi method," in *Mathematical Methods for Digital Computers*, A. Ralston and H. S. Wilf, eds.). JACOBI is given a square symmetric matrix of order n stored in the array A. The initial contents of the array S are immaterial, as S is initialized by the procedure. At exit the k^{th} column of the array S contains the k^{th} of the n eigenvectors of the given matrix, and the diagonal element A[k, k] of the array A is the corresponding k^{th} eigenvalue. The parameter rho is the "accuracy requirement" introduced in the above reference, where a detailed flow chart of the method is given. The significance of rho is that the iteration terminates when, for every off-diagonal ele-


```

ment A[i, j], abs (A[i, j]) < (rho/n) × norm1, where norm1 is a
function only of the off-diagonal elements of the original matrix;
begin real norm1, norm2, thr, mu, omega, sint, cost, intl, v1,
v2, v3;
integer i, j, p, q, ind;
comment Set array S = n × n identity matrix;
for i := 1 step 1 until n do
for j := 1 step 1 until i do
if i = j then S[i, j] := 1.0
else S[i, j] := S[j, i] := 0.0;
comment Calculate initial norm (norm1), final norm (norm2),
and threshold (thr);
intl := 0.0;
for i := 2 step 1 until n do
for j := step 1 until i-1 do
intl := intl + 2.0 × A[i, j] ↑ 2;
norm1 := sqrt (intl); norm2 := (rho/n) × norm1;
thr := norm1; ind := 0;
main: thr := thr/n;
comment The sweep through the off-diagonal elements be-
gins here;
main: for q := 2 step 1 until n do
for p := 1 step 1 until q-1 do
if abs (A[p, q]) ≥ thr then
begin ind := 1; v1 := A[p, p]; v2 := A[p, q];
v3 := A[q, q]; mu := 0.5 × (v1-v3);
omega := (if mu = 0.0 then 1 else sign (mu)) ×
(-v2)/sqrt(v2↑2 + mu↑2);
sint := omega/sqrt(2.0 × (1.0 + sqrt(1.0 -
omega↑2)));
cost := sqrt (1.0 - sint↑2);
for i := 1 step 1 until n do
begin intl := A[i, p] × cost - A[i, q] × sint;
A[i, q] := A[i, p] × sint + A[i, q] × cost;
A[i, p] := intl;
intl := S[i, p] × cost - S[i, q] × sint;
S[i, q] := S[i, p] × sint + S[i, q] × cost;
S[i, p] := intl
end;
for i := step 1 until n do
begin A[p, i] := A[i, p]; A[q, i] := A[i, q] end;
A[p, p] := v1 × cost↑2 + v3 × sint↑2 - 2.0 ×
v2 × sint × cost;
A[q, q] := v1 × sint↑2 + v3 × cost↑2 + 2.0 ×
v2 × sint × cost;
A[p, q] := A[q, p] := (v1 - v3) × sint × cost +
v2 × (cost↑2 - sint↑2)
end;
comment Now test to see if current tolerance exceeded and,
if not, whether final tolerance reached;
if ind = 1 then begin ind := 0; go to main end
else if thr > norm2 then go to main
end JACOBI

```

CERTIFICATION OF ALGORITHM 85

JACOBI [T. G. Evans, *Comm. ACM*, Apr. 1962]

J. S. HILLMORE

Elliott Bros. (London) Ltd., Borehamwood, Herts.,
England

The statement

```

omega := (if mu = 0.0 then 1 else sign (mu))
        × (-V2)/sqrt(V2 ↑ 2 + mu ↑ 2);

```

was changed to

```

omega := if mu = 0.0 then -1.0 else - sign (mu)
        × V2/sqrt (V2 ↑ 2 + mu ↑ 2);

```

When $\mu = 0$, the original statement reduces to

```

omega := -V2/sqrt (V2 ↑ 2);

```

and a truncation error in the evaluation of the square root can

make the magnitude of ω slightly greater than unity. As a result, an error stop occurs during execution of the next statement when an attempt is made to evaluate $\sqrt{1 - \omega^2}$.

In its modified form the algorithm has been successfully run using the Elliott ALGOL translator on the National-Elliott 803. Matrices of order up to fifteen have been solved, yielding eigenvalues and eigenvectors with an overall accuracy of seven decimal places.

CERTIFICATION OF ALGORITHM 85

JACOBI [Thomas G. Evans, *Comm. ACM* (Apr. 1962), 208]

P. NAUR

Regnecentralen, Copenhagen, Denmark

We have first run this algorithm in the GIER ALGOL system with the following corrections included:

1. The change given by J. S. Hillmore [*Comm. ACM* 5 (Aug. 1962), 440] with capital V changed to v .
2. The 4th for clause corrected to read:

```

for j := 1 step 1 until i - 1 do

```

3. The last for clause corrected to read:

```

for i := 1 step 1 until n do

```

On closer examination we have found, however, that a significant number of superfluous operations could be eliminated in the innermost loop by rewriting the two for statements at the center of the algorithm as a single for statement, to read as follows:

```

.....
cost := sqrt (1 - sint ↑ 2);
for i := 1 step 1 until n do
begin if i ≠ p ∧ i ≠ q then
begin intl := A[i, p]; mu := A[i, q];
A[q, i] := A[i, q] := intl × sint + mu × cost;
A[p, i] := A[i, p] := intl × cost - mu × sint
end;
intl := S[i, p]; mu := S[i, q];
S[i, q] := intl × sint + mu × cost;
S[i, p] := intl × cost - mu × sint
end;
A[p, p] := v1 × cost ↑ 2 + v3 × sint ↑ 2 - 2 × v2 × sint × cost;
.....

```

This revision is particularly advantageous in systems having a comparatively slow subscript mechanism, such as GIER ALGOL, because it eliminates more than 3 out of 8 references to subscripted variables.

JACOBI has been tried with two different sets of matrices having known eigenvalues. In both cases a test program was set up to find the range of errors of the eigenvalues computed by JACOBI. In addition, the relations $Av - \lambda v = 0$ (A is the given matrix, v an eigenvector, and λ the corresponding eigenvalue) and $A - (ST)$ LAMBDA $S = 0$ (S is the matrix having the eigenvectors as columns and ST its transpose, and LAMBDA is the diagonal matrix of the eigenvalues) were used as checks. The test matrices were TESTMATRIX calculated by the revised algorithm 52 given in *Comm. ACM* 6 (Jan. 1963), 39, and the following matrix suggested by Mr. H. B. Hansen:

```

HBH TESTMATRIX [j, i] = HBH TESTMATRIX [i, j]
                        = n + 1 - j      j ≥ i

```

having the eigenvalues $0.5/(1 - \cos((2 \times i - 1) \times \pi / (2 \times n + 1)))$.

The results were as shown in Table 1 (GIER ALGOL works with floating numbers of 29 significant bits).

The compile time for the program which produced one of these tables was about 40 seconds. Run times were as follows:

Kho	n	Original algorithm TESTMATRIX ALG. 52 HBH TESTMATRIX (seconds)		Revised algo- rithm HBH TESTMATRIX (seconds)	
10-3	5			3	
	10			22	
	15			70	
10-5	5	3		5	
	10	5	41	29	
	15	13	148	99	
10-8	5	4	7	6	
	6	5	12		
	7	5	18		
	8	5	25		
	10	13		38	
	15	22		116	

From these figures it looks as if TESTMATRIX, Algorithm 52, is atypical as far as solution by means of JACOBI is concerned. The much higher accuracy obtained for this matrix as compared with the HBH matrix points in the same direction.

For further comparison it may be mentioned that the algorithms published by J. H. Wilkinson [Num. Math. 4 (1962), 354-376] also have been tested successfully with GIER ALGOL. Wilkinson's algorithms reduce the matrix to tridiagonal form by means of Householder's method and use Sturm sequences to find the eigenvalues and inverse iteration to find the eigenvectors. In GIER ALGOL this method is about 1.3 times as fast as JACOBI for the range of matrices considered here. JACOBI has the advantage that the eigenvectors are properly orthogonal, even in the case of multiple eigenvalues, and also has a much simpler logic. On the other hand if only some of the eigenvalues and/or eigenvectors are sought Wilkinson's algorithms will often offer much higher speed than JACOBI, which always finds them all.

SEE NEXT PAGE FOR TABLES

ALGORITHM 86

PERMUTE

J. E. L. PECK AND G. F. SCHRACK

University of Alberta, Calgary, Alberta, Canada

procedure PERMUTE (x, n);

array x; **integer** n;

comment Each call of PERMUTE executes a permutation of the first n components of x. It assumes a nonlocal Boolean variable 'first', which when true causes the procedure to initialise the signature vector p. Thereafter 'first' remains false until after n! calls;

begin own **integer array** p[2:n]; **integer** i, k;

if first **then**

begin for i := 2 **step** 1 **until** n **do**

p[i] := i; first := false

end initialise;

for k := 2 **step** 1 **until** n **do**

```

begin integer km; real t;
  t := x[1]; km := k - 1;
  for i := 1 step 1 until km do
    x[i] := x[i+1];
  x[k] := t; p[k] := p[k] - 1;
  if p[k] ≠ 0 then go to EXIT;
  p[k] := k
end k;
first := true;
EXIT: end PERMUTE

```

CERTIFICATION OF ALGORITHM 86

PERMUTE [J. E. L. Peck and G. F. Schrock, *Comm.*

ACM, Apr. 1962]

D. M. COLLISON

Elliott Bros. (London) Ltd., Borehamwood, Herts.,
England

The algorithm was successfully run using the Elliott ALGOL translator on the National-Elliott 803. Values of n used were 0, 1, 2, 3, 4.

ALGORITHM 87

PERMUTATION GENERATOR

JOHN R. HOWELL

Orlando Aerospace Division, Martin Marietta Corp.,
Orlando, Florida

procedure PERMUTATION (N, K);

value K, N; **integer** K; **integer array** N;

comment This procedure generates the next permutation in lexicographic order from a given permutation of the K marks 0, 1, ..., (K-1) by the repeated addition of (K-1) radix K. The radix K arithmetic is simulated by the addition of 9 radix 10 and a test to determine if the sum consists of only the original K digits. Before each entry into the procedure the K marks are assumed to have been previously specified either by input data or as the result of a previous entry. Upon each such entry a new permutation is stored in N[1] through N[K]. In case the given permutation is (K-1), (K-2), ..., 1, 0, then the next permutation is taken to be 0, 1, ..., (K-1). A FORTRAN subroutine for the IBM 7090 has been written and tested for several examples;

begin integer i, j, carry;

for i := 1 **step** 1 **until** K **do**

if N[i] - K + i ≠ 0 **then go to** add;

for i := 1 **step** 1 **until** K **do** N[i] := i - 1;

go to exit;

add: N[K] := N[K] + 9;

for i := 1 **step** 1 **until** K-1 **do**

begin if K > 10 **then go to** B;

carry := N[K-i+1] ÷ 10; **go to** C;

B: carry := N[K-i+1] ÷ K;

C: **if** carry = 0 **then go to** test;

N[K-i] := N[K-i] + carry;

N[K-i+1] := N[K-i+1] - 10 × carry

end i;

test: **for** i := 1 **step** 1 **until** K **do if** N[i] - (K - 1) > 0 **then go to** add;

for i := 1 **step** 1 **until** K-1 **do**

for j := i+1 **step** 1 **until** K **do**

if N[i] - N[j] = 0 **then go to** add;

exit: **end** PERMUTATION GENERATOR

CERTIFICATION OF ALGORITHM 87
 PERMUTATION GENERATOR [John R. Howell,
Comm. ACM (Apr. 1962)]
 G. F. SCHRACK and M. SHIMRAT
 University of Alberta, Calgary, Alb., Canada

PERMUTATION GENERATOR was translated into FORTRAN for the IBM 1620 and it performed satisfactorily. The algorithm was timed for several small values of n . For purposes of comparison we include the times (in seconds) for PERMULEX (Algorithm 102).

n	3	4	5	6	7
PERMUTATION GENERATOR	3	41	558	—	—
PERMULEX	—	3	6	37	278

As can be seen from this table, PERMUTATION GENERATOR is considerably slower. It is probable that one could speed up PERMUTATION GENERATOR to a great extent by rearranging the algorithm in such a manner that the digits of a number to a certain base are permuted rather than the elements of a sequence.

CERTIFICATION OF ALGORITHM 85

TABLE 1
 HBH TESTMATRIX

Range of true errors of eigenvalues						Range of deviations from relation $Ax - \lambda x = 0$						Range of deviations from relation $A - (ST) \Lambda BDA S = 0$					
Order	j	$error[j]$	j	$error[j]$		Element	Vector	Error	Element	Vector	Error	Element	Vector	Error	Element	Vector	Error
rho = 1.0 ₁₀ -3																	
5	1	-1.1 ₁₀ -6	3	5.2 ₁₀ -8		1	1	-1.7 ₁₀ -4	1	3	2.0 ₁₀ -4	1	1	-2.5 ₁₀ -4	5	5	1.0 ₁₀ -4
10	9	-7.9 ₁₀ -5	8	3.5 ₁₀ -5		7	2	-3.3 ₁₀ -3	6	6	3.0 ₁₀ -3	1	1	-4.2 ₁₀ -3	6	7	3.2 ₁₀ -3
15	15	-9.2 ₁₀ -5	12	3.7 ₁₀ -5		6	3	-1.7 ₁₀ -3	11	13	1.7 ₁₀ -3	9	15	-1.5 ₁₀ -3	8	9	1.8 ₁₀ -3
rho = 1.0 ₁₀ -5																	
5	1	-1.1 ₁₀ -6	3	6.0 ₁₀ -8		2	5	-1.3 ₁₀ -7	5	2	4.1 ₁₀ -8	1	2	-1.6 ₁₀ -7	4	5	4.5 ₁₀ -8
10	1	-1.2 ₁₀ -5	2	2.2 ₁₀ -7		7	3	-2.7 ₁₀ -5	2	8	2.2 ₁₀ -5	7	7	-2.4 ₁₀ -5	2	8	2.3 ₁₀ -5
15	1	-3.5 ₁₀ -5	4	3.9 ₁₀ -7		11	9	-6.4 ₁₀ -6	7	2	4.8 ₁₀ -6	11	12	-5.3 ₁₀ -6	12	12	4.7 ₁₀ -6
rho = 1.0 ₁₀ -8																	
5	1	-1.1 ₁₀ -6	3	6.0 ₁₀ -8		2	5	-1.3 ₁₀ -7	4	2	6.5 ₁₀ -9	2	2	-1.3 ₁₀ -7	4	4	3.0 ₁₀ -8
10	1	-1.2 ₁₀ -5	2	2.2 ₁₀ -7		1	10	-1.1 ₁₀ -6	4	2	6.4 ₁₀ -8	1	2	-5.7 ₁₀ -7	9	9	8.2 ₁₀ -8
15	1	-3.5 ₁₀ -5	4	3.9 ₁₀ -7		1	14	-3.4 ₁₀ -6	4	2	3.9 ₁₀ -7	2	2	-1.3 ₁₀ -6	15	15	8.9 ₁₀ -8
TESTMATRIX, Algorithm 52																	
Range of true errors of eigenvalues						Range of deviations from relation $Ax - \lambda x = 0$						Range of deviations from relation $A - (ST) \Lambda BDA S = 0$					
Order	j	$error[j]$	j	$error[j]$		Element	Vector	Error	Element	Vector	Error	Element	Vector	Error	Element	Vector	Error
rho = 1.0 ₁₀ -5																	
5	4	-1.0 ₁₀ -8	1	.0		5	5	-3.3 ₁₀ -8	5	4	4.3 ₁₀ -8	5	5	-5.1 ₁₀ -8	4	4	3.9 ₁₀ -8
10	8	-1.1 ₁₀ -8	4	.0		7	7	-1.2 ₁₀ -8	9	6	1.3 ₁₀ -8	7	8	-5.1 ₁₀ -9	6	6	2.0 ₁₀ -8
15	13	-1.1 ₁₀ -8	6	.0		14	14	-9.3 ₁₀ -9	10	10	9.4 ₁₀ -9	8	9	-1.9 ₁₀ -9	10	10	1.3 ₁₀ -8
rho = 1.0 ₁₀ -8																	
3	3	-7.5 ₁₀ -9	1	3.7 ₁₀ -9		3	1	-2.8 ₁₀ -9	2	2	9.3 ₁₀ -9	1	3	.0	1	2	1.9 ₁₀ -8
4	4	-5.6 ₁₀ -9	3	.0		2	2	-4.5 ₁₀ -9	3	4	3.3 ₁₀ -9	2	2	.0	2	3	9.3 ₁₀ -9
5	4	-1.0 ₁₀ -8	1	.0		5	4	-4.9 ₁₀ -9	4	4	5.8 ₁₀ -9	1	1	-7.5 ₁₀ -9	3	4	7.5 ₁₀ -9
6	4	-4.7 ₁₀ -9	4	.0		4	3	-2.8 ₁₀ -9	5	4	3.6 ₁₀ -9	1	6	-2.3 ₁₀ -10	4	5	9.3 ₁₀ -9
7	4	-5.1 ₁₀ -9	5	.0		6	6	-2.8 ₁₀ -9	4	4	3.4 ₁₀ -9	5	7	-1.2 ₁₀ -10	5	6	7.5 ₁₀ -9
8	7	-7.5 ₁₀ -9	5	.0		5	5	-6.0 ₁₀ -9	5	6	3.2 ₁₀ -9	8	8	-1.2 ₁₀ -10	7	7	9.3 ₁₀ -9
9	6	-4.4 ₁₀ -9	7	.0		6	5	-5.1 ₁₀ -9	7	6	3.2 ₁₀ -9	5	5	-7.5 ₁₀ -9	8	8	1.5 ₁₀ -8
10	8	-1.5 ₁₀ -8	8	.0		8	9	-9.3 ₁₀ -9	9	7	7.2 ₁₀ -9	6	7	-2.3 ₁₀ -9	9	9	2.0 ₁₀ -8
11	10	-7.5 ₁₀ -9	1	.0		9	10	-6.5 ₁₀ -9	8	11	3.0 ₁₀ -9	1	1	-3.1 ₁₀ -9	8	8	7.5 ₁₀ -9
12	8	-5.0 ₁₀ -9	11	.0		10	6	-7.6 ₁₀ -9	10	8	2.4 ₁₀ -9	6	6	-1.7 ₁₀ -8	4	4	1.3 ₁₀ -8
13	12	-1.1 ₁₀ -8	10	.0		10	11	-6.9 ₁₀ -9	12	10	9.1 ₁₀ -9	7	7	-3.0 ₁₀ -8	12	12	3.2 ₁₀ -8
14	10	-1.5 ₁₀ -8	4	.0		13	13	-1.1 ₁₀ -8	10	10	6.7 ₁₀ -9	9	10	-3.5 ₁₀ -9	6	6	1.7 ₁₀ -8
15	13	-1.1 ₁₀ -8	6	.0		14	14	-1.1 ₁₀ -8	11	10	3.5 ₁₀ -9	8	9	-3.0 ₁₀ -9	6	11	7.5 ₁₀ -9

CERTIFICATION OF ALGORITHM 87
 PERMUTATION GENERATOR [John R. Howell,
Comm. ACM, Apr. 1962]
 D. M. COLLISON
 Elliott Bros. (London) Ltd., Borehamwood, Herts.,
 England

The array N was removed from the value list in order that the permutations might be available outside the procedure. The algorithm was then run successfully with the Elliott ALGOL translator on the National-Elliott 803. It was rather slower than Algorithm 86.

ALGORITHM 88 EVALUATION OF ASYMPTOTIC EXPRESSION FOR THE FRESNEL SINE AND COSINE INTE- GRALS

JOHN L. CUNDIFF

Engineering Experiment Station, Georgia Institute of
 Technology, Atlanta, Ga.

real procedure FRESNEL (u) Result: (frcos, frsin); **value**
 (u);

comment This procedure evaluates the Fresnel sine and cosine
 integrals for large u by expanding the asymptotic series given
 by

$$S(u) = \frac{1}{2} - \frac{\cos(x)}{\sqrt{2\pi x}} \left[1 - \frac{1 \cdot 3}{(2x)^2} + \frac{1 \cdot 3 \cdot 5 \cdot 7}{(2x)^4} - \dots \right] \\
- \frac{\sin(x)}{\sqrt{2\pi x}} \left[\frac{1}{2x} - \frac{1 \cdot 3 \cdot 5}{(2x)^3} + \frac{1 \cdot 3 \cdot 5 \cdot 7 \cdot 9}{(2x)^5} - \dots \right]$$

and

$$C(u) = \frac{1}{2} - \frac{\sin(x)}{\sqrt{2\pi x}} \left[1 - \frac{1 \cdot 3}{(2x)^2} + \frac{1 \cdot 3 \cdot 5 \cdot 7}{(2x)^4} - \dots \right] \\
- \frac{\cos(x)}{\sqrt{2\pi x}} \left[\frac{1}{2x} - \frac{1 \cdot 3 \cdot 5}{(2x)^3} + \frac{1 \cdot 3 \cdot 5 \cdot 7 \cdot 9}{(2x)^5} - \dots \right]$$

in which $x = \pi u^2/2$. Reference: PEARCEY, T. *Table of the Fresnel
 Integral to Six Decimal Places*. The Syndics of the Cambridge
 University Press, Melbourne, Australia (1956).;

```
begin  pi := 3.14159265; arg := pi * (u↑2)/2; temp := 1;
      argsq := 1/(4 * (arg↑2)); term := -3 * argsq;
      series := 1 + term; N := 3;
first:  if temp = series then go to second; temp := series;
      termi := term;
      term := -termi * (4 * N - 7) * (4 * N - 5) * (argsq);
      if abs(term) > abs(termi) then go to second;
      series := temp + term; N := N + 1; go to first;
second: series2 := 1/2 * arg; temp := 0; term := series2;
      N := 2;
loop:   if series2 = temp then go to exit; termi := term;
      term := -termi * argsq * (4 * N - 5) * (4 * N - 3);
      if abs(term) > abs(termi) then go to exit;
      temp := series2; series2 := temp + term;
      N := N + 1; go to loop;
exit:   if u < 0 then half := -1/2 else half := 1/2;
      frcos := half + (sin(arg) * series - cos(arg) * series2)/
      (pi * u);
      frsin := half - (cos(arg) * series2 + sin(arg) * series)/
      (pi * u)
end FRESNEL;
```

REMARK ON ALGORITHMS 88, 89 AND 90
 EVALUATION OF THE FRESNEL INTEGRALS
 [J. L. Cundiff, *Comm. ACM*, May 1962]
 MALCOLM D. GRAY
 The Boeing Co., Seattle, Wash.

While coding these algorithms in FORTRAN for the IBM 7094,
 modifications were required (both in the formulation and in the
 language) before execution with any degree of speed and accuracy
 could be obtained. In the process it was found that the reference,
Pearcy, contains an error in the formula for $C(u)$. This error is
 contained in Algorithm 88 in the formula

$$C(u) = \frac{1}{2} - \frac{\sin(x)}{\sqrt{2\pi x}} [] - \dots$$

The first minus sign above should be a plus sign.

After the necessary modifications were made, the three al-
 gorithms were found to be too large and uneconomical for our
 usage. A single algorithm, incorporating these three procedures,
 was written and is in current usage in a computer program which
 requires several thousand evaluations of each Fresnel integral.

ALGORITHM 89 EVALUATION OF THE FRESNEL SINE INTEGRAL

JOHN L. CUNDIFF

Engineering Experiment Station, Georgia Institute of
 Technology, Atlanta, Ga.

real procedure FRESNELSIN (u) Result: (frsin); **value** u ;

comment This algorithm computes the Fresnel sine integral
 defined by,

$$S(u) = \int_0^u \sin \pi t^2/2 dt,$$

by evaluating the series expansion

$$S(x) = \sqrt{\frac{2x}{\pi}} \left[\frac{x}{3} - \frac{x^3}{7 \cdot 3!} + \frac{x^5}{11 \cdot 5!} - \frac{x^7}{15 \cdot 7!} + \dots \right]$$

where $x = \pi u^2/2$. Reference: PEARCEY, T. *Table of the
 Fresnel Integral to Six Decimal Places*. The Syndics of the
 Cambridge University Press, Melbourne, Australia (1956).;

```
begin  Pi2 := 1.5707963; x := Pi2 * (u↑2); frsin := x/3;
      frsq := x↑2; N := 3; term := (-x * frsq)/6;
      frsini := frsin + term/7;
Loop:   if frsin = frsini then go to exit; frsin := frsini;
      term := -term * frsq/((2*N-1) * (2*N-2));
      frsini := frsin + term/(4*N-1); N := N + 1;
      go to Loop;
exit:   frsin := frsini * u
end FRESNELSIN;
```

SEE ALGORITHM 88

ALGORITHM 90 EVALUATION OF THE FRESNEL COSINE INTEGRAL

JOHN L. CUNDIFF

Engineering Experiment Station, Georgia Institute of Technology, Atlanta, Ga.

real procedure FRESNELCOS (u) result: (frcos); **value** (u);
comment This algorithm computes the Fresnel cosine integral defined by

$$C(u) = \int_0^u \cos \frac{\pi t^2}{2} dt,$$

by evaluating the series expansion

$$C(u) = \sqrt{\frac{2x}{\pi}} \left[1 - \frac{x^2}{5 \cdot 2!} + \frac{x^4}{9 \cdot 4!} - \frac{x^6}{13 \cdot 6!} + \dots \right],$$

where $x = \pi u^2/2$. Reference: PEARCEY, T., *Table of the Fresnel Integral to Six Decimal Places*. The Syndics of the Cambridge University Press, Melbourne, Australia (1956).

```
begin pi2 := 1.5707963; x := pi2 × (u ↑ 2); frcos := 1;
xsqr := x ↑ 2; N := 3; term := -xsqr/2;
frcos := 1 + (term/5);
loop: if frcos = frcos then go to exit; term := -term ×
xsqr/((2×N-2) × (2×N-3)); frcos := frcos; frcos :=
frcos + term/(4×N-3); N := N + 1; go to loop;
exit: frcos := u × frcos
end FRESNELCOS;
```

SEE ALGORITHM 88

ALGORITHM 91 CHEBYSHEV CURVE-FIT

ALBERT NEWHOUSE

University of Houston, Houston, Texas

procedure CHEBFIT(m, n, X, Y); **integer** m, n; **array** X, Y;
comment This procedure fits the tabular function $Y(X)$ (given as m points (X, Y)) by a polynomial $P = \sum_{i=0}^n A_i X^i$. This polynomial is the best polynomial approximation of $Y(X)$ in the Chebyshev sense. Reference: STIEFEL, E. *Numerical Methods of Tchebycheff Approximation*, U. of Wisc. Press (1959), 217-232;

```
begin array X[1:m], Y[1:m], T[1:m], A[0:n], AX[1:n+2],
AY[1:n+2], AH[1:n+2], BY[1:n+2], BH[1:n+2];
integer array IN[1:n+2]; real TMAX, H; integer i,
j, k, imax;
comment Initialize;
k := (m-1)/(n+1);
for 1 := 1 step 1 until n+1 do IN[i] := (i-1) × k + 1;
IN[n+2] := m;
START: comment Iteration begins;
for i := 1 step 1 until n+2 do
begin AX[i] := X[IN[i]];
AY[i] := Y[IN[i]];
AH[i] := (-1) ↑ (i-1)
end i;
DIFFERENCE: comment divided differences;
for i := 2 step 1 until n+2 do
begin
for j := i-1 step 1 until n+2 do
begin BY[j] := AY[j];
BH[j] := AH[j]
end j;
end i;
```

```
for j := i step 1 until n+2 do
begin AY[j] := (BY[j] - BY[j-1])/
(AX[j] - AX[j-1]);
AH[j] := (BH[j] - BH[j-1])/
(AX[j] - AX[j-1])
end j;
end i;
H := -AY[n+2]/AH[n+2];
POLY: comment polynomial coefficients;
for i := 0 step 1 until n do
begin A[i] := AY[i] + AH[i] × H;
BY[i] := 0
end i;
BY[1] := 1; TMAX := abs(H); imax := IN[1];
for i := 1 step 1 until n do
begin
for j := 0 step 1 until i-1 do
begin
BY[i+1-j] := BY[i+1-j] - BY[i-j] × X[IN[i]];
A[j] := A[j] + A[i] × BY[i+1-j]
end j;
end i;
ERROR: comment compute deviations;
for i := 1 step 1 until m do
begin T[i] := A[n];
for j := 0 step 1 until n do T[i] := T[i] X[i] + A[n-j];
T[i] := T[i] - Y[i];
if abs(T[i]) < TMAX then go to L1;
TMAX := abs(T[i]);
imax := i
end i;
L1: end i;
for i := 1 step 1 until n+2 do
begin
if imax < IN[i] then go to L2;
if imax = IN[i] then go to FIT end
end i;
L2: if T[imax] × T[IN[i]] < 0 then go to L3;
IN[i] := imax;
go to START;
L3: if IN[1] < imax then go to L4;
for i := 1 step 1 until n+1 do IN[n+3-i] := IN[n+2-i];
IN[i] := imax;
go to START;
L4: if IN[n+2] < imax then go to L5;
IN[i-2] := imax;
go to START;
L5: for i := 1 step 1 until n+1 do IN[i] := IN[i+1];
IN[n+2] := imax;
go to START;
FIT: end CHEBFIT
```

CERTIFICATION OF ALGORITHM 91

CHEBYSHEV CURVEFIT [A. Newhouse, *Comm. ACM*, May 1962]

ROBERT P. HALE

University of Adelaide, Adelaide, South Australia

The CHEBFIT algorithm was translated into FORTRAN and successfully run on an IBM 1620 when the following alterations were made:

(a) 2nd line after

comment Initialize;

should read

for i := 1 step 1 until n+1 do IN[i] := (i-1) × k + 1;

(b) 2nd and 3rd lines after

Poly: **comment** polynomial coefficients;

should read

begin A[i] := AY[i+1] + AH[i+1] × H; BY[i+1] := 0

(c) 3rd line after

ERROR: comment compute deviations;

should read

for $j := 1$ **step** 1 **until** n **do** $T[i] := T[i] \times X[i] + A[n-j]$;

(d) Immediately before statement *L2* insert $i := n + 2$; (as for list may be exhausted and i no longer defined).

(e) 2nd line after statement *L3* should read $IN[1] := imax$;

(f) 1st line after statement *L4* should read $IN[i-1] := imax$;

REMARKS ON ALGORITHM 91

CHEBYSHEV CURVE FIT [A. Newhouse, *Comm.*

ACM 5 (May 1962), 281; 6 (April 1963), 167]

PETER NAUR (Recd. 27 Sept. 1963)

Regnecentralen, Copenhagen, Denmark

In addition to the corrections noted by R. P. Hale [op. cit., April 1963] the following are necessary:

1. The arrays X , Y , and A cannot be declared to be local within the procedure body.

2. The identifier A must be included as a formal parameter.

3. It should be noted that the $X[i]$ must form a monotonic sequence.

4. **comment** cannot follow the colon following a label. This occurs in four places.

5. The **end** following **go to** *FIT* must be removed.

In addition, a large number of details can be made more concise and unnecessary operations can be eliminated. Also, it seems desirable to produce the maximum deviation as a result.

ALGORITHM 92

SIMULTANEOUS SYSTEM OF EQUATIONS AND MATRIX INVERSION ROUTINE

DEREK JOHANN ROEK

Applied Physics Laboratory of Johns Hopkins University,
Silver Spring, Maryland

procedure SIMULTANEOUS ($U, W, C, X, B, n, kount, eps,$
 $absf$) ;

array U, W, C, X, B ; **integer** $n, kount$;
real eps ; **real** $procedure$ $absf$;

comment This procedure solves the problem $Ux := b$ for the vector x . It assumes the problem written in the form $x'U' := b'$, where $'$ denotes transpose. The procedure is completed in n cycles and may be iterated $kount$ times ($kount \leq 6$). The transpose of U is in $U[,]$ and the row vector b' is in B . The integer n is the dimension of U , and the solution row vector x' is in X . The matrix C is a check of accuracy. It should have b' in its first row, the first element b_1 of b' along its main diagonal, and zeros elsewhere. The real number eps checks to see how close the actual result is to this theoretical one. Also if we let $b' := (1, 0, \dots, 0)$, then this procedure finds the inverse $W[,]$ of U . The function $absf$ finds the absolute value of its argument. The procedure chooses the column vectors of U as the row vectors of W in the 0th cycle of the first iteration. For all subsequent iterations, the row vectors of W , computed at the n th cycle of the last iteration, are the row vectors of W in the 0th cycle ;

begin **integer** i, j, k, p ; **real** $bh, b1, Z$;

for $j := 1$ **step** 1 **until** n **do**

for $i := 1$ **step** 1 **until** n **do** $W[j, i] := U[i, j]$;

S1: **for** $j := 1$ **step** 1 **until** n **do**

for $i := 1$ **step** 1 **until** n **do** $C[i, j] := 0$;

for $j := 1$ **step** 1 **until** n **do**

begin **for** $k := 1$ **step** 1 **until** n **do**

begin $C[j, j] := C[j, j] + W[j, k] \times U[k, j]$ **end**;

if $j = 1$ **then** $Z := B[j]/C[j, j]$ **else** $Z := 1/C[j, j]$;

for $k := 1$ **step** 1 **until** n **do**

begin $X[k] := Z \times W[j, k]$;

$W[j, k] := X[k]$

end k ;

for $k := 1$ **step** 1 **until** n **do**

begin **if** $k = j$ **then** **go to** *S2* **else**

for $p := 1$ **step** 1 **until** n **do**

$C[k, j] := C[k, j] + U[p, j] \times W[k, p]$;

if $j = 1$ **then** $bh := B[j]$ **else** $bh := 1$;

if $k = 1$ **then** $b1 := B[j]$ **else** $b1 := 0$;

for $p := 1$ **step** 1 **until** n **do**

begin $X[p] := bh \times W[k, p] + (b1 - C[k, j]) \times$

$W[j, p]$;

$W[k, p] := X[p]$

end p ;

S2: **if** $k = j \wedge j = n$ **then** **go to** *S3*

end k ;

end j ;

S3: **for** $j := 1$ **step** 1 **until** n **do**

if $absf(absf(C[j, j]) - absf(B[1])) > eps$ **then** **go to** *S4*;

go to *S6*;

S4: **if** $kount > 0$ **then** **go to** *S5* **else** **go to** *S6*;

S5: $kount := kount - 1$;

go to *S1*;

S6: **for** $j := 1$ **step** 1 **until** n **do**

$X[j] := W[1, j]$;

S7: **end** SIMULTANEOUS

ALGORITHM 93

GENERAL ORDER ARITHMETIC

MILLARD H. PERSTEIN

Control Data Corp., Palo Alto, Calif.

procedure arithmetic (a, b, c, op);

integer a, b, c, op ;

comment This procedure will perform different order arithmetic operations with b and c , putting the result in a . The order of the operation is given by op . For $op = 1$ addition is performed. For $op = 2$ multiplication, repeated addition, is done. Beyond these the operations are non-commutative. For $op = 3$ exponentiation, repeated multiplication, is done, raising b to the power c . Beyond these the question of grouping is important. The innermost implied parentheses are at the right. The hyper-exponent is always c . For $op = 4$ tetration, repeated exponentiation, is done. For $op = 5, 6, 7$, etc., the procedure performs pentation, hexation, heptation, etc., respectively.

The routine was originally programmed in FORTRAN for the Control Data 160 desk-size computer. The original program was limited to tetration because subroutine recursiveness in Control Data 160 FORTRAN has been held down to four levels in the interests of economy.

The input parameter, b, c , and op , must be positive integers, not zero;

begin **own** **integer** $d, e, f, drop$;

if $op = 1$ **then**

begin $a := b + c$; **go to** 1

end **if** $op = 2$ **then** $d := 0$;

```

else d := 1; e := c; drop := op - 1;
for f := 1 step 1 until e do
begin arithmetic (a, b, d, drop);
  d := a
end;
1: end arithmetic

```

CERTIFICATION OF ALGORITHM 93 GENERAL ORDER ARITHMETIC [Millard H. Per- stein, *Comm. ACM* (June 1962)]

RICHARD GEORGE
Particle Accelerator Div. Argonne National Laboratory,
Argonne, Ill.

Algorithm 93 was programmed for the IBM 1620, using "FORTRAN-recursion" (i.e., generous use of the copy rule). The program ran without any modifications and was tested through tetration. Further levels were available, but were too time-consuming to reach.

ALGORITHM 94 COMBINATION

JEROME KURTZBERG
Burroughs Corp., Burroughs Laboratories, Paoli, Pa.

```

procedure COMBINATION (J, N, K); value N, K; integer
array J; integer N, K;
comment This procedure generates the next combination of N
integers taken K at a time upon being given N, K and the pre-
vious combination. The K integers in the vector J(1) ... J(K)
range in value from 0 to N - 1, and are always monotonically
strictly increasing with respect to themselves in input and
output format. If the vector J is set equal to zero, the first
combination produced is N - K, ..., N - 1. That initial combina-
tion is also produced after 0, 1, ..., N - 1, the last value in that
cycle;
begin integer B, L;
  B := 1;
mainbody: if J(B) ≥ B then begin A := J(B) - B - 1;
  for L := 1 step 1 until B do J(L) := L + A;
  go to exit end;
  if B = K then go to initiate;
  B := B + 1; go to mainbody;
initiate: for B := 1 step 1 until K do J(B) := N - K - 1 + B
exit: end COMBINATION

```

CERTIFICATION OF ALGORITHM 94 COMBINATION [J. Kurtzberg, *Comm. ACM*, June, 1962]

R. E. GRENCHE*
Reactor Eng. Div., Argonne National Laboratory,
Argonne, Ill.

- * Work supported by U. S. Atomic Energy Commission
Four changes were required in the algorithm.
1. The last sentence in the comment should read: That initial combination is also produced after 0, 1, ..., K - 1, the last value in that cycle;
 2. The integer A was declared;
 3. Parentheses were replaced by brackets in the subscript expressions;

4. A semicolon was inserted at the end of the initiate statement.
After the above changes were made the body of Algorithm 94 was tested on an LGP-30 computer using the Dartmouth College ALGOL-30 translator. The body tested satisfactorily and the time required to generate one J when K = 5 and N = 15 was 30 seconds.
Various tests should be included if this algorithm is to be used as a procedure. These tests might include a statement to check if K > N and if the initial value of J is correct. These two possibilities were investigated and it was found that improper J's are generated.

CERTIFICATION OF ALGORITHM 94 COMBINATION [J. Kurtzberg, *Comm. ACM*, June 1962] RONALD W. MAY University of Alberta, Calgary, Alberta, Canada

Algorithm 94 was translated into FORTRAN for the IBM 1620 and run successfully with no corrections. The variable A, however, has not been declared.

ALGORITHM 95 GENERATION OF PARTITIONS IN PART-COUNT FORM

FRANK STOCKMAL
System Development Corp., Santa Monica, Calif.

```

procedure partgen(c, N, K, G); integer N, K; integer array c;
Boolean G;
comment This procedure operates on a given partition of the
positive integer N into parts ≤ K, to produce a consequent
partition if one exists. Each partition is represented by the
integers c[1] thru c[K], where c[j] is the number of parts of the
partition equal to the integer j. If entry is made with G = false,
procedure ignores the input array c, sets G = true, and pro-
duces the first partition of N ones. Upon each successive entry
with G = true, a consequent partition is stored in c[1] thru c[K].
For N = KX, the final partition is c[K] = X. For N = KX + r,
1 ≤ r ≤ K - 1, final partition is c[K] = X, c[r] = 1. When entry
is made with array c = final partition, c is left unchanged and G
is reset to false;
begin integer a, i, j;
  if ¬ G then go to first;
  j := 2;
  a := C[1];
test: if a < j then go to B;
  c[j] := 1 + c[j];
  c[1] := a - j;
zero: for i := 2 step 1 until j - 1
  do c[i] := 0;
  go to EXIT;
B: if j = K then go to last;
  a := a + j × c[j];
  j := j + 1;
  go to test;
first: G := true;
  c[1] := N;
  j := K + 1;
  go to zero;
last: G := false;
EXIT: end partgen

```

ALGORITHM 96

ANCESTOR

ROBERT W. FLOYD

Armour Research Foundation, Chicago, Ill

```

procedure ancestor (m, n); value n; integer n; Boolean
array m;
comment Initially  $m[i, j]$  is true if individual  $i$  is a parent of
individual  $j$ . At completion,  $m[i, j]$  is true if individual  $i$  is an
ancestor of individual  $j$ . That is, at completion  $m[i, j]$  is true
if there are  $k, l$ , etc. such that initially  $m[i, k], m[k, l], \dots, m[p, j]$ 
are all true. Reference: WARSHALL, S. A theorem on Boolean
matrices, J. ACM 9(1962), 11-12;
begin
integer i, j, k;
for i := 1 step 1 until n do
for j := 1 step 1 until n do
if m[j, i] then
for k := 1 step 1 until n do
if m[i, k] then
m[j, k] := true
end ancestor

```

CERTIFICATION OF ALGORITHM 96

ANCESTOR [Robert W. Floyd, *Comm. ACM*, June, 1962]

HENRY C. THACHER, JR.*

Argonne National Laboratory, Argonne, Ill.

* Work supported by the U.S. Atomic Energy Commission

The body of this procedure was tested on the LGP-30 using the Dartmouth translator. After inclosing conditional statements in **begin end** brackets (apparently necessary for this translator), the procedure operated satisfactorily for the following matrices:

n = 5, Time: 8'15"

FTTFF	FTTTT
FFFFT	FFFFT
FFFTF	FFFTT
FFFFT	FFFFT
FFFFF	FFFFF

n = 6, Time: 13'15"

FTTFFF	FTTTTT
FFFTFF	FFFTFT
FFFFTF	FFFTFT
FFFFFT	FFFFFT
FFFFF	FFFFF

n = 9, Time 31'2"

FTTFFFFFFF	FTTTTTTTT
FFFFTFFF	FFFFTTTTF
FFFTTFFF	FFFTTTTTT
FFFFFFFFT	FFFFFFTTT
FFFFFTTF	FFFFFTTTF
FFFFFFFTF	FFFFFTTTF
FFFFFFFTF	FFFFFTTTF
FFFFFFFTF	FFFFFTTTF
FFFFFFFTF	FFFFFTTTF
FFFFFFFTF	FFFFFTTTF

The correctness of these results was confirmed by inspection of the network diagrams.

ALGORITHM 97

SHORTEST PATH

ROBERT W. FLOYD

Armour Research Foundation, Chicago, Ill.

```

procedure shortest path (m, n); value n; integer n; array m;
comment Initially  $m[i, j]$  is the length of a direct link from
point  $i$  of a network to point  $j$ . If no direct link exists,  $m[i, j]$  is
initially  $\infty$ . At completion,  $m[i, j]$  is the length of the shortest
path from  $i$  to  $j$ . If none exists,  $m[i, j]$  is  $\infty$ . Reference: WAR-
SHALL, S. A theorem on Boolean matrices, J. ACM 9(1962), 11-12;
begin
integer i, j, k; real inf, s; inf :=  $\infty$ ;
for i := 1 step 1 until n do
for j := 1 step 1 until n do
if m[j, i] < inf then
for k := 1 step 1 until n do
if m[i, k] < inf then
begin s := m[j, i] + m[i, k];
if s < m[j, k] then m[j, k] := s
end
end shortest path

```

ALGORITHM 98

EVALUATION OF DEFINITE COMPLEX LINE INTEGRALS

JOHN L. PFALTZ

Syracuse University Computing Center, Syracuse, N. Y.

```

procedure COMPLINEINTGRL(A, B, N, RSSUM);
value A, B, N; real A, B, N; array RSSUM;
comment COMPLINEINTGRL approximates the complex line
integral by evaluating the partial Riemann-Stieltjes sum
 $\sum_{i=1}^N f(z_k)(z_i - z_{i-1})$  where  $a \leq t \leq b$  and  $z_k \in (z_{k-1}, z_k)$ . The
programmer must provide 1) the procedures GAMMA(T, Z) to
calculate  $z(t)$  on  $\Gamma$ , and FUNCT(Z, F) to calculate function
values, and 2) the end points A and B of the parametric interval
and N the number of subintervals into which  $[a, b]$  is to be
partitioned;
begin integer I; real T, DELT; real array ZT, ZTL, DELZ,
ZK, PART[1:2]; RSSUM[1] := 0.0; RSSUM[2] := 0.0;
DELT := (B - A)/N; T := A;
line: GAMMA(T, ZT);
if T = B then go to next;
for I := 1 step 1 until 2 do
begin
DELZ[I] := ZT[I] - ZTL[I]; end;
for I := 1 step 1 until 2 do
begin
ZK[I] := ZTL[I] + DELZ[I]/2.0; end;
FUNCT(ZK, FZ);
PART[1] := FZ[1]  $\times$  DELZ[1] - FZ[2]  $\times$  DELZ[2];
PART[2] := FZ[1]  $\times$  DELZ[2] + FZ[2]  $\times$  DELZ[1];
for I := 1 step 1 until 2 do
begin
RSSUM[I] := RSSUM[I] + PART[I]; end;
if T < B - (0.25  $\times$  DELT) then go to next else go to
exit;
next: for I := 1 step 1 until 2 do
begin
ZTL[I] := ZT[I]; end;
T := T + DELT;
go to line;
exit: end COMPLINEINTGRL.

```


ALGORITHM 99

EVALUATION OF JACOBI SYMBOL

STEPHEN J. GARLAND AND ANTHONY W. KNAPP
Dartmouth College, Hanover, N. H.

```

procedure Jacobi (n,m,r); value n,m;
integer n, m, r;
comment Jacobi computes the value of the Jacobi symbol (n/m),
where m is odd, by the law of quadratic reciprocity. The param-
eter r is assigned one of the values -1, 0, or 1 if m is odd. If m
is even, the symbol is undefined and r is assigned the value 2.
For odd m the routine provides a test of whether m and n are
relatively prime. The value of r is 0 if and only if m and n have
a nontrivial common factor. In the special case where m is prime,
r = -1 if and only if n is a quadratic nonresidue of m;
begin
  integer s;
  Boolean p, q;
  Boolean procedure parity (x); value x; integer x;
    comment The value of the function parity is true if x is
    odd, false if x is even;
    begin
      parity := x ÷ 2 × 2 ≠ x
    end parity;
  if ¬ parity (m) then begin r := 2; go to exit end;
  p := true;
  loop: n := n - n ÷ m × m;
    q := false;
    if n ≤ 1 then go to done;
  even: if ¬ parity (n) then
    begin
      q := ¬ q;
      n := n ÷ 2;
      go to even
    end n now odd;
  if q then if parity ((m↑2 - 1) ÷ 8) then p := ¬ p;
  if n = 1 then go to done;
  if parity ((m-1) × (n-1) ÷ 4) then p := ¬ p;
  s := m; m := n; n := s; go to loop;
  done: r := if n = 0 then 0 else if p then 1 else -1;
  exit: end Jacobi

```

REMARK ON ALGORITHM 99

EVALUATION OF JACOBI SYMBOL [S. J. Gar-
land and A. W. Knapp, *Comm. ACM* 6, June 1962]

RONALD W. MAY

University of Alberta, Calgary, Alberta, Canada

One syntactical error was found in this procedure. It occurs
in the second if statement following the label even. The state-
ment

```

if q then if parity ((m↑2-1) ÷ 8) then
  p := ¬ p;

```

might be changed as follows.

```

if q then go to CHECK;
next 1: if n = 1 then go to done;
CHECK: if parity ((m↑2 - 1) ÷ 8) then
  p := ¬ p;
  go to next 1;

```

The two statements beginning with CHECK could be inserted
before the label done and after the statement go to loop;

ALGORITHM 100

ADD ITEM TO CHAIN-LINKED LIST

PHILIP J. KIVIAT

United States Steel Corp., Appl. Research Lab., Monroeville,
Penn.

```

procedure inlist (t,info,m,list,n,first,flag,addr,listfull);
integer n,m,first,flag,t; integer array info,list,addr;
comment inlist adds the information pair {t,info} to the chain-
link structured matrix list (i,j), where t is an order key ≥ 0, and
info(k) an information vector associated with t. info(k) has di-
mension m, list(i,j) has dimensions (n × (m+3)). flag denotes
the head and tail of list(i,j), and first contains the address of the
first (lowest order) entry in list(i,j). addr(k) is a vector con-
taining the addresses of available (empty) rows in list(i,j).
Initialization: list(i,m+2) = flag, for some i ≤ n. If list(i,j) is
filled exit is to listfull;
begin integer i, j, link1, link2;
0: if addr [1] = 0; then go to listfull; i := 1;
1: if list [i,1] ≤ t
  then begin if list [i,2] ≠ 0 then begin link1 := m+2;
    link2 := m+3; go to 2 end; else begin if
    list [i,m+2] = flag then begin i := flag;
    link1 := m+3; link2 := m+2; go to 3 end;
    else begin i := i+1; go to 1 end end end;
    else begin link1 := m+3; link2 := m+2 end;
2: if list [i,link2] ≠ flag
  then begin k := i; i := list [i,link2];
    if (link2 = m+2 ∧ list [i,1] ≤ t) ∨
    (link2 ≠ m+2 ∧ list [i,1] > t) then go to 4;
    else go to 1 end;
    else begin list [i,link2] := addr [1] end;
3: j := addr [1]; list [j,link1] := i;
  list [j,link2] := flag; if link2 = m+2 then
  first := addr [1]; go to 5;
4: j := addr [1]; list [j,link1] := list [i,link1];
  list [i,link1] := list [k,link2] := addr [1];
  list [j,link2] := i;
5: list [j,1] := t; for i := 1 step 1 until m do
  list [j,i+1] := info [i]; for i := 1 step 1 until n-1 do
  addr [i] := addr [i+1]; addr [n] := 0
end inlist

```

ALGORITHM 101

REMOVE ITEM FROM CHAIN-LINKED LIST

PHILIP J. KIVIAT

United States Steel Corp., Appl. Res. Lab., Monroeville,
Penn.

```

procedure outlist (vector,m,list,n,first,flag,addr);
integer n,m,first,flag; integer array vector,list,addr;
comment outlist removes the first entry (information pair with
lowest order key) from list(i,j) and puts it in vector(k);
begin integer i;
for i := 1 step 1 until m+1 do vector[i] := list [first,i];
for i := n-1 step -1 until 1 do addr [i+1] := addr [i];
  addr [1] := first;
if list [first,m+3] = flag then
  begin list [1,m+2] := flag; first := 1;
    for i := 1 step 1 until n do addr [i] := i end;
  else begin first := list [first,m+3];
    list [first,m+2] := flag end;
  for i := 1 step 1 until m+3 do list [addr [1], i] := 0
end outlist

```

ALGORITHM 102
PERMUTATION IN LEXICOGRAPHICAL ORDER
 G. F. SCHRACK AND M. SHIMRAT
 University of Alberta, Calgary, Alberta, Canada

```

procedure PERMULEX(n,p);
integer n; integer array p;
comment Successive calls of the procedure will generate all
  permutations p of 1,2,3,...,n in lexicographical order. Before the
  first call, the non-local Boolean variable 'flag' must be set to
  true. If after an execution of PERMULEX 'flag' is false,
  additional calls will generate further permutations—if true, all
  permutations have been obtained;
begin integer array q[1:n]; integer i, k, t; Boolean flag2;
if flag then
  begin for i := 1 step 1 until n do
    p[i] := i; flag2 := true; flag := false;
  go to EXIT
  end initialize;
if flag2 then
  begin t := p[n]; p[n] := p[n-1]; p[n-1] := t;
  flag2 := false; go to EXIT
  end bypass;
  flag2 := true; for i := n-2 step -1 until 1 do
    if p[i] < p[i+1] then go to A;
    flag := true; go to EXIT;
  A: for k := 1 step 1 until n do q[k] := 0;
    for k := i step 1 until n do q[p[k]] := p[k];
    for k := p[i] + 1 step 1 until n do
      if q[k] ≠ 0 then go to B;
  B: p[i] := k; q[k] := 0;
    for k := 1 step 1 until n do
      if q[k] ≠ 0 then begin i := i + 1; p[i] := q[k] end
      else if i ≥ n then go to EXIT;
  EXIT:
end PERMULEX
  
```

ALGORITHM 103
SIMPSON'S RULE INTEGRATOR
 GUY F. KUNCIR

UNIVAC Division, Sperry Rand Corp., San Diego, Calif.

```

procedure SIMPSON(a, b, f, I, i, eps, N);
  value a, b, eps, N; integer N;
  real a, b, I, i, eps; real procedure f;
comment This procedure integrates the function f(x) using a
  modified Simpson's Rule quadrature formula. The quadrature is
  performed over j subintervals of [a,b] forming the total area I.
  Convergence in each subinterval of length (b-a)/2^n is indicated
  when the relative difference between successive three-point and
  five-point area approximations
    A3,j = (b-a)(g0 + 4g2 + g4)/(3·2n+1)
    A5,j = (b-a)(g0 + 4g1 + 2g2 + 4g3 + g4)/(3·2n+2)
  is less than or equal to an appropriate portion of the over-all
  tolerance eps (i.e., |(A5,j - A3,j)/A5,j| ≤ eps/2^n with n ≤ N).
  SIMPSON will reduce the size of each interval until this condi-
  tion is satisfied.
  
```

Complete integration over [a,b] is indicated by i = b. A value a ≤ i < b indicates that the integration was terminated, leaving I the true area under f in [a,i]. Further integration over [i,b] will necessitate either the assignment of a larger N, a larger eps, or an integral substitution reducing the slope of the integrand in that interval. It is recommended that this procedure be used between known integrand maxima and minima.

```

begin integer m, n; real d, h; array g[0:4], A[0:2], S[1:N, 1:3];
  I := i := m := n := 0;
  g[0] := f(a);
  g[2] := f((a + b)/2);
  g[4] := f(b);
  A[0] := (b - a) × (g[0] + 4 × g[2] + g[4])/2;
  AA: d := 2/n; h := (b - a)/d;
  g[1] := f(a + h × (4 × m + 1));
  g[3] := f(a + h × (4 × m + 3));
  A[1] := h × (g[0] + 4 × g[1] + g[2]);
  A[2] := h × (g[2] + 4 × g[3] + g[4]);
  if abs(((A[1] + A[2]) - A[0])/(A[1] + A[2])) > eps/d
  then begin m := 2 × m; n := n + 1;
    if n > N then go to CC;
    A[0] := A[1]; S[n,1] := A[2];
    S[n,2] := g[3]; S[n,3] := g[4];
    g[4] := g[2]; g[2] := g[1]; go to AA
  end
  else begin I := I + (A[1] + A[2])/3;
    m := m + 1; i := a + m × (b - a)/d;
  BB: if m = 2 × (m ÷ 2) then
    begin m := m ÷ 2; n := n - 1; go to BB end
    if (m ≠ 1) ∨ (n ≠ 0) then
      begin A[0] := S[n,1]; g[0] := g[4];
        g[2] := S[n,2]; g[4] := S[n,3]; go to AA end
    end
  CC: end SIMPSON
  
```

ALGORITHM 104
REDUCTION TO JACOBI

H. RUTISHAUSER

Eidg. Technische Hochschule, Zurich, Switzerland

```

procedure m2l(n, a, b, c, inform); value n;
  integer n; array a, b, c; procedure inform;
comment m2l transforms symmetric bandmatrix
  
```

represented by the arrays a, b, c by orthogonal transformation to Jacobi form which is represented by the arrays a, b. The method is described in H. RUTISHAUSER, "On Jacobi rotation patterns," to appear in Proc. Symposium in Experimental Arithmetic, Chicago, Apr. 12-14, 1962, Sect. 5. Note that declarations must be given for the arrays a, b, c with subscripts ranging from 1 to n. Also procedure inform must be declared. It may serve to use the Jacobi rotations occurring inside m2l also for other purposes;

```

begin
  real p, g, d, s;
  integer k, j;
  b[n] := c[n] := c[n-1] := 0;
  for k := 2 step 1 until n-1 do
    begin
      for j := k step 2 until n-1 do
        begin
          if k=j then
  
```

```

begin
  p := sqrt(b[k-1]^2 + c[k-1]^2);
  if p=0 then go to ex;
  d := b[k-1]/p;
  s := -c[k-1]/p;
  b[k-1] := p;
  c[k-1] := 0
end k=j
else
begin
  p := sqrt(c[j-2]^2 + g^2);
  if p = 0 then go to ex;
  d := c[j-2]/p;
  s := -g/p;
  c[j-2] := p;
  p := d×b[j-1]-s×c[j-1];
  c[j-1] := s×b[j-1]+d×c[j-1];
  b[j-1] := p
end j≠k;
common: g := 2×b[j]×d×s;
p := a[j]×d×d-g+a[j+1]×s×s;
b[j] := (a[j]-a[j+1])×d×s+b[j]×(d×d-s×s);
a[j+1] := a[j]×s×s+g+a[j+1]×d×d;
a[j] := p;
p := d×c[j]-s×b[j+1];
b[j+1] := s×c[j]+d×b[j+1];
c[j] := p;
g := -s×c[j+1];
c[j+1] := d×c[j+1];
inform (n, j, d, s);
comment: The Jacobi rotation which has been performed
in this turn of the j-loop is  $A := U^T A U$  with

$$U = \begin{pmatrix} 1 & & & & \\ & 1 & & & \\ & & d & s & \\ & & -s & d & \\ 0 & & & & 1 \end{pmatrix},$$

where the d's and s's are located at the crosspoints of
rows and columns j and j+1;
end j;
ex: end k
end m21

```

ALGORITHM 105

NEWTON MAEHLI

F. L. BAUER AND J. STOER

Johannes Gutenberg-Universität, Mainz, Germany

procedure Newton Maehly (a, n, z, eps);

value n, eps;

array a, z;

integer n;

real eps;

comment The procedure determines all zeros $z[1:n]$ of the polynomial $p(x) := a[0] \times x^n + \dots + a[n]$ of order n, if $p(x)$ has only real zeros which have to be all different. The zeros $z[i]$ are ordered according to their magnitude: $z[1] > z[2] > \dots > z[n]$. The approximations for each zero will be improved by iteration as long as $\text{abs}(x_1 - x_0) > \text{eps} \times \text{abs}(x_1)$ holds for two successive approximations x_0 and x_1 ;

```

begin real aa, pp, qq, x0, x1;
integer i, m, s;
array b, p, q[0:n-1];
procedure Horner(p, q, n, x, pp, qq);
value n, x;
array p, q;
real pp, x, qq;
integer n;
begin real s, s1;
integer i;
s := s1 := 0;
for i := 0 step 1 until n-1 do
begin s := s×x+p[i]; s1 := s1×x+q[i]; end;
pp := s×x+p[n]; qq := s1;
end;
p[0] := aa := a[0]; x0 := pp := 0; s := sign(a[0]);
for i := 1 step 1 until n do
if s × a[i] < 0 then
begin if pp=0 then pp := i;
if x0 < abs(a[i]) then x0 := abs(a[i]);
end;
x0 := if pp=0 then 0 else 1+exp(ln(abs(x0/aa))/pp);
comment x0 is a first approximation for the largest zero which
may be printed out at this point of the program;
for i := 0 step 1 until n-1 do b[i] := (n-1)×a[i];
for m := 1 step 1 until n do
begin
iteration:
Horner (a, b, n, x0, pp, qq); x1 := x0 - pp/qq;
if abs(x1-x0) > eps×abs(x1) then
begin x0 := x1;
comment x0 is the last approximation for the zero
being improved, which may be printed out at this
point;
go to iteration;
end;
z[m] := x1;
comment z[m] := x1 is the mth zero of the polynomial;
pp := b[0] := b[0] - aa; q[0] := pp;
if m < n then
begin for i := 1 step 1 until n-1 do
begin pp := p[i] := x1×p[i-1]+a(i);
pp := b[i] := b(i)-pp;
q[i] := x1×q[i-1]+pp;
end;
Horner (p, q, n-1, x1, pp, qq);
x0 := x1 - pp/qq;
comment x0 is a first approximation for the
next zero;
end
end
end Newton Maehly;

```

CERTIFICATION OF ALGORITHM 105

NEWTON MAEHLI [F. L. Bauer and J. Stoer, COMM.

ACM, July 1962]

JOANNE KONDO

Burroughs Corp., Pasadena, Calif.

Algorithm 105 was successfully run on Burroughs 220 computer after the following correction had been made:

for i := 0 step 1 until n-1 do b[i] := (n-1) × a[i]
changed to

for i := 0 step 1 until n-1 do b[i] := (n-i) × a[i].

The following polynomials were tested for real roots using this algorithm:

polynomial	epsilon	accuracy
(1) $x^3 - 2x^2 - 5x + 6$	0.0000001	10^{-8}
(2) $x^5 - 15x^4 + 85x^3 - 225x^2 + 274x - 120$	0.000001	10^{-5}

ALGORITHM 106

COMPLEX NUMBER TO A REAL POWER

MARGARET L. JOHNSON AND WARD SANGREN

Computer Applications, Inc., San Diego, California

```

procedure POWC (x, y, w, A, B); value x, y, w;
  real x, y, w, A, B;
comment This procedure takes a complex number  $(x+iy)$  to
  a real power  $w$ . The result is  $A+iB=(x+iy)^w$ . This procedure
  must be used with caution because although it is formally cor-
  rect, it may not give the desired results. For example, if  $w$  is a
  reciprocal integer it does not follow that the desired power
  (a root) will be calculated;
begin real THETA, PHI, R;
  if  $x > 0$  then begin THETA := 0.0; go to SOL 1 end;
  if  $x < 0 \wedge y \geq 0$  then begin THETA := 3.1415927;
    go to SOL 1 end;
  if  $x < 0 \wedge y < 0$  then begin THETA := 3.1415927;
    go to SOL 1 end;
  if  $x = 0 \wedge y = 0$  then begin A := B := 0.0; go to RETURN end;
  if  $x = 0 \wedge y < 0$  then begin PHI := 1.5707963; go to SOL 2 end;
  if  $x = 0 \wedge y > 0$  then begin PHI := -1.5707963;
    go to SOL 2 end;
  SOL 1: PHI := arctan (y/x)+THETA;
  SOL 2: R := sqrt (x2+y2);
    R := exp (w*ln(R));
    A := R*cos (w*PHI);
    B := R*sin (w*PHI);
  RETURN: end POWC
  
```

REMARK ON ALGORITHM 106

COMPLEX NUMBER TO A REAL POWER [Mar-
garet L. Johnson and Ward Sangren, *Comm. ACM*
5, Jul. 1962]

GRANT W. ERWIN, JR.

The Boeing Co., Renton, Wash.

The comment "if w is a reciprocal integer it does not follow that the desired power (a root) will be calculated" might better read "if w is the reciprocal of an integer N , the procedure will calculate an n th root, but possibly not the particular n th root desired. E.g. $w = \frac{1}{3}$, $x = -1$, $y = 0$ yields $A = \frac{1}{2}$, $B = \frac{1}{2}\sqrt{3}$ rather than the simpler $A = -1$, $B = 0$."

The comment should be made that it is assumed that the arctan function yields a result between $-\pi/2$ and $\pi/2$.

The following four corrections should be made:

- (1) **if** $x < 0 \wedge y < 0$ **then** **begin** THETA := 3.1415927;
should read:
... THETA := -3.1415927;
- (2) **go to** RETURN **end**;
should read:
go to RETURN **end**;
- (3) **if** $x = 0 \wedge y < 0$...
should read:
if $x = 0 \wedge y > 0$...
- (4) **if** $x = 0 \wedge y > 0$
should read:
if $x = 0 \wedge y < 0$...

ALGORITHM 107

GAUSS'S METHOD

JAY W. COUNTS

University of Missouri, Columbia, Mo.

```

procedure gauss (u, a, y);
  real array a, y; real temp; integer u;
comment This procedure is for solving a system of
  linear equations by successive elimination of the un-
  knowns. The augmented matrix is a and u the number of
  unknowns. The solution vector is y. If the system hasn't
  any solution or many solutions, this is indicated by go
  to stop;
begin
  integer i, j, k, m, n;
  n := 0;
  ck0: n := n+1;
    for k := n step 1 until u do if  $a[k, n] \neq 0$  then go to ck1;
    go to stop;
  ck1: if k=n then go to ck2;
    for m := n step 1 until u+1 do
      begin
        temp := a[n, m]; a[n, m] := a[k, m]; a[k, m] := temp;
      end;
  ck2: for j := u+1 step -1 until n do a[n, j] := a[n, j]/a[n, n];
    for i := k+1 step 1 until u do
      for j := n+1 step 1 until u+1 do
        a[i, j] := a[i, j] - a[i, n]*a[n, j];
      if n≠u then go to ck0;
    for i := u step -1 until 1 do
      begin
        y[i] := a[i, u+1]/a[i, i];
        for k := i-1 step -1 until 1 do
          a[k, u+1] := a[k, u+1] - a[k, i]*y[i];
      end end;
  end end;
  
```

REMARK ON ALGORITHM 107

GAUSS'S METHOD [J. W. Counts, *Comm. ACM*,
July 1962]

P. NAUR

Regnecentralen, Copenhagen, Denmark

Algorithm 107 cannot be recommended since it does not search for pivot and therefore will yield poor accuracy (cf. Remarks on Algorithm 42 above).

ALGORITHM 108

DEFINITE EXPONENTIAL INTEGRALS A

YURI A. KRUGLYAK

Kharkov State University, Kharkov, U.S.S.R., AND

DONALD R. WHITMAN

Case Institute of Technology, Cleveland, Ohio

```

real procedure As (n, b); value n, b; integer n; real b;
comment: This procedure computes a value of integral
   $A_{n-1}(1, b) = \int_1^{\infty} x^{n-1} \exp(-bx) dx$  for any given positive integer,  $n$ ,
  and any positive real parameter,  $b$ , by the recursion formula
   $A_n(1, b) = A_0(1, b) + (n/b)A_{n-1}(1, b)$  with  $A_0(1, b) = \exp(-b)/b$ ;
begin integer m; real db; real array a[1:n];
  a[1] := exp (-b)/b;
  if n=1 then go to exit;
  
```

```

comment integral  $a[1] = A_0(1, b)$  was evaluated;
db := 1/b; for m := 2 step 1 until n do a[m] :=
a[1] + db * (m-1) * a[m-1];
comment integral  $a[n] = A_{n-1}(1, b)$  was evaluated;
As := a[n] end As;

```

CERTIFICATION OF ALGORITHM 108

DEFINITE EXPONENTIAL INTEGRALS A [Yuri A. Kruglyak and Donald R. Whitman, *Comm. ACM* 5 (July 1962)]

YURI A. KRUGLYAK

Kharkov State University, Kharkov, U.S.S.R. and

DONALD R. WHITMAN

Case Institute of Technology, Cleveland, Ohio

Integrals $A_n(1, b) = \int_1^\infty x^n \exp(-bx) dx$ occur in physical problems involving spheroidal coordinates, particularly in quantum chemistry calculations. This algorithm was programmed for the Burrough's 220 computer using Burrough's Algebraic Compiler. The program was used to compute tables of $A_n(1, b)$ in the ranges $n=0(1)15$, and $b=0.01(0.01)30.14$. For example, for $n=0(1)15$, and $b=0.25$ and $b=24.0$, the results below were obtained. These are compared with the results (columns 3 and 5) obtained by James Miller, John M. Gerhauser, and F. A. Matsen [*Quantum Chemistry Integrals and Tables*, University of Texas Press, 1959].

n	b=0.25	b=0.25 (Miller et al.)	b=24.0	b=24.0 (Miller et al.)
0	.31152031, 01	.31152031322856, 01	.15729727, -11	.15729727267830, -11
1	.15576015, 02	.15576015661428, 02	.16385132, -11	.16385132570656, -11
2	.12772332, 03	.12772332842371, 03	.17095154, -11	.17095154982051, -11
3	.15357950, 04	.15357951442168, 04	.17866621, -11	.17866621640586, -11
4	.24575835, 05	.24575837510601, 05	.18707497, -11	.18707497541261, -11
5	.49151978, 06	.49151986541518, 06	.19627122, -11	.19627122588926, -11
6	.11796476, 08	.11796479885167, 08	.20636507, -11	.20636507915061, -11
7	.33030132, 09	.33030143989988, 09	.21748707, -11	.21748708743056, -11
8	.10569642, 11	.10569646079911, 11	.22979295, -11	.22979296848848, -11
9	.38050711, 12	.38050725887992, 12	.24346962, -11	.24346963586148, -11
10	.15220284, 14	.15220290355200, 14	.25874294, -11	.25874295428724, -11
11	.66969248, 15	.66969277562880, 15	.27588778, -11	.27588779393928, -11
12	.32145238, 17	.32145253230182, 17	.29524115, -11	.29524116937494, -11
13	.16715523, 19	.16715531679695, 19	.31721955, -11	.31721957275639, -11
14	.93606928, 20	.9360697406291, 20	.34234200, -11	.34234202345285, -11
15	.56164156, 22	.56164186443775, 22	.37126102, -11	.37126103733633, -11

The accuracy is at least six significant figures over the entire range. This accuracy is completely satisfactory for all quantum chemical calculations.

ALGORITHM 109

DEFINITE EXPONENTIAL INTEGRALS B

YURI A. KRUGLYAK

Kharkov State University, Kharkov, U.S.S.R., AND

DONALD R. WHITMAN

Case Institute of Technology, Cleveland, Ohio

real procedure Bs(n, a); value n, a; integer n; real a;

comment This procedure computes a value of the integral $B_{n-1}(a) = \int_1^{+1} x^{n-1} \exp(-ax) dx$ for any given positive integer, n, and any real parameter, a. If $|a| < \text{alim}$ an expansion of $\exp(-ax)$ is used, otherwise the recursion formula $B_n(a) = [(-1)^n e^{-a} - e^{-a} + n B_{n-1}(a)]/a$ with $b_0(a) = 2 \sinh(a)/a$ is used. The value of alim depends upon the highest n appearing in the calculations and upon the maximum errors in the last significant digits in the library procedures. For example, we have used $\text{alim} = 8$ for $n_{\max} = 16$ with $\text{gamma} = 1 \times 10^{-8}$. The intrinsic function $\text{mod}(E_1, E_2)$ which requires two integer arguments, is the conventional modulus;

```

begin integer m; real alim, delta, gamma, r, epsilon,
s, k, a2, omega, da, jp, jm, q1, q2; real array
b[1:n]; if a=0 then
L1: begin if mod(n-1, 2)=0 then
L2: begin b[n] := 2/n; go to exit end L2;
comment integral  $b[n] = B_{n-1}(0)$  for odd n was evaluated;
b[n] := 0; go to exit end L1;
comment integral  $b[n] = B_{n-1}(0)$  for even n was evaluated;
if abs(a) alim then
L3: begin delta := gamma; if mod(n-1, 2)=0 then
L4: begin r := 2/n; epsilon := r * delta; s := r;
k := 0; a2 := a^2;
Even: k := k+2;
r := r * a2 * (n+k-2) / (k * (k-1) * (n+k));
s := s+r; if r > epsilon then go to Even;
b[n] := s+r;
go to exit end L4;
comment integral  $b[n] = B_{n-1}(a)$  for odd n and  $|a| < \text{alim}$  was
evaluated;
r := 2 * a / (n+1); omega := abs(r * delta);
s := r; k := 1;
a2 := a^2;
Odd: k := k+2;
r := r * a2 * (n+k-2) / (k * (k-1) * (n+k));
s := s+r; if abs(r) > omega then go to Odd;
b[n] := -(s+r); go to exit end L3;
comment integral  $b[n] = B_{n-1}(a)$  for even n and  $|a| < \text{alim}$  was
evaluated;
da := 1/a; jp := da * exp(a); jm := (da^2)/jp;
b[1] := jp - jm;
if n=1 then go to exit;
comment integral  $b[1] = B_0(a)$  for  $|a| \geq \text{alim}$  was evaluated;
q1 := -1; q2 := 1; for m := 2 step 1 until n do
L5: begin b[m] := q1 * jp - jm + q2 * da * b[m-1];
q1 := -q1; q2 := q2+1 end L5;
comment integral  $b[n] = B_{n-1}(a)$  for integer  $n \geq 2$  and  $|a| \geq \text{alim}$ 
was evaluated;
exit: Bs := b[n] end Bs;

```

CERTIFICATION OF ALGORITHM 109

DEFINITE EXPONENTIAL INTEGRALS B [Yuri A.

Kruglyak, D. R. Whitman, *Comm. ACM* 5 (July 1962)]

YURI A. KRUGLYAK

Kharkov State University, Kharkov, U.S.S.R., and

DONALD R. WHITMAN

Case Institute of Technology, Cleveland, Ohio

Integrals $B_n(a) = \int_1^{+1} x^n \exp(-ax) dx$ occur in physical problems involving spheroidal coordinates, particularly in quantum chemistry calculations. This algorithm was programmed for the Burroughs-220 computer using a Burroughs Algebraic Compiler. The program was used to compute tables of $B_n(a)$ in the ranges $n=0(1)15$, and $a=0.00(0.01)32.54$. For example, for $n=0(1)15$ and $a=0.25$, and $a=24.0$ the results below were obtained. These are compared with the results (columns 3 and 5) obtained by James Miller, John M. Gerhauser, and F. A. Matsen [*Quantum Chemistry Integrals and Tables*, University of Texas Press, Austin, 1959].

n	a=0.25	a=0.25 (Miller et al.)	a=24.0	a=24.0 (Miller et al.)
0	.20208984, 01	.20208985344653, 01	.11037134, 10	.110371342208, 10
1	-.16771084, 00	-.16771086117520, 00	-.10577253, 10	-.105772536282, 10
2	.67921322, 00	.67921324506375, 00	.10155696, 10	.101556964184, 10
3	-.10074584, 00	-.10074585827159, 00	-.97676725, 09	-.976767216847, 09
4	.40896479, 00	.40896480211998, 00	.94091887, 09	.940918885936, 09
5	-.72008754, -01	-.72008756636929, -01	-.90768866, 09	-.907688654174, 09
6	.29268836, 00	.29268837517905, 00	.87679129, 09	.876791258533, 09
7	-.56030292, -01	-.56030294023170, -01	-.84798262, 09	-.847982638338, 09
8	.22792911, 00	.22792912573392, 00	.82105258, 09	.821052542631, 09
9	-.45856272, -01	-.45856272975462, -01	-.79581870, 09	-.795818718590, 09
10	.18664760, 00	.18664761544688, 00	.77212229, 09	.772122289331, 09

11 - .38809718, -01 - .38806719373731, -01 - .74982404, 09 - .749824039467, 09
 12 - .15803198, 00 - .15803200452627, 00 - .72880141, 09 - .728801402343, 09
 13 - .33640562, -01 - .33640563670387, -01 - .70894600, 09 - .708945995807, 09
 14 - .13702696, 00 - .13702696892367, 00 - .69016158, 09 - .690161591189, 09
 15 - .29686662, -01 - .29686663616401, -01 - .67236245, 09 - .672362427583, 09

The accuracy is at least six significant figures in the ranges mentioned above. This accuracy is enough for the majority of quantum chemistry calculations.

ALGORITHM 110 QUANTUM MECHANICAL INTEGRALS OF SLATER-TYPE ORBITALS

YURI A. KRUGLYAK

Kharkov State University, Kharkov, U.S.S.R., AND

DONALD R. WHITMAN

Case Institute of Technology, Cleveland, Ohio

real procedure INTSOLI (n, r, za, ab, As, Bs) Result:
 (s, i1, i2, i3); value n, r, za, zb; integer n; real r, za, zb;
 real array a[1:8], b[1:8], G[1:2Xn]; integer array bc[1:2Xn,
 1:2Xn]; **real procedure** As, Bs;

comment Procedure INTSOLI computes the quantum mechanical integrals $s = \langle \psi_{n00}^a | \psi_{210}^b \rangle$ (overlap integral),
 $i1 = \langle \psi_{n00}^a | Z_a^* / r_{ai} | \psi_{210}^b \rangle$ (exchange integral),
 $i2 = \langle \psi_{n00}^a | Z_b^* / r_{bi} | \psi_{210}^b \rangle$ (coulomb integral),
 and $i3 = \langle \psi_{210}^a | Z_a^* / r_{ai} | \psi_{210}^b \rangle$ (coulomb integral).

Here $|\psi_{nlm}^a\rangle$ is a Slater-type orbital of electron i centered on atomic nucleus a . The integer n is the effective principal quantum number with values 1, 2, 3 and 4. $Z_a^* = za$ and $Z_b^* = zb$ are effective nuclear charges. r_{bi} is the distance of electron i from nucleus b . The input parameter r is the distance between the two centers a and b . All physical quantities are given in atomic units;

begin integer q, t, c, m;
 real g, zsa, zsb, ks, p, pt, lilya, s, k1, exc, i1, pppt,
 k2, sue, i2, pmpt, ptmp, k3, i3;
 bc[1, 1] := bc[2, 1] := bc[2, 2] := 1;
 for q := 3 step 1 until 2Xn do
 L6: **begin** bc[g, 1] := 1; for t := 2 step 1 until g-1 do
 bc[q, t] := bc[q-1, t-1] + bc[q-1, t];
 bc[q, q] := 1 end L6;

comment binomial coefficients $bc[q, t] = \binom{q-1}{t-1}$ were computed
 using the recursion formula $\binom{q}{t} = \binom{q-1}{t-1} + \binom{q-1}{t}$;

procedure As(n, b) Result: (a[n]); value n, b; integer n;
 real b;

comment procedure As computes a value of integral $A_{n-1}(1, b)$
 [see Algorithm 108, "Definite Exponential Integrals A," by Yuri A. Kruglyak and D. R. Whitman,
Comm. ACM (July 1962)]. Any identifier occurring
 within the As is specified to be local to the As;

begin integer m; real db; a[1] := exp(-b)/b;
 if n=1 then go to exitAs; db := 1/b;
 for m := 2 step 1 until n do a[m] := a[1] +
 dbX(m-1)Xa[m-1]

exitAs: end As;

procedure Bs(n, a) Result: (b[n]); value n, a; integer n;
 real a;

comment procedure Bs computes a value of integral $B_{n-1}(a)$
 [see Algorithm 109, "Definite Exponential Integrals B" by Yuri A. Kruglyak and D. R. Whitman,
Comm. ACM (July 1962)]. Any identifier occurring
 within the Bs is specified to be local to the Bs;

begin integer m; real alim, delta, gamma, r, epsilon,
 s, k, a2, omega, da, up, jm, q1, q2;
 if a=0 then **begin** if mod(n-1, 2)=0
 then **begin** b[n] := 2/n; go to exitBs end;
 b[n] := 0; go to exitBs end;
 if abs(a)<alim then **begin** delta := gamma;
comment we have used alim=8 and gamma=1X10⁻⁸;
 if mod(n-1, 2)=0 then **begin** r := 2/n;
 epsilon := rXdelta;
 s := r; k := 0; a2 := a²;

Even: k := k+2;
 r := rXa2X(n+k-2)/((kX(k-1)X(n+k));
 s := s+r; if r>epsilon then go to Even;
 b[n] := s+r;
 go to exitBs end; r := 2Xa/(n+1);
 omega := abs(rXdelta);
 s := r; k := 1; a2 := a²;

Odd: k := k+2;
 r := rXa2X(n+k-2)/(kX(k-1)X(n+k));
 s := s+r; if abs(r)>omega then go to Odd;
 b[n] := -(s+r); go to exitBs end; da := 1/a;
 jp := daXexp(a);
 jm := (da²)/jp; b[1] := jp-jm;
 if n=1 then go to exitBs;
 q1 := -1; q2 := 1; for m := 2 step 1 until n
 do **begin** b[m] := q1Xjp-jm+q2XdaXb[m-1];
 q1 := -q1; q2 := q2+1 end

exitBs: end Bs;
 g := 1; for m := 1 step 1 until 2Xn do g := g/m;
 G[2Xn] := g;

comment 1/(2n)! = G[2Xn] was evaluated;
 zsa := za/n; zsb := zb/2; ks := (r/2)[†](n+3)X
 (2Xzsa)[†](n+1/2)Xzsb[†](5/2)XG[2Xn][†](1/2);
 p := rX(zsa+zsb)/2;
 pt := rX(zsa-zsb)/2;

for c := 1 step 1 until n+3 do
ABSI: **begin** As(c, p) Result: (a[c]);
 Bs(c, pt) Result: (b[c])
 end ABSI;

S: lilya := 0; for m := 0 step 1 until n do lilya :=
 lilya+bc[n+1, m+1]X(a[n-m+2]X(b[m+1]+
 b[m+3]) - b[m+2]X(a[n-m+1]+a[n-m+3]));
 s := ksXlilya;

I1: k1 := ksX2Xza/r; exc := 0;
 for m := 0 step 1 until n-1 do
 exc := exc+bc[n, m+1]X(a[n-m+1]X(b[m+1]+
 b[m+3]) - b[m+2]X(a[n-m]+a[n-m+2]));
 i1 := k1Xexc;

I2: pppt := p+pt; k2 := (r/2)[†](2Xn)X(2Xzsa)[†]
 (2Xn+1)XzsbXG[2Xn];
 for c := 1 step 1 until 2Xn do

BA2: **begin** As(c, pppt) Result: (a[c]);
 Bs(c, pppt) Result: (b[c])
 end BA2; sue := 0;

for m := 0 step 1 until 2Xn-1 do
 sue := sue+bc[2Xn, m+1]Xa[2Xn-m]Xb[m+1];
 i2 := k2Xsue;

I3: pmpt := p-pt; ptmp := -pmpt;
 k3 := (r/2)[†]4X2XzaXzsb[†]5;
 for c := 1 step 1 until 4 do
AB3: **begin** As(c, pmpt) Result: (a[c]);
 Bs(c, ptmp) Result: (b[c])
 end AB3; i3 := k3X(a[2]X(b[1]+2Xb[3]) - b[2]X
 (a[1]+2Xa[3]) + a[4]Xb[3] - a[3]Xb[4]) end
 INTSOLI;

CERTIFICATION OF ALGORITHM 110
QUANTUM MECHANICAL INTEGRALS OF
SLATER-TYPE ORBITALS [Yuri A. Kruglyak and
Donald R. Whitman, *Comm. ACM* 5 (July 1962)]

YURI A. KRUGLYAK

Kharkov State University, Kharkov, U.S.S.R. and

DONALD R. WHITMAN

Case Institute of Technology, Cleveland, Ohio

This procedure was written and tested in the Burroughs 220 version of the ALGOL language in the spring of 1961 at Case Institute of Technology. The program was used to compute tables of quantum mechanical integrals s , $i1$, $i2$, and $i3$ in the ranges: $r(\text{\AA})=0.64(0.02)1.40(0.10)3.10$; $Z_b^*=0.25(0.50)3.75$, 3.90, 4.25, 4.55, 4.75, 5.20, 5.25; $Z_a^*=0.7$, 1.0 for $n=1$; 1.3(1.0)3.3 for $n=2$; 0.2, 2.2(1.0)4.2 for $n=3$; and 0.2, 2.2, 3.2 for $n=4$. The table at the right shows typical results compared with values from *Integralen zur Quantenchemie* by H. Preuss (Springer-Verlag, 1957), Zweiter Band. Accuracy is at least six significant figures in the ranges mentioned above. This is ample for the overwhelming majority of quantum chemistry calculations.

Certification of INTSOLI

Input				K. and W. Result	Preuss' Result			Table No.
n	r	z_a	z_b		Notation			
1	5	0.5	0.2	s	0.14841691	0.5 0.1 [1a 3b]	0.148417	23
1	1	4.5	8.0	s	0.35203437	4.5 4.0 [1a 3b]	0.352034	30
2	1	20	20	s	$0.25032133 \times 10^{-1}$	10 10 [2a 3b]	0.250321×10^{-1}	40
1	5	0.5	0.2	i1	0.22058816	0.5 0.1 5[a ⁻¹ 1a 3b]	0.220588	59
1	1	4.5	8.0	i1	0.96587055	4.5 4.0 1[a ⁻¹ 1a 3b]	0.965871	66
2	1	20	20	i1	$0.58102500 \times 10^{-1}$	10 10 1[a ⁻¹ 2a 3b]	0.581025×10^{-1}	76
1	1	0.5	0.2	i2	0.44818080	0.5 0.5 1[b ⁻¹ 1a 1a]	0.448181	41
1	5	0.5	0.2	i2	0.97641725	0.5 0.5 5[b ⁻¹ 1a 1a]	0.976417	45
2	1	20	20	i2	0.99999530	10 10 1[b ⁻¹ 2a 2a]	0.100000×10^1	58
1	1	10	1	i3	0.26217432	0.5 0.5 1[b ⁻¹ 3a 3a]	0.262174	41
1	1	10	10	i3	0.11093011×10^1	5 5 1[b ⁻¹ 3a 3a]	0.110929×10^1	50
1	1	10	20	i3	0.10300137×10^1	10 10 1[b ⁻¹ 3a 3a]	0.103001×10^1	58

ALGORITHM 111
MOLECULAR-ORBITAL CALCULATION OF
MOLECULAR INTERACTIONS

YURI A. KRUGLYAK

Kharkov State University, Kharkov, U.S.S.R., AND

DONALD R. WHITMAN

Case Institute of Technology, Cleveland, Ohio

real procedure SOLI(n , z_a , z_b , rem , $coef2$, $r1$, $E1$, $dr1$, $drk1$, acc , $acc1$, $rk2$, $rk1$, $dr2$, asy , $rk3$, $dr3$, As , Bs , **RESULT**) **Result:** (ra , Ep , Em , ca , $ca2$, cb , $cb2$, DEa , DEb , s , $i1$, $i2$, $i3$, nn , haa , hab , hbb); **value** n , z_a , z_b , rem , $coef2$, $r1$, $E1$, $dr1$, $rk1$, $drk1$, acc ,

$acc1$, $rk2$, $dr2$, asy , $rk3$, $dr3$; **integer** n , rem ; **real** otherwise; **real array** $a[1:8]$, $b[1:8]$, $G[1:8]$, $zsap[1:9]$, $rp[1:8]$, $ans[1:rem]$; **real procedure** As , Bs , **RESULT**;

comment This procedure calculates a one-electron approximation to the energy of interaction of molecular species by the use of the molecular-orbital (MO) method with a linear combination of Slater-type orbitals (LCSTO). The wave function used is $|\phi\rangle = c_a |\psi_{n00}^a\rangle + c_b |\psi_{n10}^b\rangle$, where $|\psi_{n1m}^a\rangle$ is a STO centered on nucleus a . The effective principal quantum number n takes the integral value 1, 2, 3 or 4. The Hamiltonian used is: $\mathcal{H}_{ab} = -\Delta/2 - Z_a^*/r_a - Z_b^*/r_b + Z_a^*Z_b^*/R_{ab}$. Here Z_a^* and Z_b^* are effective nuclear charges, r_a and r_b the distances of the electron from nucleus a and b , and R_{ab} is the distance between nuclei a and b . The calculations are in atomic units, while the output ra is in Angstroms and DEa and DEb are in kcal/gm-ion. Abbreviations of the following type are used: $Za = Z_a^*$, $ra = R_{ab}(\text{\AA})$, $haa = \langle \psi_{n00}^a | \mathcal{H}_{ab} | \psi_{n00}^a \rangle$, $DEa = D(a, b + \text{electron})$, $e1 = \langle \psi_{n00}^a | -\Delta/2 - Z_a^*/r_a | \psi_{n00}^a \rangle$. The values of $coef1$ and $coef2$ are 627.71 (kcal/gm-ion) and 0.5291 $\text{\AA}$, respectively. $r1$, $E1$, $dr1$, $dr2$, $dr3$, acc , $acc1$, and asy are control parameters. The accuracy of the calculations (acc , $acc1$) is 1×10^{-5} . The initial values of R_{ab} and E_1 are conveniently: $r1=0.4(\text{\AA})$, and $E1=100(\text{a.u.})$. The steps are: $dr1=0.1$, $dr2=0.4$, and $dr3=0.01$, all in Angstroms. asy is $-1 \times 10^{-3}(\text{a.u.})$;

begin **integer** q , t , c , m , f ; **real** otherwise;
procedure $As(n, b)$ **Result:** ($a[n]$); **value** n , b ; **integer** n ; **real** b ;
comment any identifier occurring within the As is specified to be local to the As ;
begin **integer** m ; **real** db ; $a[1] := \exp(-b)/b$;
if $n=1$ **then go to** $exitAs$; $db := 1/b$;
for $m := 2$ **step 1 until** n **do** $a[m] := a[1] + db \times (m-1) \times a[m-1]$;
exitAs: **end** As ;
procedure $Bs(n, a)$ **Result:** ($b[n]$); **value** n , a ; **integer** n ; **real** a ;
comment any identifier occurring within the Bs is specified to be local to the Bs ;
begin **integer** m ; **real** otherwise; **if** $a=0$ **then begin if**
 $\text{mod}(n-1, 2)=0$ **then begin** $b[n] := 2/n$;
go to $exitBs$ **end**; $b[n] := 0$; **go to** $exitBs$ **end**;
if $\text{abs}(a) < \text{alim}$ **then begin** $\text{delta} := \text{gamma}$;
if $\text{mod}(n-1, 2)=0$ **then begin** $r := 2/n$;
 $\text{epsilon} := r \times \text{delta}$; $s := r$; $k := 0$; $a2 := a^2$;
 $k := k+2$; $r := r \times a2 \times (n+k-2)/(k(k-1)(n+k))$;
 $s := s+r$; **if** $r > \text{epsilon}$ **then go to** $Even$;
 $b[n] := s+r$; **go to** $exitBs$ **end**;
 $r := 2 \times a/(n+1)$; $\text{omega} := \text{abs}(r \times \text{delta})$;
 $s := r$; $k:=1$; $a2 := a^2$;
 $k := k+2$; $r := r \times a2 \times (n+k-2)/(k(k-1)(n+k))$;
 $s := s+r$; **if** $\text{abs}(r) > \text{omega}$ **then go to** Odd ;
 $b[n] := -(s+r)$; **go to** $exitBs$ **end**;
 $\text{da} := 1/a$; $jp := \text{da} \times \exp(a)$;
 $jm := (\text{da}^2)/jp$; $b[1] := jp - jm$;
if $n=1$ **then go to** $exitBs$; $q1 := -1$; $q2 := 1$;
for $m := 2$ **step 1**
until n **do begin** $b[m] := q1 \times jp - jm +$
 $q2 \times \text{da} \times b[m-1]$;
 $q1 := -q1$; $q2 := q2+1$ **end**;
end Bs ;
procedure $Result(coef1)$; **real** $coef1$;
comment **RESULT** computes Ep , Em , ca , $ca2$, cb , $cb2$, DEa , DEb , s , $i1$, $i2$, $i3$, nn , haa , hab , hbb . Important: **RESULT** and any identifier occurring within the **RESULT** enter SOLI as nonlocal entities;
begin $r := r \times br$; $rp[1] := r$; **for** $c := 2$ **step 1 until** $n+4$ **do** $rp[c] := rp[c-1] \times rp[1]$; $p := r \times \text{sum}$;
 $pt := r \times \text{dif}$; $ks := rp[n+3] \times \text{zss}$;

```

for c := 1 step 1 until n+3 do begin As(c, p)
Result: (a[c]); Bs(c, pt) Result: (b[c]) end;
lilya := 0; for m := 0 step 1 until n do lilya :=
lilya+bc[n+1, m+1]×(a[n-m+2]×
(b[m+1]+b[m+3])−b[m+2]×(a[n-m+1]
+a[n-m+3])); s := ks×lilya; li12 := 2×s;
k1 := ks×za/r; exc := 0; for m := 0 step 1
until n−1 do exc := exc+bc[n, m+1]×(a[n-
m+1]×(b[m+1]+b[m+3])−b[m+2]×(a[n-m]+
a[n-m+2])); i1 := k1×exc; pppt := p+pt;
k2 := rp[2×n]×zsbd; for c := 1 step 1 until
2×n do begin As(c, pppt) Result: (a[c]);
Bs(c, pppt) Result: (b[c]) end; sue := 0;
for m := 0 step 1 until 2×n−1 do sue :=
sue+bc[2×n, m+1]×a[2×n-m]×b[m+1];
i2 := k2×sue; pmpt := p−pt;
ptmp := −pmpt; k3 := rp[4]×z5;
for c := 1 step 1 until 4 do begin As(c, pmpt)
Result: (a[c]); Bs(c, ptmp) Result: (b[c]) end;
i3 := k3×(a[2]×(b[1]+2×b[3])−b[2]×(a[1]+2×
a[3])+a[4]×b[3]−a[3]×b[4]);

```

comment Two-center integrals $s, i1, i2$, and $i3$ were computed [see Algorithm 110, "Quantum Mechanical Integrals of Slater-Type Orbitals," by Yuri A. Kruglyak and D. R. Whitman, *Comm. ACM* (July 1962)]; $nn := zz/(2×r)$; $e2pnn := e2+nn$; $haa := e1−e2+nn$; $hbb := e2pnn−i3$; $hab := e2pnn×s−i1$; $den := 2−s×li12$; $bsr := haa+hbb−hab×li12$; $root := sqrt(bsr^2−2×den×(haa×hbb−hab^2))$; $Ep := (bsr+root)/den$; $Em := (bsr−root)/den$; $ans[f] := Em$; $DEa := coef1×(e2−Em)$; $DEb := coef1×(e1−Em)$; $Emhaa := Em−haa$; $Emhbb := Em−hbb$; $ES := Em×s$; $habmES := hab−ES$; $caDcb1 := habmES/Emhaa$; $cbDca2 := habmES/Emhbb$; **if** $abs(Emhaa) > abs(Emhbb)$ **then begin** $col := caDcb1^2$; $cb2 := 1/(1+li12×caDcb1+col)$; $ca2 := cb2×col$; $ca := sqrt(ca2)$; $cb := ca/caDcb1$ **go to** NATA **end**; $co2 := cbDca2^2$; $ca2 := 1/(1+li12×cbDca2+co2)$; $cb2 := ca2×co2$; $ca := sqrt(ca2)$; $cb := ca×cbDca2$

NATA: **end** RESULT;

Begin of program: $bc[1, 1] := bc[2, 1] := bc[2, 2] := 1$;
for $q := 3$ **step 1 until** 8 **do begin** $bc[q, 1] := 1$; **for** $t := 2$
step 1 until $q−1$ **do** $bc[q, t] := bc[q−1, t−1]+bc[q−1, t]$;
 $bc[q, q] := 1$ **end**;

IZM: $g := 1$; **for** $m := 1$ **step 1 until** $2×n$ **do** $g := g/m$;
 $G[2×n] := g$; $zsa := za/n$; $zsap[1] := zsa×2$;
for $c := 2$ **step 1**
until $2×n+1$ **do** $xsap[c] := zsap[c−1]×zsap[1]$;
 $D := zsap[2×n+1]×G[2×n]$; $DS := sqrt(D)$;
 $e1 := −zsap[2]×0.125×(4×n−3)/(2×n−1)$;
 $zsb := zb×0.5$; $sum := zsa+zsb$; $dif := zsa−zsb$;
 $zsb5 := zsb^5$; $zss := DS×sqrt(zsb5)$;
 $zsbd := zsb×1$; $z5 := 2×za×zsb5$; $zz := za×zb$;
 $e2 := −(zsb^2)/2$; $br := 0.5/coef2$; $f := 1$;
 $ans[1] := E1$; $ra := r1$;

KOM: $ra := ra+dr1$; **if** $ra > rk1$ **then** $ra := ra+drk1$;
 $f := f+1$; **RESULT** (coef1); **if** $ans[f]−ans[f−1] ≤$
 acc **then begin** **if** $ra > rk2$ **then go to** IZM;
go to KOM **end**; $ansf := ans[f]$; $d1 := ra$;

CLEV: $ra := ra+dr2$; **RESULT** (coef1); **if** $e1 < e2$ **then**
begin **if** $Em−e1 ≤ asy ∧ ra < rk3$ **then go to** CLEV;
go to KHAR **end**; **if** $e1 ≥ e2$ **then begin** **if** $Em−e2 ≤$
 $asy ∧ ra < rk3$ **then go to** CLEV; **go to** KHAR **end**;

KHAR: $ra := d1$; $ans[f−1] := ansf$;

CASE: $ra := ra−dr3$; $f := f+1$; **RESULT** (coef1);
if $ans[f]−ans[f−1] ≤ acc1$ **then go to** CASE;
go to IZM **end** SOLI;

ALGORITHM 112

POSITION OF POINT RELATIVE TO POLYGON

M. SHIMRAT

University of Alberta, Calgary, Alberta, Canada

Boolean procedure POINT IN POLYGON ($n, x, y, x0, y0$);

value $n, x0, y0$; **integer** n ; **array** x, y ; **real** $x0, y0$;

comment if the points $(x[i], y[i])$ ($i = 1, 2, \dots, n$) are—in this cyclic order—the vertices of a simple closed polygon and $(x0, y0)$ is a point not on any side of the polygon, then the procedure determines, by setting "point in polygon" to **true**, whether $(x0, y0)$ lies in the interior of the polygon;

begin **integer** i ; **Boolean** b ;

$x[n+1] := x[1]$; $y[n+1] := y[1]$; $b := \text{true}$;

for $i := 1$ **step 1 until** n **do**

if $(y < y[i] \equiv y > y[i+1]) \wedge$

$x0 - x[i] - (y0 - y[i]) \times (x[i+1] - x[i]) / (y[i+1] - y[i]) < 0$

then $b := \neg b$;

POINT IN POLYGON := $\neg b$;

end POINT IN POLYGON

CERTIFICATION OF ALGORITHM 112

POSITION OF POINT RELATIVE TO POLYGON

[M. Shimrat, *Comm. ACM*, Aug. 1962]

RICHARD HACKER

The Boeing Co., Seattle Wash.

The Boolean procedure POINT IN POLYGON was programmed in FORTRAN for the IBM 7090. The algorithm gave satisfactory results except for a case such as the following:

Let the polygon points be: (0, 0), (1, 0), (2, 1), (1, 2), (0, 2).

In this case the procedure would not detect that the point (1, 1) is in the polygon. However, the correct result was obtained by changing:

$\text{if } (y < y[i] \equiv y > y[i+1]) \wedge$

to read:

$\text{if } (y0 \leq y[i] \equiv y0 > y[i+1]) \wedge$

ALGORITHM 113

TREESORT

ROBERT W. FLOYD

Computer Associates, Inc., Woburn, Mass.

procedure TREESORT (UNSORTED, n , SORTED, k); **value** n, k ;

integer n, k ; **array** UNSORTED, SORTED;

comment TREESORT sorts the smallest k elements of the n -component array UNSORTED into the k -component array SORTED (the two arrays may be the same). The number of operations is on the order of $2 \times n + k \times \log_2(n)$. The number of auxiliary storage cells required is on the order of $2 \times n$. It is assumed that procedures are available for finding the minimum of two quantities, for packing one real number and one integer into a word, and for obtaining the left and right half of a packed word. The value of infinity is assumed to be larger than that of any element of UNSORTED;

begin **integer** i, j ; **array** $m[1:2 \times n - 1]$;

for $i := 1$ **step 1 until** n **do** $m[n+i-1] := \text{pack}(\text{UNSORTED}[i], n+i-1)$;


```

for i := n - 1 step - 1 until 1 do m[i] := minimum (m[2 × i],
m[2 × i + 1]);
for j := 1 step 1 until k do
begin SORTED [j] := left half (m[1]); i := right half (m[1]);
m[i] := infinity;
for i := i ÷ 2 while i > 0 do m[i] := minimum (m[2 × i], m[2 ×
i + 1])
end
end TREESORT

```

ALGORITHM 114 GENERATION OF PARTITIONS WITH CON- STRAINTS

FRANK STOCKMAL

System Development Corp., Santa Monica, Calif.

```

procedure CP GENERATOR (N, K, H, p, F, Z); integer
N, K, H; integer array p; Boolean F, Z;
comment CP GENERATOR generates a partition of N into K
parts, no part greater than H. Each partition is represented by
the array of parts p[1] thru p[K], where  $p[1] \geq p[2] \geq \dots \geq p[K]$ .
Initial entry is made with F = true and Z = true if parts = 0
are allowable, or F = true and Z = false if only nonzero parts
are desired. Upon initial entry, procedure ignores the input
array p, sets F = false, and generates the initial parti-
tion. Subsequent calls made with F = false will cause
procedure to operate upon the input partition to produce
another partition if one exists, so that all possible unpermuted
partitions with the specified constraints will be produced if CP
GENERATOR is allowed to operate upon its previous output.
When this scheme is followed, and initial entry is made with
F = true, Z = true, K = N, H = N, all possible un-
permuted partitions of N will be produced. Upon generating
the last partition, procedure resets F to true. The input param-
eters are restricted as follows:  $K \geq 1$ ,  $H \geq 1$ ,  $p[1] \geq p[2] \geq \dots \geq p[K]$ .
For Z = true, N is restricted to the range
 $0 \leq N \leq KH$ , and for Z = false,  $K \leq N \leq KH$ . A call should
not be made with  $p[1] - p[K] < 2$  and F = false;
begin integer a, b, i, j, q, r;
if F then go to first;
a := p[1] - p[2] - 2; j := 2;
test: if p[1] - p[j]  $\geq 2$  then go to divide;
a := a - 1 + j × (p[j] - p[j + 1]); j := j + 1; go to test;
first: if Z then go to alpha;
a := N - K; p[K] := 0; go to beta;
alpha: a := N; p[K] := -1;
beta: F := false; j := K;
divide: b := H - 1 - p[j]; q := entier (a/b); r := a - b × q;
for i := 1 step 1 until q do p[i] := H;
if q = K then go to last;
for i := q + 1 step 1 until j do p[i] := 1 + p[j];
p[q + 1] := r + p[q + 1];
if p[1] - p[K]  $\geq 2$  then go to exit;
last: F := true;
exit: end CP GENERATOR

```

ALGORITHM 115

PERM

H. F. TROTTER

Princeton University, Princeton, N. J.

```

procedure PERM (x, n); value n;
integer n; array x;

```

comment This algorithm was inspired by the procedure PERMUTE of Peck and Schrack (Algorithm 86, *Comm. ACM* Apr. 1962) and performs the same function. Each call of PERM changes the order of the first n components of x, and n! successive calls will generate all n! permutations. A nonlocal Boolean variable 'first' is assumed, which must be true when PERM is first called, to cause proper initialization. The first call of PERM makes 'first' false, and it remains so (unless changed by the external program) until the exit from the (n!)-th call of PERM. At that time x is restored to its original order and 'first' is made true.

The excuse for adding PERM to the growing pile of permutation generators is that, at the expense of some extra own storage, it cuts the manipulation of x to the theoretical minimum of n! transpositions, and appears to offer an advantage in speed. It also has the (probably useless) property that the permutations it generates are alternately odd and even;

```

begin own integer array p, d[2:n]; integer k, q; real t;
if first then initialize:
begin for k := 2 step 1 until n do
begin p[k] := 0; d[k] := 1 end;
first := false
end initialize;
k := 0;
INDEX: p[n] := q := p[n] + d[n];
if q = n then
begin d[n] := -1; go to LOOP end;
if q  $\neq 0$  then go to TRANSPOSE;
d[n] := 1; k := k + 1;
LOOP: if n > 2 then begin
comment Note that n was called by value;
n := n - 1; go to INDEX end LOOP;
Final exit: q := 1; first := true;
TRANSPOSE: q := q + k; t := x[q];
x[q] := x[q + 1]; x[q + 1] := t
end PERM;

```

CERTIFICATION OF ALGORITHM 115

PERM [H. F. Trotter, *Comm. ACM*, Aug. 1962]

E. S. PHILLIPS

Michigan State University, East Lansing, Mich.

PERM was translated into FORTRAN for the CDC 160-A, and it performed correctly. For n = 8, this method requires 2822 seconds. For comparison, Algorithm 86, PERMUTE, was translated and run on the same machine, requiring 3710 seconds as opposed to 1316 when run on an IBM 1620.

CERTIFICATION OF ALGORITHM 115

PERM [H. F. Trotter, *Comm. ACM* (Aug. 1962)]

G. F. SCHRACK

University of Alberta, Calgary, Alb., Canada

PERM was translated into FORTRAN for the IBM 1620 and it performed satisfactorily. Timing tests were carried out under the same conditions as for PERMUTATION (Algorithm 71) and PERMUTE (Algorithm 86).

PERM is indeed the fastest permutation generator so far encountered. For n = 8, PERM is 25% faster than PERMUTE (989 against 1316 sec.). The values for r_n are (for a definition of r_n , see Certification of Algorithm 71, *Comm. ACM*, Apr. 1962):

n	6	7	8
r_n	.92	.95	.98

ALGORITHM 116 COMPLEX DIVISION

ROBERT L. SMITH

Stanford University, Stanford, Calif.

```

procedure complexdiv (a, b, c, d) results: (e, f);
value a, b, c, d; real e, f;
comment complexdiv yields the complex quotient of  $a + ib$ 
divided by  $c + id$ . The method used here tends to avoid arith-
metic overflow or underflow. Such spills could otherwise occur
when squaring the component parts of the denominator if the
usual method were used;
begin real r, den;
if abs (c)  $\geq$  abs (d) then
  begin r := d/c;
    den := c + r  $\times$  d;
    e := (a + b  $\times$  r)/den;
    f := (b - a  $\times$  r)/den;
  end
else
  begin r := c/d;
    den := d + r  $\times$  c;
    e := (a  $\times$  r + b)/den;
    f := (b  $\times$  r - a)/den;
  end
end complexdiv

```

ALGORITHM 117 MAGIC SQUARE (EVEN ORDER)

D. M. COLLISON

Elliott Brothers (London) Limited, Borehamwood, Herts.,
England

```

procedure magiceven (n, x); value n; integer array x; in-
terger n;
comment the method of Devedec for even n is described in
"Mathematical Recreations" by M. Kraitchik, pp. 150-2. Enter
with side of square n to produce a magic square of the integers
1 - n  $\uparrow$  2 in x, where n  $\geq$  4;
begin integer a, b, n2, nn; Boolean p, q, r;
  n2 := n  $\div$  2; nn := n  $\times$  n;
  begin
    procedure alpha (p, q, a, h); value p, q, a, h; integer p, q, a;
      Boolean h;
      Comment pattern 0/0/0/...;
      begin integer r;
        for r := p step 1 until q do begin
          x[r, a] := if h then (a  $\times$  n - n + r) else (nn - a  $\times$  n +
            1 + n - r); h :=  $\neg$  h end;
        end alpha;
      procedure beta (p, q, a, h); value p, q, a, h; integer p, q, a;
        Boolean h;
        comment pattern 1 - 1 - 1 - ...;
        begin integer r;
          for r := p step 1 until q do begin
            x[r, a] := if h then (nn - a  $\times$  n + r) else (a  $\times$  n + 1 - r);
            h :=  $\neg$  h end;
          end beta;
        procedure gamma (p, q, a, h); value p, q, a, h; integer p, q, a;
          Boolean h;
          comment pattern /-/-/-...;
          begin integer r;

```

```

for r := p step 1 until q do begin
  x[r, a] := if h then (nn - a  $\times$  n + n - r + 1) else (a  $\times$  n
    + 1 - r); h :=  $\neg$  h end;
end gamma;
comment program begins;
p := q := (n - (n  $\div$  4)  $\times$  4 = 0); r := true;
for a := 1 step 1 until (n2 - 1) do begin
  beta (1, a - 1, a, r); alpha (a, n2 - 1, a, true);
  x[n2, a] := if q then (nn - a  $\times$  n + n2 + 1) else (nn - a  $\times$ 
    n + n2);
  alpha (n2 + 1, n, a,  $\neg$  q);
  q :=  $\neg$  q; r :=  $\neg$  r end;
  alpha (1, n2 - 1, n2,  $\neg$  p); alpha (n2 + 2, n, n2, false);
  gamma (1, n2 - 1, n2 + 1, p); gamma (n2 + 2, n, n2 + 1, true);
  q := p; r := true;
for a := (n2 + 2) step 1 until n do begin
  beta (1, n - a, a, q); x[n - a + 1, a] := a  $\times$  n - a + 1;
  beta (n - a + 2, n2 - 1, a, true);
  if r then for b := n2, n2 + 1 do x[b, a] := nn - a  $\times$  n +
    n - b + 1
  else begin x[n2, a] := nn - a  $\times$  n + n2;
    x[n2 + 1, a] := a  $\times$  n - n2 + 1 end;
  beta (n2 + 2, a - 1, a,  $\neg$  r); alpha (a, n, a, true);
  q :=  $\neg$  q; r :=  $\neg$  r end;
for a := n2, n2 + 1 do for b := n2, n2 + 1 do
  x[b, a] := if p then (a  $\times$  n - n + b) else (nn - a  $\times$  n + n -
    b + 1);
if  $\neg$  p then begin
  for a := n2, n2 + 1 do x[n2 - 1, a] := a  $\times$  n - n2 + 2;
  for b := n2, n2 + 1 do x[b, n2 + 2] := n  $\times$  n2 - 2  $\times$  n + b end;
end end magiceven

```

CERTIFICATIONS OF ALGORITHMS 117 and 118 MAGIC SQUARE (ODD AND EVEN ORDERS)

[D. M. Collison, *Comm. ACM*, Aug. 1962]

K. M. BOSWORTH

I.C.T. Ltd., Blyth Road, Hayes, Middlesex, England

The statement within the Boolean procedure beta should be
changed from

```

x[r, a] := if h then (nn - a  $\times$  n + r) else (a  $\times$  n + 1 - r);
to
x[r, a] := if h then (nn - a  $\times$  n + r) else (a  $\times$  n + 1 - r);

```

The procedures were then tested on magic squares of order
3 to 17 inclusive without fault.

CERTIFICATION OF ALGORITHMS 117 AND 118 MAGIC SQUARE (ODD AND, EVEN ORDERS)

[D. M. Collison, *Comm. ACM*, Aug. 1962]

D. M. COLLISON

Elliott Bros. (London) Ltd., Borehamwood, Herts.,
England

Both algorithms were checked and timed, using a special ALGOL
program, with the Elliott ALGOL translator on the National-
Elliott 803. The procedure for odd orders was the slower:

Procedure	Size of Square	Time
Odd order	9	10 sec.
	19	45 sec.
Even order	10	7 sec.
	20	23 sec.

Because of the different methods used and the length of the even
order procedure it was decided not to combine the two. The
smallest square of even order generated is given below:-

13	3	2	16
8	10	11	5
12	6	7	9
1	15	14	4

CERTIFICATION OF ALGORITHMS 117 AND 118 MAGIC SQUARES (EVEN AND ODD ORDERS)

[D. M. Collison, [Comm. ACM, Aug. 1962]

P. NAUR

Regnecentralen, Copenhagen, Denmark

MAGICEVEN needed the following correction: Within the body of **procedure** beta a left square bracket: . . . **then** [nn . . . should be changed to a left parenthesis: . . . **then** (nn . . .

With this correction it has run successfully in the GIER ALGOL system. The squares of even orders from 4 to 20 were generated and checked for magicity in rows and columns, but not in diagonals.

The algorithm contains 11 pairs of superfluous parentheses (10 of which are in conditional expressions) and if the assignments to *n2* and *nn* are moved to the place just following "end gamma;" the inner block becomes unnecessary.

MAGICODD ran without correction in GIER ALGOL and produced a few reasonable-looking squares.

Run times are as follows:

Procedure	Size of square	Time
Magicodd	9	0.6 sec
	19	2.5 sec
Magiceven	10	0.9 sec
	20	2.3 sec

ALGORITHM 118

MAGIC SQUARE (ODD ORDER)

D. M. COLLISON

Elliott Brothers (London) Limited, Borehamwood, Herts., England

procedure *magicodd* (*n*, *x*); **value** *n*; **integer** *n*; **integer** array *x*;

comment for given side *n* the procedure generates a magic square of the integers $1 - n \uparrow 2$. For the method of De la Loubère, see M. Kraitchik, "Mathematical Recreations," p. 149. *n* must be odd and $n \geq 3$;

begin **integer** *i*, *j*, *k*;

for *i* := 1 **step** 1 **until** *n* **do**

for *j* := 1 **step** 1 **until** *n* **do** *x*[*i*, *j*] := 0;

i := (*n* + 1) ÷ 2; *j* := *n*;

for *k* := 1 **step** 1 **until** *n* × *n* **do begin**

if *x*[*i*, *j*] ≠ 0 **then begin** *i* := *i* - 1; *j* := *j* - 2;

if *i* < 1 **then** *i* := *i* + *n*; **if** *j* < 1 **then** *j* := *j* + *n* **end**;

x[*i*, *j*] := *k*;

i := *i* + 1; **if** *i* > *n* **then** *i* := *i* - *n*;

j := *j* + 1; **if** *j* > *n* **then** *j* := *j* - *n*;

end;

end *magicodd*

CERTIFICATION OF ALGORITHM 118

MAGIC SQUARE (ODD ORDER) [D. M. Collison, Comm. ACM, Aug. 1962]

HENRY C. THACHER, JR.*

Reactor Engineering Div., Argonne National Lab., Argonne, Ill.

* Work supported by the U. S. Atomic Energy Commission.

The body of the procedure *magicodd* was tested on the LGP-30 using the Dartmouth ALGOL 60 translator. No syntactical errors

were found. The procedure generated odd-order magic squares satisfactorily. For orders up to 9, times were as follows (including output on the Flexowriter):

Order	Time(sec)
3	171
5	422
7	804
9	1285

The 3 × 3 square was:

4	3	8
9	5	1
2	7	6

SEE ALGORITHM 117

ALGORITHM 119

EVALUATION OF A PERT NETWORK

BURTON EISENMAN AND MARTIN SHAPIRO

United Nuclear Corp., White Plains, N. Y.

procedure *pert* (*nmax*, *i*, *j*; *te*, *st*, *emax*, *l*, *es*, *at*);

comment An algorithm describing an iterative procedure for evaluating a PERT network that permits the use of arbitrarily ordered activities and event identifiers such that an upper triangular matrix type of solution is unnecessary.

It has been observed by investigations of PERT networks, that an $N \times N$ matrix whose rows are designated as predecessor and whose columns are designated as successor events, has an entry in the (*i*, *j*)-element representing the activity time required in going from event *i* to event *j*. By elementary transformations, the matrix is transformed generally into an upper triangular matrix. The resultant upper triangular matrix is well ordered (i.e. any activity time appearing in a column is not dependent upon those activity times which appear in columns to the right of it).

This precise manipulation generally demands considerable running time. By direct evaluation not requiring a collection of elementary transformations, it is possible to evaluate the network with considerable reduction of running time;

integer *nmax*, *emax*;

real *st*;

integer array *i*, *j*, *l*;

real array *te*, *es*, *at*;

comment Given the total number of activities, *nmax*, the preceding and succeeding event identifiers, *i_n* and *j_n*, the corresponding expected time, *te*, for each activity, and the starting time, *st*, of the network, this procedure computes the early start and late finish times, *es*, and *at*, for each event, *l*, in the network;

begin

procedure *scan* (*e*, *l*, *l*);

integer *e*, *l*;

integer array *l*;

comment Given the number of events, *e*-1, contained thus far in vector array, *l*, and an event identifier *i_n* or *j_n*, stored in *l*, this procedure scans the existing array, *l*, to determine whether the event should be added to the list or not. If it is to be added, it becomes *l_e* and *e* replaces the event identifier. If it is not added, *k* replaces the event identifier.;

begin

integer *k*;

if *e* = 1 **then go to** *add*;

```

    for k := e-1 step -1 until 1 do
begin
    if t = l[k] then
begin
        t := k;
        go to out
    end
end;
add:
    l[e] := t;
    t := e;
    e := e + 1;

out:
end scan;
integer n, e, s, t, k;
real a, x;
    e := 1;
    for n := 1 step 1 until nmax do
begin
    t := j[n];
    scan (e, t, l);
    j[n] := t;
    t := i[n];
    scan (e, t, l);
    i[n] := t
end;
comment By means of the switch, s, we will either compute the
activity times,  $at_e$ , and transfer the values to the early start
vector,  $es_e$ , or we will compute  $at_e$  without any transfer process,
in which case the late finish times will be obtained.;
    emax := e - 1;
    s := 1;
    a := st;
s1:
    k := emax;
    for e := 1 step 1 until emax do
        at[e] := a;
s2:
    for n := 1 step 1 until nmax do
begin
    if l[i[n]] > 0 then
begin
        switch s := b1, b2;
b1:
        x := abs (at[i[n]]) + te[n];
        if x > abs (at[j[n]]) then go to l1;
        go to l2;
b2:
        x := abs (at[i[n]]) - te[n];
        if x < abs (at[j[n]]) then
            at[j[n]] := - x;
l1:
        at[j[n]] := - x;
l2:
        end
end;
    for e := 1 step 1 until emax do
begin
    if l[e] < 0 then
begin
        if at[e] < 0 then
begin
            l[e] := abs (l[e]);
            k := k + 1;
s3:
            at[e] := abs (at[e]);
            go to l3
        end;
        go to l3
    end;
    if at[e] ≥ 0 then
begin
        l[e] := - l[e];
        k := k - 1;
        go to l3
    end;
    go to s3;
l3:
end;
    if k ≠ 0 then go to s2;
    switch s := g1, g2;
g1:
    s := 2;

```

```

    for n := 1 step 1 until nmax do
begin
    t := i[n];
    i[n] := j[n];
    j[n] := t
end;
    a := 0;
    for e := 1 step 1 until emax do
begin
    es[e] := at[e];
    l[e] := abs (l[e]);
    if at[e] > a then
        a := at[e]
    end;
    go to s1;
g2:
    for e := 1 step 1 until emax do
        l[e] := abs (l[e]);
    end pert

```

ALGORITHM 120

MATRIX INVERSION II

RICHARD GEORGE*

Particle Accelerator Division Argonne National Laboratory
Argonne, Illinois

* Work supported by the U. S. Atomic Energy Commission.

procedure INVERSION II ($n, a, \epsilon, ALARM, \delta$);
comment This is a revision of Algorithm 58. It accomplishes inversion of the matrix a , with the result stored in matrix a . The order of the matrix is n . If in the process of calculating, any pivot element has an absolute value less than ϵ , there will be a jump to the non-local label $ALARM$. The variable δ will contain the value of the determinant of the original matrix on normal exit, zero or a very small number on exit to $ALARM$;

```

value n;
array a;
real epsilon, delta;
integer n;
begin
    array b, c[1:n]; real w, y;
    integer array z[1:n]; integer i, j, k, l, p;
    delta := 1.0;
    for j := 1 step 1 until n do
        z[j] := j;
    for i := 1 step 1 until n do
        begin
            k := i; y := a[i, i]; l := i-1; p := i+1;
            for j := p step 1 until n do
                begin
                    w := a[i, j];
                    if abs(w) > abs(y) then
                        begin
                            k := j;
                            y := w
                        end;
                end;
            end;
            delta := delta × y;
            if abs(y) < epsilon then go to ALARM;
            y := 1.0 / y;
            for j := 1 step 1 until n do
                begin
                    c[j] := a[j, k];
                    a[j, k] := a[j, i];
                    a[j, i] := - c[j] × y;
                    b[j] := a[i, j] := a[i, j] × y
                end;

```

```

a[i, i] := y;
j := z[i];
z[i] := z[k];
z[k] := j;
for k := 1 step 1 until l, p step 1 until n do
  for j := 1 step 1 until l, p step 1 until n do
    a[k, j] := a[k, j] - b[j] × c[k]
  end;
for i := 1 step 1 until n do
  begin
  REPEAT: k := z[i];
    if k=i then go to ADVANCE;
    for j := 1 step 1 until n do
      begin
        w := a[i, j];
        a[i, j] := a[k, j];
        a[k, j] := w
      end;
    p := z[i];
    z[i] := z[k];
    z[k] := p;
    delta := - delta;
    go to REPEAT;
  ADVANCE: end;
end

```

CERTIFICATION OF ALGORITHMS 120 AND MATRIX INVERSION BY GAUSS-JORDAN INVERSION II [R. George, *Comm. ACM* Aug. 1962] and gjr [by H. Rutishauser, quoted by H. R. Schwarz, *Comm. ACM* Febr. 1962]

P. NAUR

Regnecentralen, Copenhagen, Denmark

These two procedures were compared using the GIER ALGOL system (30 bits for the normalized mantissa including sign). The following changes (in part dictated by the requirements of the compiler) were included:

INVERSION II: (1) Epsilon was included in the value part.
(2) The specification label *ALARM* was added.

gjr: (1) The value part: *value n*, *eps* was inserted. (2) The second *a* in the formal parameter part was taken out.

With these changes both procedures ran smoothly through the compiler. In order to obtain a comparison each of them was tested as follows: With a given, rather large value of epsilon the procedure was called to invert a segment of the Hilbert matrix. Upon alarm exit, the value of epsilon was divided by 10 and a fresh call was made. In this way an estimate of the largest permissible epsilon was obtained. When the inverse had been obtained, that element of it which was most in error was found through a comparison with the accurate inverse as calculated by means of INVHILBERT (Algorithm 50, see certification above). A relative error was obtained through division by the largest element of the accurate inverse.

This process was carried out for segments of the Hilbert matrix of orders 2 through 15. For orders above 9, the results of the inversion are dominated by errors. Below 9 we obtained the following output:

Order	eps	Inversion by INVERSION II		
		Determinant	Maximum error Subscr. Error	Maximum error Relative
2	10 ⁻²	8.333333310 ⁻²	2,2 2.9810 ⁻⁸	2.4810 ⁻⁹
3	10 ⁻³	4.629628410 ⁻⁴	2,2 5.0110 ⁻⁵	2.6110 ⁻⁷
4	10 ⁻⁴	1.653431410 ⁻⁷	3,3 3.0610 ⁻²	4.7210 ⁻⁶
5	10 ⁻⁵	3.749000110 ⁻¹²	4,4 1.3810 ¹	7.7210 ⁻⁵
6	10 ⁻⁷	5.360187510 ⁻¹⁸	5,5 5.7810 ³	1.3110 ⁻³
7	10 ⁻⁸	4.848552910 ⁻²⁵	5,5 3.7010 ⁵	2.7710 ⁻³
8	10 ⁻¹⁰	1.522100010 ⁻³³	6,6 3.3310 ⁹	7.8410 ⁻¹

Similarly we got for gjr, and the ratio of errors of the two procedures:

Order	eps	Inversion by gjr		Ratio of errors INVERSION II to gjr
		Maximum error Subscr. Error	Maximum error Relative	
2	10 ⁻²	2,1 2.9810 ⁻⁸	2.4810 ⁻⁹	1.0
3	10 ⁻³	2,2 2.8610 ⁻⁶	1.4910 ⁻⁸	18
4	10 ⁻⁴	4,3 1.0710 ⁻⁴	1.6510 ⁻⁸	290
5	10 ⁻⁶	4,4 2.48	1.3910 ⁻⁵	5.6
6	10 ⁻⁷	5,5 4.0510 ³	9.1810 ⁻⁴	1.4
7	10 ⁻⁸	5,5 4.3210 ⁶	3.2410 ⁻²	.086
8	10 ⁻¹⁰	7,7 5.5510 ⁷	1.3110 ⁻²	60

Although the superiority of gjr, which searches for the pivot in both columns and rows, over INVERSION II, which only searches in the next column, is well brought out in the last column of the second table the behavior for *n* = 7 is curious and ought to be confirmed elsewhere.

As a further test both procedures were used to invert the matrices produced by Algorithm 52, TESTMATRIX (see certification above). Again, the error of the inverse was found by a comparison with the known inverse. The comparison of the two procedures was made for orders 2 through 23 and revealed a surprisingly small difference of accuracy. Typical output was as follows:

Order	Location and size of max. error				Ratio of errors
	INVERSION II		gjr		INVERSION II
	Subscr.	Error	Subscr.	Error	to gjr
5	5,5	8.9410-8	5,5	8.9410-8	1.00
10	10,10	3.7610-6	10,10	3.5210-6	1.07
15	15,15	2.1210-5	15,15	1.7810-5	1.19
20	20,20	6.8110-5	20,20	6.7110-5	1.02

The relative errors of the determinants calculated by INVERSION II increased slowly with *n*, reaching 2.310⁻⁷ for *n* = 24.

Typical execution times were found as follows:

Order	INVERSION II	gjr
5	2 seconds	3 seconds
10	5 "	8 "
15	16 "	17 "
20	53 "	57 "

However, it should be noted that owing to the automatic segmentation of the program into drum tracks in GIER ALGOL the execution time may vary somewhat from one program in which a procedure is used to another. The above times do not, in fact, refer to the same program.

SEE ALGORITHM 42

ALGORITHM 121 NORMDEV

DAVID SHAFER

University of Chicago, Chicago, Ill.

procedure NormDev(Random, A, x);

procedure Random; **real** A, x;

comment 'NormDev' uses (1) a procedure 'Random(y)' assumed to produce a random number, 0 < *y* < 1, and (2) the constant *A* = $\sqrt{2/\pi} \times \int_0^1 \exp(-x^2/2) dx$, to produce a positive normal deviate 'x';

begin **real** y;

Random(x); **if** x > A **then** go to large;

x := x/A;

1: Random(y); **if** y < $\exp(-x^2/2)$ **then** go to EndND;

Random(x); **go** to 1;

large: x := (x - A)/(1 - A);

2: x := $\sqrt{1 - 2 \times \log(x)}$;

Random(y); **if** y < 1/x **then** go to EndND;

Random(x); **go** to 2;

80 EndND: **end**

ALGORITHM 122
TRIDIAGONAL MATRIX
GERARD F. DIETZEL
Burroughs Corp., Pasadena, Calif.

```

procedure TRIDIAG (n, A, U);
integer n; array A, U;
comment This procedure reduces a real symmetric matrix A of
order n to tridiagonal form (UT)AU (UT = transpose of U) by
a sequence of at most  $(n-1)(n-2)/2$  binary orthogonal trans-
formations. Also, the matrix U is calculated. [Cf. W. Givens,
"Numerical computation of the characteristic values of a real
symmetric matrix," Report ORNL1574 (1954), Oak Ridge Nat.
Lab., Tenn., and D. E. Johansen, "A modified Givens method
for the eigenvalue evaluation of large matrices," J. ACM 8, 3
(1961)];
begin real fact, c1, c2, loc1, loc2, temp; integer i, j, j1, j2, j3, j4, n1;
comment Set array U = identity matrix of order n;
for i := 1 step 1 until n do
begin
for j := i + 1 step 1 until n do U[i, j] := U[j, i] = 0;
U[i, i] := 1.0
end;
comment The reduction of the matrix A begins here. Only the
upper triangular elements of A are used in the computation;
n1 := n - 2;
for i := 1 step 1 until n1 do
begin
j1 := i + 1; j2 := i + 2;
for j := j2 step 1 until n do
begin
if A[i, j] = 0 then go to lab;
fact := 1 /  $\sqrt{A[i, j1]^2 + A[i, j]^2}$ ;
c1 := fact × A[i, j1]; c2 := fact × A[i, j];
loc1 := A[j1, j1]; loc2 := A[j1, j];
A[j1, j1] := c12 × loc1 + 2.0 × c1 × c2 × loc2 + c22 ×
A[j, j];
A[j1, j] := -c1 × c2 × loc1 + (c12 - c22) × loc2 + c1 ×
c2 × A[j, j];
A[j, j] := c22 × loc1 - 2.0 × c1 × c2 × loc2 + c12 ×
A[j, j];
j3 := j + 1;
for k := j3 step 1 until n do
begin
temp := A[j1, k];
A[j1, k] := c1 × temp + c2 × A[j, k];
A[j, k] := -c2 × temp + c1 × A[j, k]
end;
j4 := j - 1;
for k := j2 step 1 until j4 do
begin
temp := A[j1, k];
A[j1, k] := c1 × temp + c2 × A[k, j];
A[k, j] := -c2 × temp + c1 × A[k, j]
end;
A[i, j1] := c1 × A[i, j1] + c2 × A[i, j];
A[i, j] := 0;
for k := 1 step 1 until n do
begin
temp := U[k, j1];
U[k, j1] := c1 × temp + c2 × U[k, j];
U[k, j] := -c2 × temp + c1 × U[k, j]
end;
lab: end
end;
for i := 1 step 1 until n do
for j := i + 1 step 1 until n do
A[j, i] := A[i, j]
end TRIDIAG

```

CERTIFICATION OF ALGORITHM 122
TRIDIAGONAL MATRIX [Gerard F. Dietzel, *Comm.*
ACM 5 (Sept. 1962), 482]
PETER NAUR (Recd 27 Sept. 63)
Regnecentralen, Copenhagen, Denmark

TRIDIAG needed the following corrections:

1. Insert *k* among the local integers to read:
integer *i*, *j*, *j1*, *j2*, *j3*, *j4*, *n1*, *k*;
2. At the end of line 5 of the procedure body, insert the colon to
read *U*[*j*, *i*] := 0;
3. Change the round parenthesis to a square bracket following
for *k* := *j3* ... to read *temp* := *A*[*j1*, *k*];

With these corrections the algorithm worked satisfactorily with
the GIER ALGOL system. As a test it was tried with the following
matrix:

$$HBH\ TESTMATRIX[j, i] = HBH\ TESTMATRIX[i, j] \\ = n + 1 - j \quad (j \geq i)$$

(cf. the Certification of Alg. 85, *Comm. ACM* 6 (Aug. 1963), 447).
As a check the resulting matrix was rotated back again, using the
resulting *U*-matrix, and the largest deviation of any element from
the original was found.

For comparison the figures obtained by using the algorithms
given by Wilkinson in *Numerische Mathematik* 4 (1962), 354-376,
may be used. Wilkinson's algorithms use Householder's method of
obtaining the tridiagonal form. It should be noted that the devi-
ations given in the table below for Householder's method refer to
the final result of obtaining the eigenvalues and vectors, and not
only the tridiagonal form, and thus include error contributions
from a rather longer chain of calculations than the ones given for
TRIDIAG. The times, however, only refer to the tridiagonalisa-
tion process in both cases.

	<i>n</i> =5	<i>n</i> =10	<i>n</i> =15
Largest deviation			
TRIDIAG,	1.4 ₁₀ - 7	7.0 ₁₀ - 7	2.4 ₁₀ - 6
householder tridiagonalisation		1.4 ₁₀ - 7	1.3 ₁₀ - 6
Time of execution, in GIER			
ALGOL, seconds			
TRIDIAG	2	7	34
householder tridiagonalisation	1	4	10

These figures clearly demonstrate the superiority of the House-
holder process. Since, in addition, the Householder method in the
form given by Wilkinson uses much less storage for variables.
Algorithm 122 cannot be recommended.

ALGORITHM 123
REAL ERROR FUNCTION, ERF(*x*)
MARTIN CRAWFORD AND ROBERT TECHO
Georgia Institute of Technology, Atlanta, Ga.

```

real procedure Erf(x); real x;
comment  $\Phi(x) = \text{Erf}(x) = (2/\sqrt{\pi}) \int_0^x e^{-u^2} du$  can be computed
by using the recursive relation for derivatives with  $\Phi^{(1)}(x) =$ 
 $(2/\sqrt{\pi})e^{-x^2}$ , where  $\Phi^{(n)}(x) = -2x\Phi^{(n-1)}(x) - 2(n-2)\Phi^{(n-2)}(x)$ ,
for  $n = 2, 3, \dots$ . The Taylor's series expansions of  $\Phi(a_k)$  are
taken about  $k+1$  points on the interval  $0 < a_k \leq x$  and summed
to get  $\Phi(x)$ ;
begin real A, U, V, W, Y, Z, T; integer N;
Z := 0; 1: if x ≠ 0 then
begin if 0.5 < abs (x) then A := - sign (x) × 0.5

```

```

else A := -x;
U := V := 1.12837917 × exp(-x2/2); Y := T := -V ×
A; N := 1;
2: if abs(T) ≥ 10-10 then
begin N := N + 1; W := -2 × x × V - 2 × U × (N-2);
T := T × W × A/(V × N);
U := V; V := W; Y := Y + T; go to 2 end;
Z := Z + Y; x := x + A; go to 1 end;
Erf := Z end Erf

```

CERTIFICATION OF ALGORITHM 123

REAL ERROR FUNCTION, ERF (x) [Martin Crawford and Robert Techo, *Comm. ACM*, Sept. 1962]

HENRY C. THACHER, JR.*

Argonne National Laboratory, Argonne, Ill.

* Work supported by the U. S. Atomic Energy Commission.

The body of *Erf*(x) was tested using the Dartmouth SCALP compiler for the LGP-30. For $x = 0(0.01)0.3$, the results agreed with tabulated values to 8 in the 7th decimal place, and for $x = 0.4(0.2)1.6$ the error was less than 1 in the 6th decimal. These results are compatible with the roundoff error in the arithmetic used. The computing time increased rapidly (by a factor of more than 10) as x increased from 0.01 to 1.6.

The following comments should be considered by users of the algorithm:

1. The parameter x should be called by value, both to allow the use of expressions, and also to avoid destruction of the actual parameter.
2. The constant $10-10$ in statement 2 determines the accuracy of the computation. Its value should be adjusted to the arithmetic being used, and the accuracy required. A machine-independent test could be made by substituting $if Y - T = Y$ then ...
3. For large x , the error function is more efficiently calculated from the Laplace continued fraction for *erfc*(x). Algorithm 180 is based on this method.

REMARK ON ALGORITHM 123

ERF(x) [Martin Crawford and Robert Techo, *Comm. ACM*, Sept. 1962]

D. IBBETSON

Elliott Brothers (London) Ltd.

Elstree Way, Borehamwood, Herts., England

(1) The specification value x ; was added to allow x to be an expression and to prevent side effects.

(2) The algorithm was then modified to give the Gaussian integral $(1/\sqrt{2\pi}) \int_{-\infty}^x \exp(-\frac{1}{2}u^2) du$ by

(a) changing its name to *Gauss* (x),

(b) inserting $x := x + 0.70710678$; immediately before $Z := 0$; , and

(c) changing the final statement to

Gauss := (Z+1)/2 end *Gauss*

(3) The algorithm with the above changes was tested on a National Elliott 803 computer using the Elliott-ALGOL translator with $10-8$ substituted for $10-10$. It was found to produce wrong answers when $x = \pm 1$ (corresponding to *Erf*($\pm 1/\sqrt{2}$)) giving 0.5 ± 0.3467899 instead of 0.5 ± 0.3413447 .

REMARK ON ALGORITHM 123

ERF(x) [Martin Crawford and Robert Techo, *Comm. ACM* 5 (Sept. 1962), 483; 6 (June 1963), 316; 6 (Oct. 1963), 618]

STEPHEN P. BARTON AND JOHN F. WAGNER (Recd 2 Dec. 63)
General Telephone and Electronics Laboratories, Bayside,
New York

This algorithm may err when the Taylor series expands about a root of the n th-order Hermite polynomial; one such error has already been noted [Remark on Algorithm 123, D. Ibbetson, *Comm. ACM* 6 (Oct. 1963), 618]. The difficulty springs from the Taylor-series truncation criterion, which assumes that the magnitude of successive terms in the Taylor series decreases. This is not always so, as may be seen by relating

$$\Phi^{(n)}(x) = \frac{2}{\sqrt{\pi}} \frac{d^{n-1}}{dx^{n-1}} (e^{-x^2}), \quad (n \geq 1)$$

to the Hermite polynomial $H_n(x)$, which can be defined as

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} (e^{-x^2}).$$

Therefore

$$\Phi^{(n)}(x) = \frac{2}{\sqrt{\pi}} (-1)^{n-1} e^{-x^2} H_{n-1}(x).$$

As a result, $\Phi^{(n)}(x)$ vanishes when x is a root of $H_{n-1}(x)$ and the Taylor series may be terminated prematurely.

The algorithm was translated into FORTRAN II and run on a Scientific Data Systems 910 computer (39-bit mantissa) with the following changes:

(1) The argument was decremented by 0.25 rather than 0.5.

(2) The truncation criterion for *abs* (T) was 10^{-12} rather than 10^{-10} .

Errors, detected for $x = 1/\sqrt{2}$ and $x = 2.652$, were traced to the above described premature truncation of the relevant Taylor series. These arguments correspond to the roots of $H_2(x)$ and $H_7(x)$.

The program was therefore modified to sum a fixed number of terms, with special attention to the difficulties that might arise when expanding about roots of $H_n(x)$. In particular, in Algorithm 123, line 9, the coefficient, $A^n/n!$, of the n th term in the Taylor expansion, is obtained via the intermediate step of dividing the $(n-1)$ -term, T , by the $(n-1)$ -derivative, V . The possibility of dividing by $V = 0$ when the Taylor expansion takes place about roots of $H_{n-2}(x)$ was avoided by modifying the program to compute coefficients directly from the recursion relation,

$$A^n/n! = [A^{n-1}/(n-1)!][A/n].$$

In selecting the number of terms to be included in each Taylor series, consideration should also be given to the size of the standard decrement (specified as 0.5 in line 3 of Algorithm 123), for it is the combination of these two parameters which largely determines the accuracy and running time. A brief survey suggested that at least 10-digit accuracy could be obtained if a decrement of 0.4 were employed with 16 terms in each Taylor series; this resulted in an average running time of about 3.5 seconds per computation for arguments in the range $0 \leq x \leq 5.0$.

REFERENCE: H. MARGENAU and G. M. MURPHY, *The Mathematics of Physics and Chemistry*, pp. 119, 122. D. van Nostrand, 1943.

ALGORITHM 124 HANKEL FUNCTION

LUIS J. SCHAEFER

Purdue University, West Lafayette, Ind.

```

procedure HANKEL(N,X,H); value N,X; integer N;
real X; array H;
comment This procedure evaluates the complex valued hankel
function of the first kind for real argument X and integral order
N and assigns it to H. The individual Bessel- and Neuman-func-
tion series are not evaluated separately. Both the real and
imaginary parts are generated from the same terms;
begin real K, P, R, A, S, T, D, L; integer Q;
A := R := 1; H[1] := H[2] := S := 0;
for Q := 1 step 1 until N do begin R := R × Q; S := S +
1/Q end; D := R/N;
R := 1/R; K := X × X/4; P := (X/2)↑N; T := ln(K) +
1.1544313298631;
for Q := 0, Q+1 while Q ≤ N√L ≠ H[2] do
begin L := H[2]; H[1] := H[1] + A × K × R;
H[2] := H[2] + A × (R × K × (T - S) - (if Q < N then D/P
else 0));
A := A × K/Q; R := -R/(Q+N); S := S + 1/Q + 1/(Q+N);
if Q < N then D := D/(N-Q)
end; H[2] := H[2] × .31830989
end

```

ALGORITHM 125 WEIGHTCOEFF

H. RUTISHAUSER

Eidg. Technische Hochschule, Zurich, Switzerland

```

procedure weightcoeff (n,q,e,eps,w,x); value n; real eps;
integer n; array q,e,w,x;
comment Computes abscissae  $x_i$  and weight coefficients  $w_i$  for
a Gaussian quadrature method  $\int_0^b w(x)f(x) dx \approx \sum_{i=1}^n w_i f(x_i)$ ,
where  $\int_0^b w(x) dx = 1$  and  $w(x) \geq 0$ . The method requires the order
n, a tolerance eps and the 2n-1 first coefficients of the continued
fraction

```

$$\int_0^b \frac{w(x)}{z-x} dx = \frac{1}{z} - \frac{q_1}{1} - \frac{e_1}{z} - \frac{q_2}{1} - \frac{e_2}{z} - \dots$$

to be given, the latter as two arrays $q[1:n]$ and $e[1:n-1]$ all com-
ponents of which are automatically positive by virtue of the con-
dition $w(x) \geq 0$. The method works as well if the upper bound b
is actually infinity (note that b does not appear directly as param-
eter!) or if the density $w(x) dx$ is replaced by $d\alpha(x)$ with a mono-
tonically increasing $\alpha(x)$ with at least n points of variation. The
tolerance eps should be given in accordance to the machine ac-
curacy, e.g. as 10^{-10} for a computer with a ten-digit mantissa. The
result is delivered as two arrays $w[1:n]$ (the weight coefficients)
and $x[1:n]$ (the abscissae). For a description of the method see
H. Rutishauser, "On a modification of the QD-algorithm with
Graeffe-type convergence" [Proceedings of the IFIPS Congress,
Munich, 1962].;

```

begin
integer k;
Boolean test;
real m, p;
array g[1:n];

```

```

procedure red (a,f,n); value n; integer n; array a,f;
comment Subprocedure red reduces a heptadiagonal matrix
a to tridiagonal form as described in the paper loc. cit. Since
the bulk of the computing time of the whole method is spent
in this subprocedure, it would pay to write it in machine
code.;

```

```

begin
real c; integer j,k;
for k := 1 step 1 until n-1 do
begin
for j := k step 1 until n-1 do
begin
c := -f[j] × a[j,7]/a[j,2];
a[j,7] := 0;
a[j+1,2] := a[j+1,2] + c × a[j,5];
a[j,1] := a[j,1] - c × f[j] × a[j,4];
a[j,6] := a[j,6] - c × a[j+1,1];
a[j+1,3] := a[j+1,3] - c × a[j+1,6];
end j;
for j := k step 1 until n-1 do
begin
c := -f[j] × a[j,4]/a[j,1];
a[j,4] := 0;
a[j+1,1] := a[j+1,1] + c × a[j,6];
a[j+1,6] := a[j+1,6] + c × a[j+1,3];
a[j,5] := a[j,5] - c × a[j+1,2];
a[j+1,0] := a[j+1,0] - c × a[j+1,5];
end j;
for j := k+1 step 1 until n-1 do
begin
c := -a[j,3]/a[j-1,6];
a[j,3] := 0;
a[j,6] := a[j,6] + c × a[j,1];
a[j-1,5] := a[j-1,5] - c × f[j] × f[j] × a[j,0];
a[j,2] := a[j,2] - c × f[j] × f[j] × a[j,5];
a[j,7] := a[j,7] - c × f[j] × a[j+1,2];
end j;
for j := k+1 step 1 until n-1 do
begin
c := -a[j,0]/a[j-1,5];
a[j,0] := 0;
a[j+1,2] := a[j+1,2] + c × f[j] × a[j,7];
a[j,5] := a[j,5] + c × a[j,2];
a[j,1] := a[j,1] - c × f[j] × f[j] × a[j,6];
a[j,4] := a[j,4] - c × f[j] × a[j+1,1];
end j;
end k;
end red;

```

```

procedure qdgraeffe (n,h,g,f); value n;
integer n; array h,g,f;
comment Subprocedure qdgraeffe computes for a given
finite continued fraction

```

$$f(z) = \frac{1}{z} - \frac{q_1}{1} - \frac{e_1}{z} - \frac{q_2}{1} - \dots - \frac{q_n}{1}$$

another one, the poles of which are the squares of the poles of
 $f(z)$. However $qdgraeffe$ uses not the coefficients $q_1, \dots, q_n$
and $e_1, \dots, e_{n-1}$ of $f(z)$, but the quotients

$$\begin{cases} f_k = q_{k+1}/q_k \\ g_k = e_k/q_{k+1} \end{cases} \quad (k := 1, 2, \dots, n-1)$$

and the $h_k = \ln(\text{abs}(q_k))$ ($k := 1, 2, \dots, n$), and the results are
delivered in the same form. Procedure $qdgraeffe$ can be used
independently, but requires subprocedure red above;


```

begin
  integer k; array a[0:n,0:7];
  g[n] := f[n] := 0;
  for k := 1 step 1 until n do
    begin
      a[k-1,4] := a[k-1,5] := 1;
      a[k,1] := a[k,2] := 1 + g[k] × f[k];
      a[k,6] := a[k,7] := g[k];
      a[k,0] := a[k,3] := 0;
      comment The array a represents the heptadiagonal
        matrix Q of the paper loc. cit., but with the modifications
        needed to avoid the large numbers and with a peculiar
        arrangement.;
    end k;
    a[n,5] := 0;
    red(a,f,n);
    for k := 1 step 1 until n do
      h[k] := 2 × h[k] + ln(abs(a[k,1] × a[k,2]));
      comment A saving might be achieved by economizing the
        log-computation in the range .8 ≤ x ≤ 1.2;
    for k := 1 step 1 until n-1 do
      begin
        f[k] := f[k] × f[k] × a[k+1,2] × a[k+1,1]/(a[k,1] × a[k,2]);
        g[k] := a[k,5] × a[k,6]/(a[k+1,1] × a[k+1,2])
      end k;
    end qdgraeffe;
  L1: x[1] := q[1] + e[1];
    for k := 2 step 1 until n do
      begin
        g[k-1] := e[k-1] × q[k]/x[k-1];
        x[k] := q[k] + (if k=n then 0 else e[k]) - g[k-1];
        g[k-1] := g[k-1]/x[k];
        w[k-1] := x[k]/x[k-1];
        x[k-1] := ln(x[k-1]);
      end k;
    x[n] := ln(x[n]);
  L2: p := 1;
  L25: begin
    test := true;
    for k := 1 step 1 until n-1 do
      test := test ∧ abs(g[k] × w[k]) < eps;
    if test then go to L3;
    qdgraeffe (n,x,g,w);
  end;
  p := 2 × p;
  go to L25;
  comment What follows is a peculiar method to compute
    the wk from given ratios gk = wk+1/wk such that  $\sum_{k=1}^n w_k = 1$ ,
    but the straightforward formulae to do this might well
    produce overflow of exponent.;
  L3: w[1] := m := 0;
    for k := 1 step 1 until n-1 do
      begin
        w[k+1] := w[k] + ln(g[k]);
        if w[k] > m then m := w[k];
      end k;
    for k := 1 step 1 until n do w[k] := exp(w[k]-m);
    m := 0;
    for k := 1 step 1 until n do m := m + w[k];
    for k := 1 step 1 until n do begin w[k] := w[k]/m;
      x[k] := exp(x[k]/p) end;
  end weightcoeff

```

ALGORITHM 126

GAUSS' METHOD

JAY W. COUNTS

University of Missouri, Columbia, Mo.

```

procedure gauss (u,a,y);
real array a,y; integer u;
comment This procedure is for solving a system of linear equa-
tions by successive elimination of the unknowns. The augmented
matrix is a and u is the number of unknowns. The solution vector
is y. If the system hasn't any solution or many solutions, this is
indicated by the go to error where error is a label outside the
procedure.;
begin
  integer i,j,k,m,n;
  n := 0;
ck0: n := n + 1;
  for k := n step 1 until u do if a[k,n] ≠ 0 then go to ck1;
  go to error;
ck1: if k = n then go to ck2;
  for m := n step 1 until u+1 do
    begin
      temp := a[n,m]; a[n,m] := a[k,m]; a[k,m] := temp
    end;
ck2: for j := u + 1 step -1 until n do a[n,j] := a[n,j]/a[n,n];
  for i := k + 1 step 1 until u do
    for j := n + 1 step 1 until u + 1 do
      a[i,j] := a[i,j] - a[i,n] × a[n,j];
    if n≠u then go to ck0;
  for i := u step -1 until 1 do
    begin
      y[i] := a[i,u + 1]/a[i,i];
      for k := i - 1 step -1 until 1 do
        a[k,u + 1] := a[k,u + 1] - a[k,i] × y[i]
      end end;

```

ALGORITHM 127

ORTHO

PHILIP J. WALSH

National Bureau of Standards, Washington, D. C.

```

procedure ORTHO(W,Y,Z,X,DEV,COF,STD,CV,V,VCV,Q,Q2,E,EP,A,GF,ENF);
COF,STD,CV,V,VCV,gmdt,Q,Q2,E,EP,A,GF,ENF);
value n,m,p,r,ai,au,mi,zei,X,DEV;
real fn,gmdt;
array W,Y,Z,X,DEV,COF,STD,CV,V,VCV,Q,Q2,E,EP,A,GF,ENF;
integer n,m,p,r,ai,au,mi,zei;
switch at := at1,at2; switch ze := ze1,ze2;
switch au := au1,au2; switch mu := mu1,mu2,mu3;
comment ORTHO is a general purpose procedure which is
capable of solving a wide variety of problems. For a detailed
discussion of the applications listed below and other applica-
tions, see (1) Philip Davis and Philip Rabinowitz, "A Multiple
Purpose Orthonormalizing Code and Its Uses," J. ACM 1
(1954), 183-191, (2) Philip Davis, "Orthonormalizing Codes in
Numerical Analysis," in J. Todd (Ed.), A Survey of Numerical
Analysis, Ch. 10 (McGraw-Hill, 1962), (3) Philip Davis and
Philip Rabinowitz, "Advances in Orthonormalizing Computa-
tion," in F. L. Alt (Ed.), Advances in Computers, Vol. 2, pp. 55-
133 (Academic Press, 1961), (4) Philip J. Walsh and Emilie V.
Haynsworth, General Purpose Orthonormalizing Code, SHARE
Abstr. #850. APPLICATIONS: (a) orthonormalizing a set of

```

vectors with respect to a general inner product, (b) least squares approximation to given functions by polynomial approximations or any linear combination of powers, rational functions, transcendental functions and special functions, such as those defined numerically by a set of values, (c) curve fitting of empirical data in two or more dimensions, (d) finding the best solution in the l.s.s. to a system of m linear equations in n unknowns ($n \leq m$), (e) matrix inversion and solution of linear systems of equations, (f) expansion of functions in a series of orthogonal functions, such as a series of Legendre or Chebyshev polynomials.

The following information must be supplied to the procedure. (We are considering here the approximation feature of the procedure.)

- n the number of components per vector (excluding augmentation)
- m the number of vectors used in the approximation. For a polynomial fit of degree t , set $m=t+1$.
- p the number of augmented components per vector. A feature of this procedure is that once the approximating vectors have been orthonormalized, they may be used in approximating r functions without repeating the orthonormalization procedure on the original approximating vectors.
- r the number of functions to be approximated.
- ai a switch control concerning the approximating vectors. With $ai=1$, the procedure selects the first n components of the first row of $[Z]$, supplied by user. The i powers of these values are computed and stored into working location $[X]$, $i=0(1)m-1$. This is the usual set up for a polynomial fit. With $ai=2$, the procedure selects the first n components of the first m rows of $[Z]$ supplied by user and stores them into working location $[X]$.
- au a switch control concerning augmentation on the approximating vectors. If $p=0$, this switch is ignored. With $au=1$, regular augmentation is applied to the vectors in $[X]$. p zeros are stored after the n th component of the first m rows of $[X]$. The $(n+i)$ th component is replaced by 1.0, $i=1(1)m$. With $au=2$, special augmentation is applied to the vectors in $[X]$. The p components located after the n th component of the first m rows of $[Z]$ supplied by the user augment $[X]$.
- ze a switch control concerning augmentation on the functions to be approximated. If $r=0$, this switch is ignored. With $ze=1$, regular augmentation is applied to the functions during the calculation. The n components of the first r rows of $[Y]$ supplied by user will be augmented by p zeros when moving $[Y]$ to $[X]$. With $ze=2$, special augmentation is applied. The first n components of the first r rows of $[Y]$ are the functional values supplied by user. The next p components of the first r rows of $[Y]$ are special values also supplied by user.
- mu a switch control concerning weights. $[W]$ is an $n \times n$ real, positive definite, symmetric matrix of weights. It is generally diagonal and often the Identity matrix. $mu=1$ when $[W]=I_n$, the matrix $[W]$ need not be supplied. $mu=2$ when $[W]$ is diagonal, but not I_n . The procedure is supplied the n diagonal elements of $[W]$, but stored in the first row of matrix $[W]$. $mu=3$ when the full weighting matrix is supplied to the procedure.

The following list of matrix arrays is given to aid the user in determining the number of components and vectors in the input and results. $W[1:n,1:n]$, $Y[1:r,1:n+p]$, $Z[1:m,1:n+p]$, $X[1:m+1,1:n+p]$, $DEV[1:r,1:n]$, $COF[1:r,1:p]$, $STD[1:r]$, $CV[1:p+1,1:p]$, $VCV[1:r,1:p+1,1:p]$, $Q[1:r,1:m+1]$, $Q2$, E , $EP[1:r,1:m]$, $A[1:m,1:p]$, $GF[1:m+r]$, $ENF[1:m]$.

The results of the procedure are stored in the following locations. The user must be sufficiently familiar with the theory to know which results are relevant to his application of the procedure. All vectors are stored row-wise in the matrices listed below.

X orthonormal vectors
 DEV deviations
 COF coefficients
 STD standard deviations
 CV covariance matrix, stored in upper triangular form. The $(p+1)$ st row contains the square root of the diagonal elements of the matrix.
 VCV variance-covariance matrices, stored in upper triangular form with the $(p+1)$ st rows containing the square root of the diagonal elements. There are r such matrices, the first subscript running over the r values.
 $gmdt$ Gram determinant value
 Q Fourier coefficients
 $Q2$ squared Fourier coefficients
 E sum of the squared residuals
 EP residuals
 A a lower triangular matrix used to calculate the covariance matrix. $CV = A'A$.
 GF Gram factors
 ENF norms of the approximating vectors;
begin
integer $npp, npm, m1, n2, m2, r1, rbar, p2, bei, rhi, i18, gai, sii, i, j, dei, mu1, elz1, elz2, k, thi, ali, om1, nui$;
array $PK, XP[1:n+p], QK[1:m+1]$;
real $denom, sum, dk2, dk, fi, ss, ssq$;
switch $be := be1, be2$; **switch** $rh := rh1, rh2$; **switch** $ga := ga1, ga2$;
switch $si := si1, si2$; **switch** $de := de1, de2$; **switch** $nu := nu1, nu2$;
switch $th := th1, th2, th3$; **switch** $al := al1, al2$;
switch $om := om1, om2$;
 $npp := n+p$; $npm := n+m$; $m1 := m-1$; $n2 := n+1$; $m2 := m+1$;
 $r1 := 0$; $rbar := r$; $p2 := p+1$; $denom :=$ if $n=m$ then 1.0
else $\sqrt{n-m}$; $bei := rhi := i18 := 1$;
if ($p \neq 0$) **then** $gai := sii := 2$ **else** $gai := sii := 1$;
box1: **go to** $at[ai]$;
at1: **for** $j := 1$ **step** 1 **until** n **do begin**
 $X(2,j) := Z(1,j)$; $X[1,j] := 1.0$ **end**;
for $i := 2$ **step** 1 **until** $m1$ **do begin**
for $j := 1$ **step** 1 **until** n **do**
 $X[i+1,j] := X[i,j] \times X[2,j]$ **end**; **go to** $box2$;
at2: **for** $i := 1$ **step** 1 **until** m **do begin**
for $j := 1$ **step** 1 **until** n **do**
 $X[i,j] := Z[i,j]$ **end**;
box2: **if** $p=0$ **then** **go to** $box3$ **else** **go to** $au[au]$;
au1: **for** $i := 1$ **step** 1 **until** m **do begin**
for $j := n2$ **step** 1 **until** npp **do**
 $X[i,j] := 0.0$; $X[i,n+i] := 1.0$ **end**; **go to** $box3$;
au2: **for** $i := 1$ **step** 1 **until** m **do begin**
for $j := n2$ **step** 1 **until** npp **do**
 $X[i,j] := Z[i,j]$ **end**;
box3: $dei := nui := elz1 := elz2 := k := 1$;
box4: $thi := 1$;
box5: $ali := omi := 1$; **if** $p=0$ **then** **go to** $box6$ **else**
for $j := 1$ **step** 1 **until** p **do** $PK[n+j] := 0.0$;
box6: **go to** $mu[mu]$;
mu1: **for** $i := 1$ **step** 1 **until** n **do** $PK[i] := X[k,i]$;
go to $box7$;
mu2: **for** $i := 1$ **step** 1 **until** n **do**
 $PK[i] := X[k,i] \times W[1,i]$; **go to** $box7$;
mu3: **for** $i := 1$ **step** 1 **until** n **do begin** $sum := 0.0$;
for $j := 1$ **step** 1 **until** n **do** $sum := sum + X[k,j] \times W[i,j]$; $PK[i] := sum$ **end**;
box7: **go to** $om[om]$;
om1: **for** $i := 1$ **step** 1 **until** k **do begin** $sum := 0.0$;
for $j := 1$ **step** 1 **until** npp **do**
 $sum := sum + PK[j] \times X[i,j]$; $QK[i] := sum$ **end**;
go to $box8$;

```

om2: dk2 := 0.0; for i := 1 step 1 until npp do
    dk2 := dk2 + PK[i] × X[k,i];
    dk := sqrt(dk2);
    GF[i18] := dk; i18 := i18 + 1;
    for i := 1 step 1 until npp do
        X[k,i] := X[k,i]/dk;
        omi := 1; go to box6;
box8: go to de[dei];
    del: elz1 := -elz1; if elz1 < 0 then go to box8b else
        go to box8a;
box8a: for i := 1 step 1 until k-1 do
    QK[i] := -QK[i]; QK[k] := 1.0;
    for i := 1 step 1 until npp do begin
        sum := 0.0; for j := 1 step 1 until k do
            sum := sum + X[j,i] × QK[j];
        XP[i] := sum end; go to box9;
box8b: ENF[i18] := sqrt(QK[k]); go to box8a;
    de2: elz2 := -elz2; if elz2 < 0 then go to box8c else
        go to box8a;
box8c: for i := 1 step 1 until m do begin
    Q[r1,i] := QK[i]; Q2[r1,i] := QK[i] × QK[i] end;
    Q[r1,m2] := QK[m2]; E[r1,1] := Q[r1,m2] - Q2[r1,1];
    for j := 2 step 1 until m do
        E[r1,j] := E[r1,j-1] - Q2[r1,j];
    fi := 1.0;
    for i := 1 step 1 until m do begin
        if (fn-fi) > 0.0 then begin if E[r1,i] < 0.0 then begin
            EP[r1,i] := -sqrt(abs(E[r1,i])/(fn-fi)); go to box8d
        end
        else EP[r1,i] := sqrt(E[r1,i]/(fn-fi));
        go to box8d; end else E[r1,i] := -1.0;
box8d: fi := fi + 1.0; end go to box8a;
box9: go to th[thi];
    th1: for i := 1 step 1 until npp do
        X[k,i] := XP[i]; go to box10;
    th2: for i := 1 step 1 until n do
        DEV[r1,i] := XP[i];
        for i := 1 step 1 until p do
            COF[r1,i] := -XP[n+i]; thi := 3; go to th1;
    th3: go to box11;
box10: go to al[ali];
    al1: omi := ali := 2; go to box6;
    al2: if k < m then begin k := k+1; go to box4; end
        else go to box12;
box11: go to nu[nui];
    nu1: nui := 2; go to box14;
    nu2: ss := dk/denom; ssq := ss × ss;
        STD[r1] := ss; go to box14;
box12: go to be[bei];
    be1: for i := 1 step 1 until m do begin
        for j := 1 step 1 until p do
            A[i,j] := X[i,n+j] end;
        gmdt := 1.0; for i := 1 step 1 until m do
            gmdt := gmdt × (GF[i]/ENF[i]);
        gmdt := gmdt × gmdt; dei := bei := thi := 2;
        k := k+1; go to box13;
    be2: go to box11;
box13: go to ga[gai];
    ga1: go to box11;
    ga2: for i := 1 step 1 until p do begin
        for j := i step 1 until p do begin
            sum := 0.0;
            for nii := 1 step 1 until m do
                sum := sum + A[nii,i] × A[nii,j];
            CV[i,j] := sum end end;
        for i := 1 step 1 until p do
            CV[p2,i] := sqrt(CV[i,i]); gai := 1; go to box11;

```

```

box14: go to rh[rhi];
    rh1: if rbar = 0 then go to final else rbar := rbar - 1;
        r1 := r1 + 1; thi := rhi := 2; go to ze[zei];
    ze1: for i := 1 step 1 until n do
        X[m2,i] := Y[r1,i];
        for i := 1 step 1 until p do
            X[m2,n+i] := 0.0; go to box5;
    ze2: for i := 1 step 1 until npp do
        X[m2,i] := Y[r1,i]; go to box5;
    rh2: go to si[sii];
    si1: go to rh1;
    si2: for i := 1 step 1 until p do begin
        for j := i step 1 until p do
            VCV[r1,i,j] := ssq × CV[i,j] end;
        for i := 1 step 1 until p do
            VCV[r1,p2,i] := ss × CV[p2,i]; go to rh1;
    final: end ortho

```

ALGORITHM 128 SUMMATION OF FOURIER SERIES M. WELLS University of Leeds, Leeds 2, England*

* Currently with Burroughs Corp., Pasadena, Calif.

```

procedure Fourier (X, r, w, n, A, B);
    value n; real X, w, A, B; integer r, n;
    comment Fourier sums a one-dimensional Fourier series,
        using a recurrence relation described by Watt [Computer
        J. 1, 4 (1959) 162]. The parameters are the coefficients X, which
        are selected by r, w, the argument and n the total number of
        terms in the series. On exit A =  $\sum_{r=0}^{n-1} X_r \cos(rw)$  and
        B =  $\sum_{r=0}^{n-1} X_r \sin(rw)$ . Fourier is particularly efficient
        where  $X_r = 0$  for all  $r > \text{some } r_1$  and  $X_r \neq 0$  for all  $r \leq r_1$ ;
    begin real t, tr, tr1, cosw2;
        tr1 := 0; cosw2 := 2 × cos(w);
        for r := n-1 step -1 until 0 do
            begin if X ≠ 0 then go to term end search for nonzero term;
            tr := 0; go to all zeroes;
        term: tr := X; for r := r-1 step -1 until 0 do
            begin t := tr × cosw2 + X - tr1; tr1 := tr; tr := t end
            recurrence;
        all zeros: A := tr - tr1 × cosw2/2; B := tr1 × sin(w)
    end Fourier series

```

CERTIFICATION OF ALGORITHM 128 [C6] SUMMATION OF FOURIER SERIES [M. Wells, Comm.

ACM 5 (Oct. 1962), 513]

HENRY C. THACHER, JR.* (Recd. 18 Mar. 1964)

Argonne National Lab., Argonne, Ill.

* Work supported by the U.S. Atomic Energy Commission

The body of *Fourier* was transcribed for the Dartmouth SCALP translator for the LGP-30 computer. After uniformizing the spelling of zeros (lines 5 and 9 in the procedure body), the program compiled and ran without difficulty.

In the procedure statement for *Fourier*, the actual parameter corresponding to X should be an expression depending on the actual parameter corresponding to r.

The SCALP program was tested for the finite series:

$$A = \sum_{r=0}^{n-1} \cos rw = \frac{\sin((n-1)w/2)}{\sin(w/2)} \cos(nw/2) + 1$$

$$B = \sum_{r=0}^{n-1} \sin rw = \frac{\sin((n-1)w/2)}{\sin(w/2)} \sin(nw/2)$$

for $w = 0.1, 0.2, 0.5$ and 1.0 , and for $n = 1(1)51$. Although the algorithm appears to be numerically correct, the results showed evidence of serious numerical instability, particularly for small values of w . For $w = 0.1$, and $n = 51$, the error in A was .00109, and in B , -.00231. Since the largest A for $n < 51$ is 10.5, and the largest B about 20, the best result obtainable with the 7+ significant digit arithmetic of the SCALP system is about .00001. For comparison, a program summing the same series using a forward recurrence based on the addition formulas for the sine and cosine gave errors of .00012 and -.00018. It was, however, only about half as fast.

ALGORITHM 129

MINIFUN

V. W. WHITLEY

Signal Missile Support Agency, White Sands Missile Range, N. Mex.

procedure MINIFUN ($t1, b1, eps, n, ncnt, fmin, xmin, k1, GFUN$);

value $t1, b1, eps, n, ncnt$; **integer** $n, ncnt, k1$; **real** $fmin$;

real procedure $GFUN$; **array** $t1, b1, eps, xmin$;

comment MINIFUN is a subroutine to find the minimum of a function of n variables, using the method of steepest descent. Input is:

1. $t1(i)$, $i = 1, 2, \dots, n$, the upper limits of the search region
2. $b1(i)$, $i = 1, 2, \dots, n$, the lower limits of the search region
3. $eps(i)$, $i = 1, 2, \dots, n$, the convergence criteria. The function must be a minimum in the region $|x(i) - xmin(i)| \leq eps(i)$
4. n , the number of variables (the dimension of the arrays)
5. $ncnt$, the maximum number of iterations. The routine searches for a minimum until $|x(i) - xmin(i)| \leq eps(i)$ for all i , or until $icnt = ncnt$, whichever happens first.

Output is:

1. $fmin$, the minimum value of the function
2. $xmin(i)$, $i = 1, \dots, n$, the point at which the minimum occurs
3. $k1$, an error code

If $k1 = 1$, a minimum has been found within the specified number of iterations and the minimum is less than all values of the function at the centers of the planes forming the boundary of the epsilon-cube

If $k1 = 2$, $\Delta x(i) \leq eps(i)$ but a new minimum has been found

If $k1 = 3$, $ncnt$ has been exceeded without $\Delta x(i) \leq eps(i)$. In this case, a test is made to see if the current minimum is a minimum in the epsilon-cube.

MINIFUN has been written as a FORTRAN II subroutine and is available from the SMSA Computation Center. It should be noted that the FORTRAN II deck has been tested only on some relatively simple functions of two variables, such as $GFUN(x, y) = \cos(xy)$. The writer does not claim that the algorithm has been thoroughly tested;

begin **integer** $j, i, icnt, k$; **real** $w, dmax, alamb, ft$;
array $wnew[1:n], xt[1:n], xlb[1:n], xub[1:n]$,
 $delx[1:n], d12x[1:n], xmin[1:n], x[1:n, 1:4], g[1:n, 1:4]$,
 $dxmin[1:n], d2xmn[1:n]$;

comment start looking for a minimum at midpoint of region;
for $j := 1$ **step** 1 **until** n **do**

begin $wnew[j] := (t1[j] + b1[j])/2$; $xt[j] := wnew[j]$;
 $xub[j] := t1[j]$; $xl[b[j] := b1[j]$; $delx[j] := (xub[j]$
 $- xlb[j])/5$;
 $d12x[j] := delx[j]^2$; $xmin[j] := xt[j]$

end;

$fmin := GFUN(xmin)$;

for $j := 1$ **step** 1 **until** n **do**

begin $w := xt[j]$; **for** $i := 1$ **step** 1 **until** 4 **do**

begin $x[j, i] := xlb[j] + i \times delx[j]$;

$xt[j] := x[j, i]$; $g[j, i] := GFUN(xt)$;

end;

$xt[j] := w$;

$dxmin[j] := (g[j, 3] - g[j, 2])/delx[j]$;

$d2xmn[j] := (g[j, 4] - g[j, 3] - g[j, 2] + g[j, 1])/d12x[j]$

end;

comment first and second difference quotients have been computed;

$icnt := 0$; $dmax := dxmin[1]$; $k := 1$;

nustep: **for** $j := 2$ **step** 1 **until** n **do**

begin **if** $abs(dmax) < abs(dxmn[j])$ **then**

begin $dmax := dxmn[j]$; $k := j$

end;

end;

$alamb := dxmin[k]/d2xmn[k]$; $w := xt[k] - alamb$;

comment a new coordinate has been computed for the variable having the largest first partial derivative. It will be checked to see if the new point still lies within the region and search will continue;

if $w < b1[k]$ **then** $w := b1[k]$ **else if** $w > t1[k]$ **then** $w := t1[k]$;

$xt[k] := w$; $ft := GFUN(xt)$;

if $ft < fmin$ **then go to check else**

restart: **if** $xt[k] < wnew[k]$ **then go to** $1bdchk$

else if $xt[k] = wnew[k]$ **then go to** $stnubds$

else if $t1[k] > xt[k]$ **then go to** $nupbds$

else $xt[k] := 1.5 \times wnew[k]$;

$nupbds$: $xub[k] := t1[k]$; $xl[b[k] := 2 \times xt[k] - t1[k]$; **go to** $newdel$;

$stnubds$: $xlb[k] := xt[k] - 0.5 \times wnew[k]$; $xub[k] := xt[k] + 0.5 \times wnew[k]$;

$newdel$: $delx[k] := 0.2 \times (xub[k] - xlb[k])$; $d12x[k] := delx[k]^2$;

for $i := 1$ **step** 1 **until** 4 **do**

begin $x[k, i] := xlb[k] + i \times delx[k]$; $w := xt[k]$;

$xt[k] := x[k, i]$; $g[k, i] := GFUN(xt)$; $xt[k] := w$

end;

$dxmin[k] := (g[k, 3] - g[k, 2])/delx[k]$;

$d2xmn[k] := (g[k, 4] - g[k, 3] - g[k, 2] + g[k, 1])/d12x[k]$;

$icnt := icnt + 1$;

if $icnt > ncnt$ **then go to** $outed$ **else go to** $nustep$;

$1bdchk$: **if** $xt[k] \leq b1[k]$ **then** $xt[k] := 0.5 \times wnew[k]$

else $xlb[k] := b1[k]$; $xub[k] := 2.0 \times xt[k] - b1[k]$;

go to $newdel$;

check: $fmin := ft$; $xmin[k] := xt[k]$;

for $j := 1$ **step** 1 **until** n **do if** $delx[j] > eps[j]$ **then go to** $restart$;

recheck: **for** $j := 1$ **step** 1 **until** n **do**

begin $w := xmin[j]$; $xmin[j] := w + eps[j]$; $ft := GFUN(xmin)$;

if $ft < fmin$ **then go to** $set2$; $xmin[j] := w - eps[j]$;

$ft := GFUN(xmin)$; **if** $ft < fmin$ **then go to** $set2$; $xmin[j] := w$

end;

if $k1 < 3$ **then** $k1 := 1$; **go to** $bgend$;

$set2$: $k1 := 2$; **go to** $bgend$;

$outed$: $k1 := 3$; **go to** $recheck$;

$bgend$: **end** MINIFUN;

REMARK ON ALGORITHM 129 MINIFUN
 MINIFUN [V. W. Whitley, *Comm. ACM*, Nov. 1962]
 E. J. WASSCHER
 Philips Research Laboratories
 N. V. Philips' Gloeilampenfabrieken
 Eindhoven-Netherlands

Some errors found in Algorithm 129 MINIFUN [*Comm. ACM*, Nov. 1962] are given below.

In addition, the way "steepest descent" is used to compute the minimum of a function of n variables is not entirely satisfactory. The method for computing first derivatives may be improved in two ways:

1. Instead of computing $\frac{f(x+h)-f(x)}{h}$ it is better to take $\frac{f(x+h)-f(x-h)}{2h}$. As $f(x-h)$ has been computed by MINIFUN this does not give rise to extra computations.

2. In MINIFUN the choice of h seems rather deliberate. Indeed, h is taken as $2 \times (xub - xlb)$, where xub and $xl b$ are variable bounds of x . In the beginning of the program these bounds are put equal to the fixed bounds $b1$ and ub ; afterwards in the iteration process they should tend towards each other, and in the limit they provide the minimum. So especially when a good approximation to the minimum is unknown, $b1$ and ub have to be taken well apart from each other, which means that h is rather large. At the limit, however, h is very small. It is better to take h in such a way that the nominator $f(x+h)-f(x-h)$ attains an appropriate value.

As the method used by MINIFUN is the Newton-Raphson method applied to the first derivatives, convergence is not always secured—especially since first and second partial derivatives are estimated with numerical methods.

It should be noted that the test on end of program is not correct. For a further possible decrease of the function one has not to look in the direction of the coordinate axes but in the direction of the steepest descent.

ALGOL descriptions of some "steepest descent" programs which were written in the symbolic code of the Philips computer Pascal [cf. H. J. Heijn and J. C. Selman, *IRE Trans. EC10* (June 1961), 175-183] are given in Algorithms 203, 204 and 205.

CORRECTIONS OF MINIFUN:

Printing errors: The line below label *nustep* should read:

begin if abs(dmax) < abs(dxmin[j]) then

The label 1 *bdcchk* should be *lbdchk*

In comment MINIFUN: $k1=2$: a new minimum has not been found.

The label *nustep* should be placed before the statement: $dmax := dxmin[j]$; The declaration of $xmin$ should be removed from the blockhead of the procedure body. The 2-dimensional arrays $x[1:n, 1:4]$ and $g[1:n, 1:4]$ can be replaced by a real x and a 1-dimensional array $g[1:4]$ respectively.

An improvement could be the insertion of the statement

$k1 := 1$;

just before the label *nustep*.

I am having considerable trouble with the obviously important part played by the array *wnew*, although it does not change after being set in the first statement of the program. Furthermore it seems to me that *wnew* plays a double rôle: first the component $wnew[k]$ is the value of $xt[k]$ before an iteration on $xt[k]$. But then one should insert another statement after label *nustep*: $wnew[k] := xt[k]$; Secondly $wnew[k]$ is to be understood as half the distance between upper and lower bound $tl[k]$ and $b1[k]$, which is only true when $b1[k] = 0$.

Convergence of $delx[j]$ to 0 is only achieved when $xlb[k]$ and $xub[k]$ are tending towards each other. This indicates that $wnew[k]$ should go to 0 too. (See statements after label *stnubds*.)

The following modifications could remove these objections (starting with the line above label *restart*):

```

    if  $ft < fmin$  then go to check else  $xt[k] := wnew[k]$ ;
restart: if  $xt[k] < wnew[k]$  then go to lbdchk;
        if  $xt[k] = wnew[k]$  then go to stnubds;
        if  $xt[k] < tl[k]$  then go to nupbds;
         $xt[k] := 0.5 \times (wnew[k] + tl[k])$ ;
nupbds:  $xub[k] := tl[k]$ ;  $xlb[k] := 2 \times xt[k] - tl[k]$ ; go to
        newdel;
stnubds:  $xlb[k] := xt[k] - 0.5 \times (wnew[k] - xlb[k])$ ;
         $xub[k] := xt[k] + 0.5 \times (wnew[k] - xlb[k])$ ; (etc.)
lbdchk: if  $xt[k] = b1[k]$  then  $xt[k] := 0.5 \times (wnew[k] + b1[k])$ ;
         $xlb[k] := b1[k]$ ;  $xub[k] := 2 \times xt[k] - b1[k]$ ; go to
        newdel; (etc.)

```

ALGORITHM 130
 PERMUTE

Lt. B. C. EAVES

U.S.A. Signal Center and School, Fort Monmouth, N. J.

procedure PERMUTE (A, n, x)

array A ; integer n, x ;

comment Each entry into PERMUTE generates the next permutation of the first n elements of A . If A is read as a number ($A[1]A[2] \dots A[n]$), each generation is larger than the last:

$n := 4, x := 1$
 $A[1] \quad 1 \quad 1 \quad 1 \quad 8 \quad 8 \quad 8$
 $A[2] \quad 1 \quad 8 \quad 8 \quad 1 \quad 1 \quad 8$
 $A[3] \quad 8 \quad 1 \quad 8 \quad 1 \quad 8 \quad 1$
 $A[4] \quad 8 \quad 8 \quad 1 \quad 8 \quad 1 \quad 1$ end
 Permutations = $\frac{4!}{2!2!}$

Identical elements in A reduce the number of permutations. The array should be ordered before the first call on PERMUTE. Integer x specifies the first elements whose order should be preserved: $n := 4, x := 3$

$A[1] \quad 1 \quad 1 \quad 1 \quad 4$
 $A[2] \quad 2 \quad 2 \quad 4 \quad 1$
 $A[3] \quad 3 \quad 4 \quad 2 \quad 2$
 $A[4] \quad 4 \quad 3 \quad 3 \quad 3$ end
 Permutations = $\frac{4!}{3!}$

Before the first call on PERMUTE for a given array, *first* should be made true. If *more* is true, then PERMUTE was able to give another permutation;

```

begin array  $B[1:n]$ ; integer  $f, i, k, m, p$ ; real  $r$ ; own real  $t$ ;
if first then  $t := A[x]$ ; first := false;
for  $i := 1$  step 1 until  $n$  do  $B[i] := 0$ ;
for  $i := n$  step -1 until 2 do

```

```

    begin if  $A[i] > t \wedge A[i] > A[i-1]$  then go to find; end;
    more := false; go to exit;

```

```

find: for  $k := n$  step -1 until  $i$  do
    begin if  $A[k] > t \wedge A[k] > A[i-1]$  then
        begin  $B[k] := A[k]$ ;  $m := k$ ; end; end;

```

```

for  $k := n$  step -1 until  $i$  do
    begin if  $B[k] > 0 \wedge B[k] < B[m]$  then
        begin  $B[m] := B[k]$ ;  $f := k$ ; end; end;

```

```

 $r := A[i-1]$ ;  $A[i-1] := B[m]$ ;  $A[f] := r$ ;

```

```

schell:  $p := i-1$ ;  $m := n-p$ ;
for  $m := m/2 - 1$  while  $m > 0$  do
    begin  $k := n-m$ ;
    for  $f := p+1$  step 1 until  $k$  do

```

```

        begin  $i := f$ ;
        if  $A[i] > A[i+m]$  then
            begin  $r := A[i+m]$ ;  $A[i+m] := A[i]$ ;
             $A[i] := r$ ;  $i := i+m$ ;
            if  $i \geq p+1$  then go to comp;
            end end end schell;

```

exit: end PERMUTE

ALGORITHM 131 COEFFICIENT DETERMINATION*

V. H. SMITH AND M. L. ALLEN

Georgia Institute of Technology, Atlanta 13, Ga.

* This procedure pertains to research work sponsored in part by NSF Grant G-7361.

procedure DET (*n*, *G*, *H*);
array *G*, *H*; **integer** *n*;
comment Given the first *n* coefficients of the power series $G(z) = g_1 + g_2z + g_3z^2 + \dots + g_nz^{n-1} + \dots$, and $H(z) = h_1 + h_2z + h_3z^2 + \dots + h_nz^{n-1} + \dots$, this procedure determines the coefficients d_i , $i = 1, \dots, n$, of the power series which is the expansion of the quotient $H(z)/G(z)$. It is assumed that $g_1 \neq 0$. The arrays *G* and *H* initially contain the coefficients of $G(z)$ and $H(z)$, respectively. The integer *n* is the number of known coefficients in the expansion of $G(z)$ and $H(z)$. At the conclusion, *H*, contains the coefficient d_i . The procedure may also be useful in calculating residues for certain complex functions. Suppose $F(z) = H(z)/G(z)$ is a complex valued function of a complex variable and that *F* has a pole of order *m* at $z = b$, where $H(z) = \sum_{k=1}^{\infty} h_k(z-b)^{k-1}$, $G(z) = \sum_{k=1}^{\infty} g_k(z-b)^{k+m-1}$, and $g_1 \neq 0$, $h_1 \neq 0$. The required residue at $z = b$ is d_m where

$$D(z) = \left[\sum_{k=1}^{\infty} h_k(z-b)^{k-1} \right] / \left[\sum_{k=1}^{\infty} g_k(z-b)^{k-1} \right] \\ = \sum_{i=1}^{\infty} d_i(z-b)^{i-1}.$$

For more on this, one is referred to Einar Hille, "Analytic Function Theory, Vol. I," Ginn and Co., 1959, pages 242-244;

```
begin integer i, j, n; real alpha, beta;  
    alpha := 1/G[1];  
    for j := 1 step 1 until n do  
    begin beta := alpha × H[j];  
    for i := j + 1 step 1 until n do  
        H[i] := H[i] - (beta × G[i - j + 1]) end;  
    for j := 1 step 1 until n do  
        H[j] := H[j] × alpha;  
end DET
```

ALGORITHM 132 QUANTUM MECHANICAL INTEGRALS OVER ALL SLATER-TYPE INTEGRALS

J. C. BROWNE

The University of Texas, Austin, Tex.

real procedure: *allslater* (*p*, *q*, *pe*, *qe*, *np*, *nq*, *lp*, *lq*, *mp*, *mq*, *na*, *nb*)
internuclear distance: (*r*);
real *pe*, *qe*, *r*; **integer** *p*, *q*, *np*, *nq*, *lp*, *lq*, *mp*, *mq*,
na, *nb*;

comment The Slater-type orbitals frequently used in quantum mechanical calculations on atoms and molecules are defined as $p = k(np, pe) r^{np-1} e^{-(pe)r} Y_{lp}^{mp}(\theta, \phi)$, where $k(np, pe)$ is a normalization constant, $Y_{lp}^{mp}(\theta, \phi)$ is a spherical harmonic with the phase convention $[Y_{lp}^{mp}(\theta, \phi)]^* = (-1)^m Y_{lp}^{-m}(\theta, \phi)$, *np* is a positive integer, *lp* is an integer, $lp < np$, *mp* is an integer, $-lp \leq mp \leq lp$; and *pe* is a real positive constant. Algorithm 110, Y. A. Kruglyak and D. R. Whitman (Comm. ACM, July 1962) serves to compute integrals over certain operators of a quite restricted class of Slater-type orbitals, $np \geq 4$, $lp = 1$, $mp = 0$. The algorithm given here will compute all integrals of the form

$$\int p_c(r_c^{n_c}) q_c dr$$

which can be expressed in terms of the simple $A_n(b)$ and $B_n(a)$ functions. The subscript *c* denotes either of the two nuclei of a diatomic molecule. These integrals include all those one-electron integrals necessary for a conventional energy calculation on a diatomic molecule. In the arguments of *allslater* *p* and *q* are numerical designations for the respective orbitals. *p* and *q* are even or odd as they respectively are associated with the "left," *a*, nucleus or "right," *b*, nucleus of a diatomic molecule. Global arrays, *fact* 1, of factorials and *binom*, of binomial coefficients are assumed. We first define some procedures utilized by *allslater*. The main program begins at the label *set*;

```
begin real norm, r2, alpha, beta, s, clp, clq, bpci;  
integer nsum, lsum, peven, qeven, podd, godd, limitp, limitq,  
g, h, i, j, nlp, nlq, lmp, lmq, gama, gamb, aidaa, aidab, gami,  
aida, num2; real array avalues [0:21], bvalues [0:21]; real procedure cl, bpc, modulus;  
real procedure cl (l, m, j); value l, m, j, integer l, m, j;  
    begin cl := ((-1)j) × fact1[2 × (l - j)] / ((2l) × fact1[l - 2 × j - m] × fact1[l - j] × fact1[j])  
    end cl;  
real procedure bpc (i, j, k); value i, j, k, integer i, j, k;  
    begin real t; integer m; t := 0;  
    for m := 0 step 1 until k do  
        begin t := t + ((-1)j) × (k - m) × binom [i, m] × binom [j, k - m]  
        end  
    end bpc;  
real procedure modulus (i, j); value i, j; integer i, j;  
    begin modulus := 1 - abs (i ÷ j) × j  
    end modulus;  
procedure avector (b, nmax, avalues); value b, nmax;  
    real b; integer nmax; real array avalues;  
    begin integer m;  
    avalues[0] = exp (-b) / b;  
    if nmax = 0 then go to exit;  
    for m = 1 step 1 until nmax do  
        avalues[m] = avalues[0] + (m / b) × avalues[m - 1]  
    end;  
exit: end avector;  
procedure bvector (a, nmax, bvalues); value a, nmax; real a;  
    integer nmax; real array bvalues; real procedure modulus;  
comment This procedure computes a sequence of values for the integral,  $B_n(a) = \int_{-1}^1 x^n e^{-ax} dx$ , for  $n = 0$  to  $n = nmax$ . If  $a \geq alim$  then  $B_0(a)$  is computed and upward recursion is used to generate the higher n values. If  $a < alim$  then  $B_{nmax}(a)$  is computed by series expansion and downward recursion is used to generate the smaller n values. alim is determined within the program by a simplification of a result of Gautschi (J. ACM 8, 21 (1961)). Gautschi has made an analysis of the recursive procedures for the  $B_n(a)$  which could be taken as a model for workers in molecular quantum mechanics;  
begin real fx, fy, numerator, denom, sum, factor1, tsum,  
factor2, t, aa; integer m, mn;  
    begin if abs (a) ≥ ((nmax + nmax / 6 + 3) / 2.3) then  
        up: begin fx := exp (a);  
        fy := 1 / fx;  
        bvalues [0] := (fx - fy) / a;  
        for m := 1 step 1 until nmax do  
            begin fx := - fx;  
            bvalues [m] := (fx - fy + m × bvalues [m - 1]) / a  
            end;  
        go to exit;  
    end up;  
    down: begin aa := axa;
```

```

    if modulus (nmax, 2) ≠ 0 then
    setodd: begin numerator := nmax + 2;
            sum := a/numerator;
            factor1 := -2;
            factor2 := 3;
            go to compute;
        end setodd;
    seteven: begin numerator := nmax + 1;
            sum := 1/numerator;
            factor1 := factor2 := 2;
            end seteven;
    compute: begin denom := numerator + 2;
            t := sum;
            t := (((t/factor2)×aa)
                /(factor2-1))×numerator
                /denom;
            tsum := t + sum;
            if (sum-tsum)=0 then
            begin bvalues[nmax] := sum × factor1;
                go to recur;
            end;
            begin factor2 := factor2 + 2;
                numerator := denom;
                sum := tsum;
                go to compute;
            end compute;
    recur: begin fxx := exp(a);
            fxy := 1/fxx;
            mn := nmax - 1;
            if modulus(nmax, 2) ≠ 0 then
            fxx := -fxx;
            for m := mn step -1 until 0 do
            begin fxx = -fxx;
                bvalues[m] := (fxx+fxy + a ×
                    bvalues[m+1])/(m+1);
            end
            end recur;
        end down;
    end;
exit: end bvector;
set: begin if (mp + mq) ≠ 0 then
        begin allslater := 0.0; go to exit end;
    set: begin norm := sqrt (((2×pe)↑
        (2×np+1) × (2×lp+1) × fact1[lp-mp] × (2×qe)↑
        (2×ng+1) × (2×lq+1) × fact1[lq-mq])/(fact1[2×
        np] × fact1[lp+mp] × fact1[2×ng] × fact1[lq+mq] ×
        4));
        nsum := np+ng;
        lsum := lp+lq;
        r2 := r/2;
        norm := norm × (r2↑(nsum+1+na+nb));
        alpha := r2 × (pe+qe);
        beta := r2 × (((-1)↑p)×pe + ((-1)↑q) × qe);
        num2 := 2;
        avector (alpha, nsum, avalues);
        bvector (beta, nsum, bvalues);
        peven := modulus (p+1,2);
        qeven := modulus (q+1,2);
        podd := modulus (p,2);
        qodd := modulus (q,2);
        limitp := (lp-mp)÷num2;
        limitq := (lq-mq)÷num2;
        s := 0;
    end set;
sum: begin for g := 0 step 1 until limitp do
        begin clp := cl(lp,mp,g);
        for h := 0 step 1 until limitq do

```

```

        begin clq := cl(lq,mq,h);
            nlp := np-lp+2×g-1;
            nlp := nq-lq+2×h-1;
            lmp := lp-mp-2×g;
            lmp := lq-mq-2×h;
            gama := nlp × peven + nlp × qeven + 1 + na;
            gamb := nlp × podd + nlp × godd + 1 + nb;
            aidaa := lmp × peven + lmq × qeven;
            aidab := lmp × podd + lmq × godd;
            gam = gama + gamb;
            aida = aidaa + aidab;
            for i := 0 step 1 until gam do
            begin bpci := bpc(gama, gamb, i);
            for j := 0 step 1 until aida do
            begin
                s := s + clp × clq × bpci ×
                    bpc(aidaa, aidab, j) ×
                    avalues[nsum+na+nb-i-j]
                    × bvalues[lsum-2 × (g+h) + i-j];
            end
            end
            end;
            allslater := s × norm;
        end sum;
    exit: end;
end allslater;

```

ALGORITHM 133

RANDOM

PETER G. BEHRENS

Mathematikmaskinnämnden, Stockholm, Sweden

real procedure *RANDOM* (A, B, X0);

value A, B, X0;

real A, B;

integer X0;

comment *RANDOM* generates a rectangular distributed pseudo-random number in the interval $A < B$. *X0* is an integer starting-value. The first time *RANDOM* is used in a program *X0* should be a positive odd integer with 11 digits, $X0 < 2^{25} = 34\,359\,738\,368$. The following times *RANDOM* is used, *X0* should be $X0 = 0$. The mathematical method used is $X_{n+1} = 5 X_n \pmod{2^{25}}$. This sequence has period 2^{25} . *RANDOM* was successfully run on *FACIT EDB* using *FACIT-ALGOL 1*, which is a realization of *ALGOL 60* for *FACIT EDB*, except for the declarator *own*, which is not included in *FACIT-ALGOL 1*. To test *RANDOM*, we computed $1/N \sum X_n$ and $1/N \sum X_n^2$ in the interval 0,1 for $N = 500, 1000, 5000$. The starting-value was $X0 = 28\,395\,423\,107$. The results were 0.50625, 0.48632, 0.50304 and 0.34304, 0.31681, 0.33469. Theoretically one expects 0.50000 and 0.33333;

begin

integer *M35*, *M36*, *M37*;

own integer *X*;

if $X0 \neq 0$ then begin

$X := X0$; $M35 := 34\,359\,738\,368$; $M36 := 68\,719\,476\,736$;

$M37 := 137\,438\,953\,472$ end; $X := 5 \times X$;

if $X \geq M37$ then $X := X - M37$;

if $X \geq M36$ then $X := X - M36$;

if $X \geq M35$ then $X := X - M35$;

RANDOM := $X/M35 \times (B - A) + A$ end

CERTIFICATION OF ALGORITHM 133

RANDOM [Peter G. Behrenz, *Comm. ACM*, Nov. 1962]

JESSE H. POORE, JR.

Louisiana Polytechnic Institute, Ruston, La.

Algorithm 133 was transliterated into FORTRAN II for the IBM 1620 computer. A monitor program performed the test indicated in Algorithm 133 on the generated numbers.

Results of the test are shown in the following chart. The notation used is identical to that used in the algorithm.

N_n	$\frac{1}{N} \sum X_n$	$\frac{1}{N} \sum X_n^2$	
13543288579	.4986480931	.3280561242	$N = 500$
	.4840396640	.3141520616	$N = 1000$
	.4996829627	.3321160892	$N = 5000$
24376589411	.4971414796	.3297990588	$N = 500$
	.4997720126	.3326801987	$N = 1000$
	.4986380784	.3319949173	$N = 5000$
34359738367	.4962408238	.3339214303	$N = 500$
	.4974837457	.3335720239	$N = 1000$
	.4929612237	.3253421270	$N = 5000$
11324679915	.5313808305	.3691599122	$N = 500$
	.5167083685	.3498558251	$N = 1000$
	.5043814637	.3383429327	$N = 5000$

REMARK ON ALGORITHM 133

RANDOM (P. G. Behrenz, *Comm. ACM*, Nov. 1962)

PETER G. BEHRENTZ

Matematikmaskinnämnden, Box 6131, Stockholm 6, Sweden

Replace the declarations in the body of the procedure,
integer M35, M36, M37; own integer X;

by:

own integer X, M35, M36, M37;

This sequence of 2^{25} random numbers contains about 15 numbers which are not really random numbers. For details, see R. W. Hamming, *Numerical Methods for Scientists and Engineers*, p. 384 [McGraw-Hill, 1962].

REMARK ON ALGORITHM 133

RANDOM [Peter G. Behrenz, *Comm. ACM* 11, Nov. 1962]

DONALD L. LAUGHLIN

Missouri School of Mines and Metallurgy, Rolla, Missouri

Algorithm 133 was translated into FORTRAN II for the IBM 1620 and run successfully. The starting value was changed to 21 348 759 609 and significant results followed.

For $N = 500$ and 1000, the resulting values were: 0.4990157688, 0.4986269653 and 0.3318717863, 0.3290401482.

ALGORITHM 134

EXPONENTIATION OF SERIES

HENRY E. FETTIS

Aeronautical Research Laboratories, Wright-Patterson Air Force Base, Ohio

procedure SERIESPWR(A, B, P, N);

comment This procedure calculates the coefficients $B[i]$ for the series $(f(x))^P = g(x) \div 1 + \sum B[i] \times x \uparrow i, (i = 1, 2, \dots, N)$ given the coefficients of the series $f(x) = 1 + \sum A[i] \times x \uparrow i$.
 P may be any real number;

value A, P, N;

array A, B;

integer N;

begin integer i, k;

real p, s;

B[1] := P × A[1];

for i := 2 step 1 until N do

begin s := 0;

for k := 1 step 1 until i-1 do

S := s + (P × [i-k] - k) × B[k] × A[i-k];

B[i] := P × A[i] + (s/i)

end for i;

end SERIESPWR

CERTIFICATION OF ALGORITHMS 134 AND 158

EXPONENTIATION OF SERIES [Henry E. Fettis,

COMM. ACM, Oct. 1962 and Mar. 1963]

HENRY C. THACHER, JR.

Reactor Engineering Div., Argonne National Laboratory
Argonne, Ill.

Work supported by the U.S. Atomic Energy Commission.

The bodies of SERIESPWR were transcribed for the Dartmouth SCALP processor for the LGP-30 computer. In addition to the modifications required by the limitations of this translator, the following corrections were necessary:

1. Add "real P;" to the specifications.
2. Delete "p," from the declarations in the procedure body.
3. (134 only) Replace "S" by "s" and [i-k] by "(i-k)" in the statement $S := s + \dots$
4. (158 only) Changes last sentence of comment to "Setting $P = 0$ gives the coefficients of $\ln(f(x))$. In this series, the constant term is 0, instead of 1 as elsewhere;"
5. (158 only) Add the identifier P2 to the declared real variables.
6. (158 only) Make the first statements read:

"if P = 0 then P2 := 1 else P2 := P;

B[1] := P2 × A[1];

7. (158 only) Make the statement of the for k loop read

"S := S + (P × (i-k) - k) × B[k] × A[i-k];"

8. Change the last statement to

"B[i] := P2 × A[i] + S/i end for i;

In addition, the following modifications would improve the efficiency of the program:

1. Remove A from the value list.
2. Omit the statement $B[1] := P \times A[1]$; ($P2 \times A[1]$ in 158 according to correction 6) and change the initial value of i in the statement following from 2 to 1.

When these changes were made, both procedures produced the first ten coefficients of the series for $(\exp(x)) \uparrow 2.5$ from the first ten coefficients of the exponential series. The procedures were also used to generate the binomial coefficients by applying them to $(1+x)^P$, for $P = 2.0$, and 0.5000000. Algorithm 158 was also tested with $P = 0$ for $1+x$ and for the series expansions for $(\sin x)/x$, $\cos x$, and $\exp x$. In all cases, the coefficients agreed with known values within roundoff.

ALGORITHM 135 CROUT WITH EQUILIBRATION AND ITERATION

WILLIAM MARSHALL MCKEEMAN*

Stanford University, Stanford, Calif.

* This work was supported in part by the Office of Naval Research under contract Nonr 225(37).

procedure LINEARSYSTEM (*A*) order:(*n*) right-hand sides:(*B*)
number of right-hand sides:(*m*) answers:(*X*) determinant:(*det*,
ex) condition of *A*:(*cnr*);

integer *n, m, ex*; **real** *det, cnr*; **real array** *A, B, X*;

comment, *LINEAR SYSTEM* uses Crout's method with row equilibration, row interchanges and iterative improvement for solving the matrix equation $AX = B$ where *A* is $n \times n$ and *X* and *B* are $n \times m$. As special cases one sees that: for $m \leq 0$, only the determinant of *A* is evaluated, for $m = 1$, the algorithm solves a system of *n* equations in *n* unknowns, for $m = n$ and *B* = the identity matrix, the algorithm inverts *A*.

If the algorithm breaks down for a singular or nearly singular matrix *A*, exit to a non-local label "singular" is provided. Five auxiliary procedures: *EQUILIBRATE*, *CROUT*, *PRODUCT*, *RESIDUALS* and *SOLVE* are declared with appropriate comments after the end of this procedure. This code is the result of the joint efforts of G. Guthrie, W. McKeeman, Cleve Moler, Margaret Salmon, Alan Shaw and R. Van Wyk. It was written following ideas presented by J. H. Wilkinson as a visiting lecturer in Professor George E. Forsythe's class in Advanced Numerical Analysis at Stanford, 1962;

begin integer array pivot [1:*n*]; **integer** *i, j, k*; **real** *mz*;

real array *LU*[1:*n*, 1:*n*], *y, res, mult*[1:*n*];

comment, remove appropriate factors from the rows of *A*...;

EQUILIBRATE(*A, n, mult*);

comment ... and save the result for the eventual computation

of residuals during iteration;

for *i* := 1 **step** 1 **until** *n* **do**

for *j* := 1 **step** 1 **until** *n* **do** *LU*[*i, j*] := *A*[*i, j*];

comment, decompose the matrix into triangular factors;

CROUT(*LU, n, pivot, det*);

comment, assuming that there was no exit to "singular",

evaluate the determinant in the form $det \times (10.0 \uparrow ex)$;

for *i* := 1 **step** 1 **until** *n* **do** *y*[*i*] := *LU*[*i, i*] $\times mult$ [*i*];

det := *det* $\times PRODUCT$ (*y, 1, n, ex*);

comment, now begin to process right-hand sides;

for *k* := 1 **step** 1 **until** *m* **do**

begin integer *i, count, limit*; **real** *normy, kr*;

kr := *k*;

comment, scale the right-hand side;

for *i* := 1 **step** 1 **until** *n* **do** *res*[*i*] := *B*[*i, k*] := *B*[*i, k*]/*mult*[*i*];

comment, store the first approximation and its *L*(1) norm;

normy := 0;

SOLVE(*LU, n, res, pivot, y*);

for *i* := 1 **step** 1 **until** *n* **do**

begin

normy := *normy* + *abs*(*y*[*i*]);

X[*i, k*] := *y*[*i*];

end;

comment, enter the iterating loop. The iteration is terminated on the integer "limit" which itself is determined on the basis of the success of the first iteration and a machine-dependent real number designated here by "eps". For "eps", the programmer must insert the largest real number such that $eps + 1.0 = 1.0$;

for *count* := 1, 2 **step** 1 **until** *limit* **do**

begin integer *i*; **real** *t*;

comment, compute the residuals of the solution *y*;

RESIDUALS(*A, n, B, k, X, res*);

comment ... and find the next increment to the solution;

SOLVE(*LU, n, res, pivot, y*);

comment, set up termination conditions;

if *count* = 1 **then**

begin real *normdy*;

normdy := 0;

for *i* := 1 **step** 1 **until** *n* **do** *normdy* := *normdy* + *abs*(*y*[*i*]);

if *normdy* = 0 **then** **begin** *cnr* := 1.0; **go to** *enditer* **end**;

t := *normy*/*normdy*;

comment, The quantity $\|A\| \cdot \|A^{-1}\|$ (spectral norm) is called the condition number of the matrix *A*. It is a measure of the difficulty in solving the input equation and appears naturally in error bounds for the solution (see Wilkinson [3]). *cnr* is a direct measure of the error and experimentally approximates the condition number;

cnr := ((*kr* - 1.0) $\times$ *cnr* + 1.0/(*eps* $\times$ *t*))/*kr*;

if *t* < 2.0 **then** **go to** *singular*;

limit := *ln*(*eps*)/*ln*(1.0/*t*);

end;

comment, store the new approximation;

for *i* := 1 **step** 1 **until** *n* **do** *X*[*i, k*] := *X*[*i, k*] + *y*[*i*];

end iteration;

enditer:

end right-hand sides

end LINEAR SYSTEM;

procedure EQUILIBRATE (*A*) order:(*n*) multipliers:(*mult*);

integer *n*; **real array** *A, mult*;

comment, scaling the rows of the matrix *A* to roughly the same maximum magnitude (here, dividing by the largest element) allows the procedure *CROUT* to select effective pivotal elements for the Gaussian decomposition of the matrix. The iterating procedure will converge to the solution for the equilibrated matrix rather than the input matrix. If the matrix is badly conditioned then the solution is sensitive to perturbations in the input and the scaling division must be done not by the largest element but rather by the power of the machine number base (2 and 10 for binary and decimal machines, respectively) nearest the largest element so as to avoid rounding errors. Equilibration is discussed in reference [3] p. 284;

begin integer *i*; **real** *mz*;

for *i* := 1 **step** 1 **until** *n* **do**

begin integer *j*;

mz := 0.0; **comment**, find the largest element;

for *j* := 1 **step** 1 **until** *n* **do**

if *abs*(*A*[*i, j*]) > *mz* **then** *mz* := *abs*(*A*[*i, j*]);

if *mz* = 0.0 **then** **go to** *singular*;

comment, now store the multiplier and scale the row;

mult[*i*] := *mz*; **comment** := base $\uparrow ex$ for exact scaling;

if *mz* $\neq$ 1.0 **then**

for *j* := 1 **step** 1 **until** *n* **do** *A*[*i, j*] := *A*[*i, j*]/*mz*

end

end EQUILIBRATE;

procedure CROUT (*A*) order:(*n*) pivots:(*pivot*) interchanges:(*sg*).

integer *n*; **integer array** *pivot*; **real array** *A*; **real** *sg*;

comment, this is Crout's method with row interchanges as formulated in reference [1] for transforming the matrix *A* into the triangular decomposition *LU* with all the $L[k, k] = 1.0$. *pivot*[*k*] stores the index of the pivotal row at the *k*-th stage of the elimination for use in the procedure *SOLVE*;

begin integer *i, j, k, imax, p*; **real** *t, quot*;

real procedure *IP1* (*A*) extra term:(*t*) length:(*f*);

integer *f*; **real** *t*; **real array** *A*; **comment** non-local *i, j, k*;

comment, *IP1* forms a row by column inner product of *A*, namely the sum of $A[i, p] \times A[p, k]$ for $p = 1, 2, \dots, f$, and then adds the extra term *t*. If $f < 1$, the value of *IP1* is *t*. This procedure is the inner loop of the algorithm. The pro-

grammer can expect a substantial advantage from substituting a faster and more accurate inner product here;

```

begin real sum; integer p;
  sum := t;
  for p := 1 step 1 until f do sum := sum + A[i,p] × A[p,k];
  IP1 := sum
end IP1;
sg := 1.0;
comment, k is the stage of the elimination;
for k := 1 step 1 until n do
begin
  t := 0;
  for i := k step 1 until n do
begin comment, compute L. Note that the first calls on IP1
are empty;
  A[i,k] := -IP1(A, -A[i,k], k-1);
  if abs(A[i,k]) > t then
begin t := abs(A[i,k]); imax := i end
end;
if t = 0 then go to singular;
comment, A[imax,k] is the largest element in the remainder
of column k. Interchange rows if necessary and record the
change;
pivot[k] := imax;
if imax ≠ k then
begin
  sg := -sg;
  for j := 1 step 1 until n do
begin
    t := A[k,j]; A[k,j] := A[imax,j]; A[imax,j] := t
  end
end;
comment, compute a column of multipliers;
quot := 1.0/A[k,k];
for i := k+1 step 1 until n do A[i,k] := A[i,k] × quot;
comment, and compute a row of U;
for j := k+1 step 1 until n do
  A[k,j] := -IP1(A, -A[k,j], k-1)
end
end CROUT;
real procedure PRODUCT (factors) start:(s) finish:(f)
  exponent:(ex);
integer s,f,ex; real array factors;
comment, PRODUCT multiplies the numbers stored from index
s through f inclusive in the array "factors", preventing ex-
ponent overflow. The answer is normalized so that 1.0 > abs
(PRODUCT) ≥ 0.1. The exponent appears in ex;
begin integer i; real p, pl;
  ex := 0; p := 1.0;
  for i := s step 1 until f do
begin
  pl := factors[i];
  if abs(pl) < 0.1 then begin pl = 10.0 × pl; ex := ex-1
  end;
  p := p × pl;
  if p = 0 then begin ex := 0; go to fin end;
1: if abs(p) < 0.1 then
  begin p := p × 10.0; ex := ex-1; go to 1 end;
2: if abs(p) ≥ 1.0 then
  begin p := p/10.0; ex := ex+1; go to 2 end;
end;
fin: PRODUCT := p
end PRODUCT;
procedure RESIDUALS (A) order:(n) right-hand sides:(B)
  column of B:(k) approximate solution:(X) residuals:(res);
integer n, k; real array A, B, X, res;
comment, RESIDUALS computes b - Ay where b is the kth
column of the right-hand side matrix B and y is the kth column
of X;

```

```

real procedure IP2 (A) row: (i) order:(n) approximate
  solution:(X)
  column:(k) extra term:(t);
integer i, k, n; real t real array A, X;
comment, IP2 forms the inner product of row i of the matrix
A and column k of the solution matrix X, then adds the
single term t. It is essential that IP2 be an "accumulating"
or double precision inner product as discussed in reference
[3] p. 296. The value of IP2 is the rounded single precision
result of the double precision arithmetic. The body of the
procedure is left undefined;
begin integer i;
for i := 1 step 1 until n do
  res[i] := -IP2(A, i, n, X, k, -B[i,k])
end RESIDUALS;
procedure SOLVE (A) order:(n) right-hand side:(b) pivots:
  (pivot) answer:(y);
integer n; integer array pivot; real array A, b, y;
comment, SOLVE processes a right-hand side b and then back-
solves for the solution y using the LU decomposition provided
by CROUT;
begin integer k, p; real t;
for k := 1 step 1 until n do
begin
  t := b[pivot[k]]; b[pivot[k]] := b[k];
  for p := 1 step 1 until k-1 do t := t - A[k,p] × b[p];
  b[k] := t
end ...having modified b by L inverse;
comment, now the back solution for y;
for k := n step -1 until 1 do
begin
  t := b[k];
  for p := k+1 step 1 until n do t := t - A[k,p] × y[p];
  y[k] := t
end backsolution
end SOLVE

```

REFERENCES

1. GEORGE E. FORSYTHE, Crout with Pivoting. Algorithm 16. *Comm. ACM* 3, 2 (Sept. 1960), 507.
2. DEREK JOHANN ROEK, Simultaneous System of Equations and Matrix Inversion Routine. Algorithm 92. *Comm. ACM* 5, 5 (May 1962), 286.
3. J. H. WILKINSON, Error Analysis of Direct Methods of Matrix Inversion, *J. ACM* 8, 3 (July 1961), 281-330.

CERTIFICATION OF ALGORITHM 135 CROUT WITH EQUILIBRATION AND ITERATION [William Marshall McKeeman,* *Comm. ACM*, Nov. 1962]

WILLIAM MARSHALL MCKEEMAN,
Stanford University, Stanford, Calif.

* This work was supported in part by the Office of Naval Research under contract Nonr 225(37).

A BALGOL translation of the algorithm was tested for accuracy, proper termination and running time on the Burroughs 220. The exact inverse of the Hilbert segment of order 6 can be stored in the 8-decimal-digit floating word of the B220 and was used in the accuracy and termination tests. The Hilbert segment H_6 is very ill-conditioned (for the spectral norm, $\|H_6\| \cdot \|H_6^{-1}\| = 1.3 \times 10^7$). Hence the number of iterations required should not be taken as typical.

The $[n,n]$ element (mathematically $t_1^1 = .090909 \dots$) is representative of the behavior of the rest:

	"exact" equilibration (by powers of 10)	equilibration by largest element in row
initial solution	.092587535	.094091506
first iteration	.090877240	.091498265
second iteration	.090909695	.091570311
third iteration	.090909080	.091568310
fourth iteration	.090909091	.091568365
fifth iteration	terminated	.091568364 terminated

Conclusions: The iterating procedure terminated correctly, or performed one extra iteration in each case. If the equilibration procedure alters the data, the iteration will converge to the solution for the altered matrix. If the matrix is ill-conditioned, as in the case above, the equilibration may cost a great deal more than it gains. As a practical matter, a machine language substitute for EQUILIBRATE which will not cause rounding of the data is probably the best course of action.

The running time is approximately proportional to n^3 as expected. If for a given machine, μ is the floating multiply time in seconds, one can expect that run time will be given by $rt := 1.3 \times \mu \times (n + 7) \uparrow 3$ seconds for a call on LINEARSYSTEM with one right-hand side.

The division of run time between the various phases of the algorithm is as follows:

REFERENCE:

1. SAVAGE AND LUKACS, Tables of inverses of finite segment of the Hilbert matrix. In Olga Taussky (Ed.), Contributions to the Solution of Systems of Linear Equations and the Determination of Eigenvalues, pp. 105-108, Nat. Bur. Standards Appl. Math. Series no. 39, U. S. Government Printing Office, Wash., D.C., 1954.

REMARK ON ALGORITHM 135 [F4]

CROUT WITH EQUILIBRATION AND ITERATION
[W. M. McKeeman, *Comm. ACM* 5 (Nov. 1962), 555-557, 559].

WILLIAM MARSHALL MCKEEMAN (Recd. 1 Apr. 1964)
Computation Center, Stanford University, Stanford, Calif.

The following corrections to the published algorithm are recommended:

1. Two lines above the bottom line of procedure SOLVE one must change

$$y[k] := t \quad \text{to} \quad y[k] := t/A[k,k]$$

2. In procedure EQUILIBRATE, all occurrences of the subscript k must be changed to j .

3. The statement $cnr := 1.0$ should be added at the start of the body of procedure LINEARSYSTEM, so that cnr will have a value the first time it is used.

4. Line 19 from the end of LINEARSYSTEM should be changed from

if normdy = 0 then begin cnr := 1.0; go to enditer end;

to read

if normdy = 0 then go to enditer;

This correction makes sure that cnr retains a reasonable value in case normdy should be 0 for some column.

5. The symbol "." must be removed from the parameter delimiters in the declarations of procedures LINEARSYSTEM, RESIDUALS and SOLVE.

6. Four lines above the bottom line of procedure LINEARSYSTEM, delete the first occurrence of $X[i,k] :=$

7. In the third line of the heading of procedure IP2, the parameter delimiter

) extra term:(

should be changed to

) extra term:(

ALGORITHM 136

ENLARGEMENT OF A GROUP

M. WELLS*

University of Leeds, England

* Currently with Burroughs Corporation, Pasadena, California

```

procedure Enlarge group (G, n, g, Abelian);
array G, g; integer n; Boolean Abelian;
comment This procedure combines the element g with the sub-
group G, of n elements, to form a new group. The Boolean
Abelian has the value true if the group to which G and g belong
is Abelian. Two procedures, multiply and equal are assumed
to be declared: multiply (G[i]) by : (G[j]) to give : (G[k]) will set
the element Gk equal to the product of the elements Gi and Gj.
equal (G[i], G[j]) is a Boolean procedure whose value is true
if, and only if, the elements Gi and Gj are equal. On leaving the
procedure the enlarged group is in G, and n is equal to the
number of elements in the new sub-group G. The procedure
will function correctly if g is included in G on entry. It is prob-
able that g and the elements of G will be arrays, and the pro-
cedure body will, in practice, need to be altered considerably.
The procedure has been used successfully in connection with
problems of space-group theory;
begin integer i, j, k;
for i := 1 step 1 until n do
if equal (G[i], g) then go to not new generator;
n := n + 1; G[n] := g;
for i := n step 1 until n do
begin for j := 1 step 1 until n do
begin multiply (G[i], G[j], G[n+1]);
for k := 1 step 1 until n do
if equal (G[k], G[n+1]) then go to not new element 1;
n := n + 1;
not new element 1: if Abelian then go to take next element;
multiply (G[j], G[i], G[n+1]);
for k := 1 step 1 until n do
if equal (G[k], G[n+1]) then go to not new element 2;
n := n + 1;
not new element 2: take next element:
end of j-loop;
end of i-loop;
not new generator: end of group enlargement

```

ALGORITHM 137

NESTING OF FOR STATEMENT I

DAVID M. DAHM & M. WELLS*

Burroughs Corp., Pasadena, Calif.

* On leave of absence from the University of Leeds, England.

```

procedure Fors 1 (n, P);
  value n; integer n; procedure P;
  comment Fors 1 generates a nest of n for statements with the
  procedure P at their center. Two non-local arrays I and U,
  which give the value of the controlled variable and its upper
  bound for each level are assumed to be declared;
  begin integer j;
  if n = 0 then P
  else for j := 1 step 1 until U[n] do
    begin I[n] := j; Fors 1 (n-1, P) end end Fors 1

```

ALGORITHM 138

NESTING OF FOR STATEMENT II

DAVID M. DAHM & M. WELLS*

Burroughs Corp., Pasadena, Calif.

* On leave of absence from the University of Leeds, England.

```

procedure Fors 2 (P);
  procedure P;
  comment Fors 2 performs the same function as Fors 1, but is
  more economic of storage space. It is expected, however,
  that Fors 1 would be more economic of time. The formal
  parameter n is now replaced by the non-local integer n;
  begin if n = 0 then P
  else for I[n] := 1 step 1 until U[n] do
    begin n := n-1; Fors 2 (P) end;
    n := n + 1 end Fors 2

```

ALGORITHM 139

SOLUTIONS OF THE DIOPHANTINE EQUATION

J. E. L. PECK

University of Alberta, Calgary, Alberta, Canada

```

procedure Diophantus (a,b,c); integer a,b,c;
  comment This procedure seeks the integer solutions of the
  equation  $ax + by = c$ , where the integers a,b,c are given. It
  assumes a non-local integer M, which should be as large as
  storage will allow, two nonlocal labels INDETERMINATE
  and NO SOLUTION and two non-local Boolean variables
  'general solution' and 'time permits' which are self explanatory.
  It also assumes the procedures abs, sign and print;
  begin integer n,r,s,d,i; integer array q[1:M];
  n := i := 0; d := s := abs(a); r := abs(b);
  comment d will become the greatest common divisor of a and b.
  If b = 0 then d = |a|. The vector q will retain the successive
  quotients in the Euclidean algorithm  $r_{i-1} = r_{iq_i} + r_{i+1}$ ,
  i = 1, 2, ..., n, where  $0 \leq r_{i+1} < r_i$ ,  $r_0 = |a|$ ,  $r_1 = |b|$ ,
  and  $r_{n+1} = 0$ ;
  for i := i + 1 while r ≠ 0 do
    begin n := i; d := r; q[i] := s ÷ d;
    r := s - d × q[i]; s := d end This records the quotients and

```

```

the number n of divisions for use below;
if d = 0 then go to if c = 0 then INDETERMINATE
else NO SOLUTION; comment The case d = 0 occurs when
 $a^2 + b^2 = 0$ . If d now does not divide c then the equation can-
not be solved so;
if (c ÷ d) × d ≠ c then go to NO SOLUTION;
if d ≠ 1 then
  begin a := a/d, b := b/d; c := c/d end, which removes
  the common factor and reduces the equation to the case
  where a and b are relatively prime;
  begin comment We shall now find  $u_1$  and  $v_1$  in order to
  express
   $1 = au_1 + bv_1$ , using the relations  $r_n = r_{i-1}u_i + r_{i-2}v_i$ ,
   $i = n, n-1, \dots, 1, v_n = 1, u_n = 0$ , and  $r_{i+1} = -r_iq_i + r_{i-1}$ ,
   $i = n-1, n-2, \dots, 1$ ; integer u,v;
  if n = 0 then
    begin v := 0; u := 1 end, which takes care of the case
    b = 0
  else
    begin v := 1; u := 0;
    for i := n-1 step -1 until 1 do
      begin integer t;
      t := v; v := u - v × q[i]; u := t
      end i
    end the case n ≠ 0. It remains now to multiply the equality
     $1 = au_1 + bv_1$  through by c;
    begin integer x0, y0;
    x0 := c × u × sign(a); y0 := c × v × sign(b); print (x0,y0);
    comment If  $x_0, y_0$  is a particular solution then  $x_0 \pm ib$ ,
     $y_0 \mp ia$ , i=1,2, ... gives the general solution. Therefore;
    if general solution then
      begin u := b; v := a;
      A: print(x0 + u, y0 - v); print(x0 - u, y0 + v);
      u := u + b; v := v + a;
      if time permits then go to A
      end general solution and
    end solution.
  end u,v
end Diophantus.

```

ALGORITHM 140

MATRIX INVERSION

P. Z. INGERMAN

University of Pennsylvania, Philadelphia, Penn.

```

procedure invert (a) of order:(n) with tolerance:(eps) and
  error exit:(oops);
  value n, eps; array a; integer n; real eps; label oops;
  comment This procedure inverts a matrix by using elementary
  row operations. Although the method is not particularly good
  for ill-conditioned matrices, the simplicity of the algorithm
  and the fact that the inversion occurs in place make it useful
  on occasion;
  begin integer i;
  for i := 1 step 1 until n do
    begin integer j, k; real q;
    q := a[i,i];
    if abs(q) ≤ abs(eps) then go to oops;
    a[i,i] := 1;
    if q ≠ 1 then for k := 1 step 1 until n do a[i,k] := a[i,k]/q;
    for j := 1 step 1 until n do
      if i ≠ j then
        begin q := a[j,i]; a[j,i] := 0;
        for k := 1 step 1 until n do
          a[j,k] := a[j,k] - q × a[i,k] end end end

```

CERTIFICATION OF ALGORITHM 140 MATRIX INVERSION [P. Z. Ingerman, *Comm. ACM*, Nov. 1962]

RICHARD GEORGE*

Argonne National Laboratory, Argonne, Ill.

* Work supported by the United States Atomic Energy Commission.

Algorithm 140 was tested on the LGP-30, using SCALP, a load-and-go compiler from the Dartmouth College Computation Center, and it was shown to be syntactically correct.

It is indeed a simple procedure. It is so simple because the author has eliminated the very necessary search for largest elements and the row interchanges. As a result, this procedure will fail to invert many non-singular matrices. To be invertible by this procedure, a matrix must be such that all of its leading diagonal submatrices will have non-zero determinants.

One would do well to avoid this algorithm and use one (such as 120) which employs the pivoting process.

ALGORITHM 141 PATH MATRIX

P. Z. INGERMAN

University of Pennsylvania, Philadelphia, Penn.

```

procedure findpath (a, n);
value n; Boolean array a; integer n;
comment This procedure is merely an Algol implementation
of the method of Warshall (JACM 9(1962), 11-12). Some advantage
is taken of the characteristics of the problem to increase the efficiency;
begin integer i, j, k;
  for j := 1 step 1 until n do
    for i := 1 step 1 until n do
      if a[i,j]  $\wedge$  i  $\neq$  j then
        for k := 1 step 1 until n do
          a[i,k] := a[i,k]  $\vee$  a[j,k] end findpath

```

ALGORITHM 142 TRIANGULAR REGRESSION

W. L. HAFLEY AND J. S. LEWIS

Aluminum Company of America, Pittsburgh, Penn.

```

procedure trireg (n, nob, dep, pmax);
real pmax; integer n, nob, dep;
comment trireg is a multiple regression procedure which
develops and inverts only the upper triangular portion of a
correlation matrix of order n. The  $i,j$ th ( $i \leq j$ ) matrix element
is  $r(c_i + j)$  where the  $c$ 's are cram numbers (ref. Algorithm 67,
J. Caffey, Comm. ACM 4, July 1961).  $dep < n$  dependent
variables are regressed simultaneously. Read (u) is an input
procedure for single elements. The input consists of nob observations
on n variables. The first dep variables are considered dependent
and the remaining  $n - dep$  are considered independent variables.
Independent variables are dropped when the pivotal element exceeds pmax
during the inversion. Total variable storage is  $14 + 3n + n(n+1)/2$ ;

```

```

begin integer i1, i2, i3, c1, c2, c3, df; integer array c[1:n];
  real d, p, a; real array r[1:n(n+1)/2], v[1:n], m[1:n];
initial: df := 0; for i1 := 1 step 1 until n do m[i1] := 0;
  for i1 := 1 step 1 until n(n+1)/2 do r[i1] := 0;
input: for i1 := 1 step 1 until nob do
  begin for i2 := 1 step 1 until n do Read (v[i2]);
    c1 := 0; for i2 := 1 step 1 until n do
      begin d := v[i2]; m[i2] := m[i2] + d;
        for i3 := i2 step 1 until n do
          begin c1 := c1 + 1; r[c1] := r[c1] + v[i3]  $\times$  d end
        end i2;
      end i1;
    correlation: c1 := 1; a := 1/nob; for i1 := 1 step 1 until n do
      begin v[i1] := 1/sqrt(r[c1] - (m[i1]2  $\times$  a));
        r[c1] := 1; c1 := c1 + n - i1
      end i1;
      c1 := 1; for i1 := 1 step 1 until n do
        begin d := a  $\times$  m[i1]; p := v[i1]; c1 := c1 + 1;
          m[i1] := d;
          for i2 := i1 + 1 step 1 until n do
            begin r[c1] := (r[c1] - d  $\times$  m[i2])  $\times$  v[i2]  $\times$  p;
              end i2;
            end i1;
          comment variable i may be dropped from the
          regression by setting  $v_i = 0$  and df equal to the
          number of variables dropped;
        cram: i1 := -n; i2 := n + 1; for i3 := 1 step 1 until n do
          begin i1 := i1 + i2 - i3; c[i3] := i1
          end i1;
        inversion: for i1 := dep + 1 step 1 until n do
          begin c1 := c[i1]; if v[i1]  $\neq$  0 then
            begin p := 1/r[c1+i1]; if p > pmax then
              begin df := df + 1; go to YY end else
                begin r[c1+i1] := p; for i2 := 1 step 1
                  until i1 - 1 do
                  begin c2 := c[i2]; a := p  $\times$  r[c2+i1];
                    for i3 := i2 step 1 until n while i3  $\neq$  i1 do
                      begin if i3 < i1 then
                        begin c3 := c[i3]; d := r[c3+i1] end
                        else d := -r[c1+i3];
                          r[c2+i3] := r[c2+i3] + d  $\times$  a
                        end i3;
                      end i2;
                    for i2 := i1 + 1 step 1 until n do
                      begin a := p  $\times$  r[c1+i2]; c2 := c[i2];
                        for i3 := i2 step 1 until n do
                          r[c2+i3] := r[c2+i3] - a  $\times$  r[c1+i3];
                        end i3;
                      end i2;
                    ZZ: for i2 := 1 step 1 until i1 - 1 do
                      begin c2 := c[i2+i1]; r[c2] := -p  $\times$  r[c2]
                      end i2;
                    for i2 := c1 + i1 + 1 step 1 until n + c1 do
                      r[i2] := p  $\times$  r[i2]
                    end
                  end else
                    YY: begin p := 0; r[c1+i1] := 0; go to ZZ end
                coeff: d := 1/(nob - n + dep - 1 + df); for i1 := 1 step 1 until
                  dep do
                  if v[i1]  $\neq$  0 then
                    begin a := 0; p := 1/v[i1]; c1 := c[i1]; for i2 := dep
                      + 1 step 1 until n do
                      begin if r[i2]  $\neq$  0 then
                        begin r[c1+i2] := -r[c1+i2]  $\times$  v[i2]  $\times$  p; a :=
                          a + r[c1+i2]  $\times$  m[i2]
                        end
                      end i2;
                    v[i1] := (2 - r[c1+i1])  $\times$  d / (v[i1]2)

```

comment: $v[1:dep]$ now contains the mean square deviations from regressions for the dependent variables. The coefficients of determination R^2 may be obtained as $r[c1+i1] - 1$;
 $r[c1+i1] := m[i1] - a$ else
 begin $c1 := c[i1]$; for $i2 := c1 + i1$ step 1 until $c1 + n$ do $r[i2] := 0$
 end

end

comment The r -array now contains the constants and coefficients of regression, and the inverse of the correlation matrix of the independent variables that have been kept. The following example will help to locate the information in the r array.

Example: $n = 6$ $dep = 3$

r_1	r_2	r_3	r_4	r_5	r_6	b_{01}	b_{11}	b_{21}	b_{31}
r_7	r_8	r_9	r_{10}	r_{11}		b_{02}	b_{12}	b_{22}	b_{32}
r_{12}	r_{13}	r_{14}	r_{15}			b_{03}	b_{13}	b_{23}	b_{33}
r_{16}	r_{17}	r_{18}					r_{11}	r_{12}	r_{13}
r_{19}	r_{20}						r_{21}	r_{22}	r_{23}
r_{21}							r_{31}	r_{32}	r_{33}

The variances and covariances of the regression coefficients for the j th dependent variable can be determined by—

$$\text{Var}(b_{ji}) = r_{ii}^{-1} \times v_j \times v_i^2$$

$$\text{Covar}(b_{ji}, b_{kj}) = r_{ik}^{-1} \times v_j \times v_i \times v_k$$

end trireg

ALGORITHM 143

TREESORT 1

ARTHUR F. KAUPÉ, JR.

Westinghouse Electric Corp., Pittsburgh, Penn.

```

procedure TREESORT 1 (UNSORTED, n, SORTED, k);
  value n, k;
  integer n, k; array UNSORTED, SORTED;
  comment TREESORT 1 is a revision of TREESORT (ALGORITHM 113) which requires neither the "packed" array m nor the machine procedures pack, left half, right half, and minimum. The identifier infinity is used as nonlocal real variable with value greater than any element of UNSORTED;
  begin integer i, j; array m1 [1:2×n-1];
    integer array m2 [1:2×n-1];
  procedure minimum; if m1 [2×i] ≤ m1 [2×i+1] then
    begin m1[i] := m1 [2×i]; m2[i] := m2 [2×i] end else
    begin m1[i] := m1 [2×i+1]; m2[i] := m2 [2×i+1] end minimum;
  for i := n step 1 until 2 × n - 1 do begin m1[i] := UNSORTED [i-n+1]; m2[i] := i end
  for i := n - 1 step -1 until 1 do minimum;
  for j := 1 step 1 until k do
    begin SORTED [j] := m1 [1]; i := m2 [1]; m1[i] := infinity;
    for i := i ÷ 2 while i > 0 do minimum end
  end TREESORT 1

```

ALGORITHM 144

TREESORT 2

ARTHUR F. KAUPÉ, JR.

Westinghouse Electric Corp., Pittsburgh, Penn.

```

procedure TREESORT 2 (UNSORTED, n, SORTED, k, ordered);
  value n, k;
  integer n, k; array UNSORTED, SORTED; Boolean procedure ordered;
  comment TREESORT 2 is a generalized version of TREESORT 1. The Boolean procedure ordered is to have two real arguments. The array SORTED will have the property that ordered (SORTED[i], SORTED[j]) is true when j > i if ordered is a linear order relation;
  begin integer i, j; array m1 [1:2×n-1]; integer array m2 [1:2×n-1];
  procedure minimum; if ordered (m1 [2×i], m1 [2×i+1]) then
    begin m1[i] := m1 [2×i]; m2[i] := m2 [2×i] end else
    begin m1[i] := m1 [2×i+1]; m2[i] := m2 [2×i+1] end minimum;
  for i := n step 1 until 2 × n - 1 do begin m1[i] := UNSORTED [i-n+1]; m2[i] := i end
  for i := n - 1 step -1 until 1 do minimum;
  for j := 1 step 1 until k do
    begin SORTED [j] := m1 [1]; i := m2 [1]; m1[i] := infinity;
    for i := i ÷ 2 while i > 0 do minimum end
  end TREESORT 2

```

ALGORITHM 145

ADAPTIVE NUMERICAL INTEGRATION BY SIMPSON'S RULE

WILLIAM MARSHALL McKEEMAN*

Stanford University, Stanford, Calif.

* This work was supported in part by the Office of Naval Research under contract Non4 225(37).

```

real procedure Integral (F) limits: (a, b) tolerance: (eps);
real procedure F; real a, b, eps;
begin comment Integral will numerically approximate the integral of the function F between the limits a and b by the application of a modified Simpson's rule. Although eps is a measure of the relative error of the result, the actual error may be very much larger (e.g. whenever the answer is small because a positive area cancelled a negative area). The procedure attempts to minimize the number of function evaluations by using small subdivisions of the interval only where required for the given tolerance;
  integer level;
  real procedure Simpson (F, a, da, Fa, Fm, Fb, absarea, est, eps);
  real procedure F; real a, da, Fa, Fm, Fb, absarea, est, eps;
  begin comment Recursive Simpson's rule;
    real dx, x1, x2, est1, est2, est3, F1, F2, F3, F4, sum;
    dx := da/3.0; x1 := a + dx; x2 := x1 + dx;
    F1 := 4.0 × F(a+dx/2.0); F2 := F(x1);
    F3 := F(x2); F4 := 4.0 × F(a+2.5×dx);
    est1 := (Fa+F1+F2) × dx/6.0;
    est2 := (F2+Fm+F3) × dx/6.0;
    est3 := (F3+F4+Fb) × dx/6.0;
    absarea := absarea-abs(est) + abs(est1) + abs(est2) + abs(est3);
    sum := est1 + est2 + est3;
    level := level + 1;
  end

```

```

Simpson := if (abs(est-sum) ≤ eps × absarea ∧ est ≠ 1.0) ∨
level ≥ 7 then sum
else Simpson (F, a, dx, Fa, F1, F2, absarea, est1, eps/3.0)
+ Simpson (F, x1, dx, F2, Fm, F3, absarea, est2, eps/3.0)
+ Simpson (F, x2, dx, F3, F4, Fb, absarea, est3, eps/3.0);
level := level - 1;
end Simpson;
level := 1;
Integral := Simpson (F, b-a, F(a), 4.0 × F((a+b)/2.0), F(b),
1.0, 1.0, eps)
end Integral 13

```

CERTIFICATION OF ALGORITHM 145 ADAPTIVE NUMERICAL INTEGRATION BY SIMPSON'S RULE [W. McKeeman, *Comm. ACM*, Dec. 1962]

WM. M. McKEEMAN
Stanford University, Stanford, Calif.

Suggested changes in the code:

1. Replace all occurrences of $eps/3.0$ by $eps/1.7$.
2. Replace $level \geq 7$ by $level \geq 20$.
3. The second parameter a in the final call of *Simpson* was omitted; insert it.

With the above changes, a BALGOL translation of *Integral* has been tested successfully on a large number of functions. An example of its behavior is given below:

Machine: Burroughs 220, 8 decimal digit floating-point mantissa.
 $f(x) = 1.0/\sqrt{\text{abs}(x)}$; which has a pole at the origin.
 $a = -9.0$; $b = 1000.0$; correct answer = 206.0;

eps	computer answer	relative error
0.1	200.22251	0.028
0.01	206.00226	0.0000107
0.001	206.00092	0.0000045
0.0001	205.99985	0.0000007

If the recursion was allowed to go thirty levels deep we found:

0.0001 206.00005 0.0000002

The graph below shows the adaptive clustering of the points of evaluation around the pole of the function (taken from the first example above).

Each vertical line represents a point of evaluation for the function during the execution of the call:

`integral(f, -9.0, 10000.0, 0.1);`

ALGORITHM 146 MULTIPLE INTEGRATION WILLIAM MARSHALL McKEEMAN* Stanford University, Stanford, Calif.

* This work was supported in part by the Office of Naval Research under contract Non4 225(37).

```

real procedure MultipleIntegral (F) limits: (a, b) order: (n)
tolerance: (eps);
real procedure F; real array a, b; real eps; integer n;
begin comment F is a function of n variables which are stored
in an internal array x. MultipleIntegral approximates the
multiple integral of F between the n pairs of limits stored in
the parameter arrays a and b. For a mesh of k steps on each
axis, the number of function evaluations required for an
integral of nth order is approximately k^n. One consequence
is that the practical limit on n is quite small. Another is that
any inefficiency in the (undefined) procedure Integral will
reflect itself to the nth power in MultipleIntegral. The adap-
tive procedure Integral is recommended;
real array x[1:n+1]; integer axis;
real procedure Integral (F) limits: (a, b) tolerance: (eps);
real procedure F; real a, b, eps;
begin comment The body of procedure Integral is left
undefined. For it one may substitute any procedure of the
same name that evaluates the integral of a function of a single
variable between the real limits a and b;
end Integral;
real procedure MI(y); real y;
begin comment Recursive multiple integration;
x[axis] := y;
axis := axis - 1;
MI := if axis = 0 then F(x) else
Integral (MI, a[axis], b[axis], eps/n);
axis := axis + 1;
end MI;
axis := n + 1;
MultipleIntegral := MI(0)
end MultipleIntegral

```

CERTIFICATION OF ALGORITHM 146 MULTIPLE INTEGRATION [W. M. McKeeman, *Comm. ACM* 5 (Dec. 1962), 604] NIKLAUS WIRTH (Recd. 6 Jan. 1964) Computer Science Div., Stanford U., Stanford, Calif.

Algorithm 146 was translated into a generalized ALGOL [cf. N. Wirth, A generalization of ALGOL, *Comm. ACM* 6 (Sept. 1963), 547-554] and successfully run on the Stanford IBM 7090 computer. Algorithm 60, Romberg Integration [*Comm. ACM* 4 (June 1961), 255; 5 (Mar. 1962), 168; 5 (May 1962), 281] was used for the real procedure *Integral*.

The main disadvantage of Algorithm 146 is that the bounds of the domain of integration must be constant, i.e. the domain must always have the form of a rectangular hyperbox.

ALGORITHM 147 PSIF D. AMIT Ministry of Defense, Israel

```

real procedure psif(x, a, tan, ln) exit: (errexit);
value x, a; label errexit; real procedure tan, ln;

```

comment Computes the logarithmic derivative of the factorial function defined by:

$$\Psi(x) = \frac{(x)!'}{x!} = \frac{\Gamma'(x+1)}{\Gamma(x+1)}$$

We make use of the expansion: (1) $\Psi(x) = \ln x + 1/2x - 1/12x^2 + 1/120x^4 - 1/252x^6 + \epsilon$, (2) $\epsilon < 1/240x^2$ and of the recursion relation, (3) $\Psi(x) = \Psi(x+n) - (1/(x+1) + \dots + 1/(x+n))$. For $x < -1$ we use: (4) $\Psi(-x) = \pi \tan \pi(x+0.5) + \Psi(x-1)$. The value of x is increased up to a . Then Ψ is calculated by $\Psi_1(3)$ and (1). The error is then less than $1/240a^2$;

```
begin real psi, pei; psi := 0;
if x > -1 ^ x ≠ 0 then go to pos;
if x = 0 then begin psi := -0.5772156649; go to exit end;
begin integer x1; x1 := x;
if x = x1 then go to errezit end
comment psi is infinite;
pei := 3.141592654; x := -x - 1;
psi := pei × tan(pei × (x+0.5));
pos: if x ≥ a then go to large;
x := x + 1; psi := psi - 1/x; go to pos;
large: begin real y; y := 1/x;
psi := psi + ln(x) + y/2 - y ↑ 2/12 + y ↑ 4/120 - y ↑ 6/252;
exit: psif := psi;
end psif.
```

CERTIFICATION OF ALGORITHM 147

PSIF [D. Amit, *Comm. ACM*, Dec. 62]

HENRY C. THACHER, JR.*

Reactor Eng. Div., Argonne National Lab., Argonne, Ill.

* Work supported by the U. S. Atomic Energy Commission.

The following minor errors were noted in this algorithm:

- (3) in the comment should read $\epsilon < 1/240 x^2$.
- The function $\tan$ is not a standard ALGOL function. It should be declared, or replaced by $\sin(\)/\cos(\)$.
- The block labelled *large* should be closed by inserting **end** immediately after 252.

The efficiency of the program would be improved by the following modifications:

- Let the statement

if x = 0 then begin ... end;

be the first statement of the procedure body.

- Delete the condition $x \neq 0$ from the if clause,

if x > -1 ^ x ≠ 0 then ...

- Delete the declaration of *pei*, and the assignment of the value of 3.141592654 to *pei* in the statement

psi := *pei* × $\sin(\text{pei} \times (x+0.5)) / \cos(\text{pei} \times (x+0.5))$;
replace *pei* by the value 3.141592654.

- Replace the block labelled *large* by:

large: begin real y; x := 1/x; y := x × x;
psi := *psi* - $\ln(x) + x/2 - ((y/252 - 0.008333333333) \times y + 0.08333333333) \times y$ **end;**

With these changes, the body of the procedure was translated and run on the LGP-30 computer using the Dartmouth SCALP processor. The program was used to tabulate $\text{psif}(x)$ for $x = -1(0.5)0(0.005)1.250$. With $a = 3.0$ the results agreed with tabulated values to within 3 in the 6th decimal place. This is considered satisfactory, since one decimal place is lost in applying the recurrence. Running time, including output on the Flexowriter and computation of new values of the independent variable, averaged about 30 seconds per value.

It should be observed that $\text{psif}(x)$ is $\Psi(x+1)$ as tabulated, for example, by Jahnke-Emde-Losch.

ALGORITHM 148

TERM OF MAGIC SQUARE

D. M. COLLISON

Elliott Brothers (London) Ltd., Borehamwood, Herts.

integer procedure *magicterm* (*x*, *y*, *n*); **value** *x*, *y*, *n*; **integer** *x*, *y*, *n*;

comment for the magic square $s[1:n, 1:n]$, *magicterm* generates the element $s[x, y]$, where $n > 2$ and n is odd. De la Loubère's method is used;

begin integer *b*, *c*;

b := $y - x + (n-1) \div 2$; *c* := $y + y - x$;

if *b* ≥ *n* **then** *b* := *b* - *n* **else if** *b* < 0 **then** *b* := *b* + *n*;

if *c* > *n* **then** *c* := *c* - *n* **else if** *c* ≤ 0 **then** *c* := *c* + *n*;

magicterm := *b* × *n* + *c*

end magicterm

CERTIFICATION OF ALGORITHM 148

TERM OF MAGIC SQUARE [D. M. Collison, *Comm.*

ACM, Dec. 62]

DMITRI THORO

San Jose State College, San Jose, Calif.

This algorithm was translated into FORTRAN and FORGO for the IBM 1620. No changes in the program were necessary. The elements of magic squares of odd orders up to 15 were generated satisfactorily.

CERTIFICATION OF ALGORITHM 148

TERM OF MAGIC SQUARE [D. M. Collinson, *Comm.*

ACM, Dec. 1962]

J. N. R. BARNECUT

University of Alberta, Calgary; Calgary, Alberta, Canada

MAGICTERM was translated into FORTRAN for the IBM 1620. The procedure was tested for terms of squares up to order 13. Correct results were obtained. For determination of complete squares operating time was not significantly different from Algorithm 118.

ALGORITHM 149

COMPLETE ELLIPTIC INTEGRAL

J. N. MERNER

Burroughs Corp., Pasadena, Calif.

comment The following two procedures, along with a test program were compiled and run by Peter Naur on the DISADEC computer. Compilation time for the 9 pass compiler was less than 10 seconds. The elliptic integral of the form

$$\int_0^{\pi/2} \frac{dt}{\sqrt{a^2 \cos^2 t + b^2 \sin^2 t}}$$

is evaluated by replacing *a* and *b* by their arithmetic and geometric means, respectively. *ELIP 2* is a nonrecursive procedure to accomplish the same thing;

real procedure *ELIP 1* (*a*, *b*); **value** *a*, *b*; **real** *a*, *b*;

ELIP 1 := **if** $\text{abs}(a-b) <_{10} -8 \times a$

then 3.14159265/2/*a*

else *ELIP 1* ((*a*+*b*)/2, $\text{sqrt}(a \times b)$);

real procedure *ELIP 2* (*a*, *b*); **value** *a*, *b*; **real** *a*, *b*;

begin real *C*;

L: *C* := (*a*+*b*)/2; *b* := $\text{sqrt}(a \times b)$; *a* := *c*;

if $\text{abs}(a-b) <_{10} -8 \times a$ **then** *ELIP 2* := 3.14159265/2/*a*;

else go to *L* **end**

SEE ALGORITHM 55

ALGORITHM 150

SYMINV2

H. RUTISHAUSER

Eidg. Technische Hochschule, Zurich, Switzerland

procedure *syminv2*(*a*,*n*) **result**: (*a*) **exit**: (*fail*); **value** *n*; **integer** *n*; **array** *a*; **label** *fail*;

comment *syminv2* obtains inverse of a symmetric matrix *a* of order *n* by a method which is similar to that given by Busing and Levy [Comm. ACM 5 (1962), 446] but requires no interchanges of rows and columns nor storage space for an additional matrix *Q*, yet is numerically equivalent. The procedure requires the upper triangular part of *a* to be given and overwrites it by the upper triangular part of the inverse which is again denoted by *a*. All pivots are chosen on the diagonal, and if all further diagonal elements which are eligible as pivots vanish (this is impossible for a positive definite matrix *a*) then exit through *fail* occurs;

begin

real *bigajj*;

integer *i*, *j*, *k*;

real array *p*, *q*[1:*n*];

Boolean array *r*[1:*n*];

for *i* := 1 **step** 1 **until** *n* **do** *r*[*i*] := **true**;

grand loop:

for *i* := 1 **step** 1 **until** *n* **do**

begin

search for pivot:

bigajj := 0;

for *j* := 1 **step** 1 **until** *n* **do**

begin

if *r*[*j*] $\wedge$ *abs*(*a*[*j*,*j*]) > *bigajj* **then**

begin

bigajj := *abs*(*a*[*j*,*j*]);

k := *j*

end;

end;

if *bigajj* = 0 **then go to** *fail*;

preparation of elimination step i:

r[*k*] := **false**;

q[*k*] := 1/*a*[*k*,*k*];

p[*k*] := 1;

a[*k*,*k*] := 0;

for *j* := 1 **step** 1 **until** *k*-1 **do**

begin

p[*j*] := *a*[*j*,*k*];

q[*j*] := (**if** *r*[*j*] **then** -*a*[*j*,*k*] **else** *a*[*j*,*k*] $\times$ *q*[*k*]);

a[*j*,*k*] := 0

end;

for *j* := *k*+1 **step** 1 **until** *n* **do**

begin

p[*j*] := **if** *r*[*j*] **then** *a*[*k*,*j*] **else** -*a*[*k*,*j*];

q[*j*] := -*a*[*k*,*j*] $\times$ *q*[*k*];

a[*k*,*j*] := 0

end;

elimination proper:

for *j* := 1 **step** 1 **until** *n* **do**

for *k* := *j* **step** 1 **until** *n* **do**

a[*j*,*k*] := *a*[*j*,*k*] + *p*[*j*] $\times$ *q*[*k*]

end grand loop

end syminv2

CERTIFICATION OF ALGORITHM 150

SYMINV2 [H. Rutishauser, Comm. ACM 6 (Feb. 1963), 67]

PETER NAUR (Recd 27 Sept. 63)

Regnecentralen, Copenhagen, Denmark

Since the translator refuses to run programs with more than one occurrence of the same identifier in a formal parameter list, the second *a* was taken out when this procedure was run with the GIER ALGOL system [cf. also the discussion in Comm. ACM 6 (July 1963), 390]. Otherwise it ran smoothly. For testing the accuracy, segments of the Hilbert matrix were inverted and the results multiplied by the original segment and compared with the unit matrix. The largest deviation in any element was found to be:

Order	Max. deviation from elements of the unit matrix	Order	Max. deviation from elements of the unit matrix
2	-1.49 ₁₀ -8	6	-7.32 ₁₀ -3
3	-2.38 ₁₀ -7	7	-3.59 ₁₀ -1
4	-1.53 ₁₀ -5	8	-2.95 ₁₀ 1
5	-3.36 ₁₀ -4	9	-1.25 ₁₀ 1

These figures may be compared directly with the ones related to Algorithms 120, INVERSION II, and *gjr* [Comm. ACM 6 (Aug. 1963), 445]. A comparison shows that all three algorithms yield about the same accuracy, with *syminv2* being the best in most cases, however. This is not too surprising since the knowledge that the matrix is symmetric ought to simplify the calculation considerably.

The lengths of the three procedures after translation are as follows:

	Number of GIER words
<i>syminv2</i>	216
INVERSION II	279
<i>gjr</i>	302

Execution times for *syminv2* in GIER ALGOL are:

Order	Time (sec)
5	1
10	3.5
15	10.5
20	23

This is about half the time of execution of INVERSION II or *gjr*.

REMARK ON ALGORITHM 150

SYMINV2 [H. Rutishauser, COMM. ACM, Feb. 1963]

H. RUTISHAUSER

Eidg. Technische Hochschule, Zurich, Switzerland

procedure *syminv2* (*a*, *n*) **result** : (*a*) **exit** : (*fail*); ... indicates that the value of parameter "*a*" is changed by the computing process (the matrix *a* is changed into its inverse, whereby the given matrix is destroyed). In any procedure call, the two actual parameters corresponding to the two *a*'s must be identical, otherwise the action of the procedure will be undefined (by virtue of the substitution rule). The user may also change the procedure heading into *syminv2* (*a*, *n*) **exit** : (*fail*); ... without changing the effect of the procedure.

EDITOR'S NOTE: The ALCOR group has adopted the rule that if the value of a parameter is changed by the execution of the procedure, then the parameter should be listed twice. Although the ALGOL 60 Report does not forbid listing a formal parameter twice, it would appear that a compiler which thus restricts the language could not accept some of the examples given in the ALGOL 60 Report.

REMARK ON ALGORITHM 150

SYMINV2 [H. Rutishauser, COMM. ACM, Feb. 1963]

ARTHUR EVANS, JR.

Carnegie Institute of Technology, Pittsburgh, Pennsylvania

The identifier "a" appears twice in the procedure heading as a formal parameter. It is not clear that this situation has any meaning in ALGOL. Indeed, it is not at all obvious how one might translate the procedure. If the actual parameters corresponding to the two formal parameters with the same identifier are different there is no way for the translator (or for the reader) to distinguish which 'a' is to be used. Further, it would take a detailed examination of the published algorithm to determine how this situation might be corrected. It is certainly not clear that it would be safe merely to delete one occurrence of the formal parameter 'a', since the operation of the algorithm might require that two separate matrices be available.

ALGORITHM 151

LOCATION OF A VECTOR IN A LEXICOGRAPHICALLY ORDERED LIST

HENRY F. WALTER

United States Steel Corp., Applied Research Laboratory, Monroeville, Penn.

```
integer procedure LOCATE (min, n, c, v, combinatorial);
value v; integer min, n, c; integer array v;
integer procedure combinatorial;
comment This procedure locates the position, LOCATE, of a
given vector in a list of vectors without searching the list. The
list consists of all the combinations of n consecutive digits taken
d at a time. Min is the smallest of the n integers. Each vector
(combination) is written in ascending order from left to right,
as, for example, 378 and the vectors are listed lexicographically,
by which is meant, that, considered as d digit numbers, the
vectors are listed in ascending order. For example, with min = 1,
d = 3, and n = 6, the vectors in order are 123, 124, 125, 126, 134,
135, ..., 456. Given the vector, v = 356, the procedure locates
this vector as the 19th in the list;
begin integer i, r, max, part, whole;
r := 1; v[0] := min - 1; max := min - 1 + n;
for i := 0 step 1 until c-1 do
begin part := c - i - 1;
ask: if v[i+1] - v[i] > 1 then
begin whole := max - v[i] - 1;
r := r + combinatorial (whole, part);
v[i] := v[i] + 1;
go to ask
end;
end;
locate := r
end;
```

ALGORITHM 152

NEXCOM

JOHN HOPLEY

Peat, Marwick, Mitchell & Co., London, England

```
procedure nexcom (char, N, setcomplete, nullvector);
array char; integer N;
label setcomplete, nullvector;
comment char is a column vector containing N elements each of
which is either 1 or 0. Nexcom transforms char into another
vector containing the same number of 1's and 0's, but in a differ-
ent sequence. Startin; with char in the state of having 1 in each of
the element positions 1, ..., r and zeros elsewhere then repeated
application of nexcom generates all 2^N patterns of char. The
procedure terminates if the presented vector char has 1 in each
of the positions N, N-1, ..., N-r+1 and zeros elsewhere. Termination
is indicated by exit through the formal label 'setcomplete'.
If char is the null vector then procedure exists through the
formal label 'nullvector';
begin integer n, p, m;
comment find the first 1 in char;
for n := 1 step 1 until N do if
char [n] = 1 then go to A;
go to nullvector;
comment how many adjacent 1's;
A: p := 0;
for m := n + 1 step 1 until N do
if char [m] = 1 then p := p + 1 else go to B;
comment Have all combinations been generated;
B: if p + n = N then go to setcomplete;
comment Set up next combination; char[n+p+1] := 1;
for m := n + p step - 1 until n do char [m] := 0;
for m := 1 step 1 until p do char [m] := 1;
end nexcom;
```

ALGORITHM 153

GOMORY

F. L. BAUER

Johannes Gutenberg-Universität, Mainz, Germany

```
procedure Gomory (a, m, n) result: (a) exit: (no solution);
value m, n;
integer m, n;
integer array a;
label no solution;
comment Gomory algorithm for all-integer programming. The
objective of this procedure is to determine the integer solution
of a linear programming problem with integer coefficients only.
The tableau-matrix a consists of m + 1 rows and n columns.
The top row of a is the objective row, the last column represents
the right-hand sides. The tableau-columns, with the exception
of the last column, have to be lexicographically positive. The
algorithm is finished if all entries in the last column, except the
top most entry, are nonnegative. Then the top most entry of
the last column represents the value of the objective function.
The other entries of the last column define the coordinates of
the optimal solution. There are always the same variables connected
with the same rows. The exit no solution is used if a row
is found which has a negative entry in the last column, but
otherwise only nonnegative entries;
begin integer i, k, j, l, r;
real lambda;
integer array l[1:n-1], c[1:n];
```

```

1:   for i := 1 step 1 until m do if a[i,n] < 0 then
      begin r := i; go to 2 end;
      go to end;
2:   for k := 1 step 1 until n-1 do if a[r,k] < 0 then
      go to 4;
      go to no solution;
4:   l := k;
      for j := k+1 step 1 until n-1 do if a[r,j] < 0 then
          begin i := 0;
              3: if a[i,j] < a[i,l] then l := j else
                  if a[i,j] = a[i,l] then
                      begin i := i+1; go to 3 end
                  end;
              for j := 1 step 1 until n-1 do if a[r,j] < 0 then
                  begin if a[0,l] ≠ 0 then t[j] := entier(a[0,j]/a[0,l])
                          else t[j] := 1
                      end;
                  lambda := abs(a[r,1]/t[1]);
                  for j := 2 step 1 until n-1 do if a[r,j] < 0 then
                      begin if abs(a[r,j]/t[j]) > lambda then
                          lambda := abs(a[r,j]/t[j]) end;
                      for j := 1 step 1 until n do if j ≠ l then
                          begin c[j] := entier(a[r,j]/lambda);
                              if c[j] ≠ 0 then
                                  for i := 0 step 1 until m do a[i,j] := a[i,j] + c[j] ×
                                      a[i,l]
                              end;
                          go to 1;
                      end;
                  end;
          end;
end: end;

```

CERTIFICATION OF ALGORITHM 153
 GOMORY [F. L. Bauer, *Comm. ACM* 6, Feb. 1963]
 B. LEFKOWITZ AND D. A. D'ESORO*
 Stanford Research Institute, Menlo Park, California

* Work supported by Office of Naval Research.

GOMORY was hand-coded in BALGOL for the Burroughs 220 and in FORTRAN for the CDC 1604. The following corrections should be made:

The statement
 $\lambda := \text{abs}(a[r,1]/t[1]);$
 should read
 $\lambda := \text{abs}(a[r,l]/t[l]);$
 The statement
 for j := 2 step 1 until n-1 do if a[r,j] < 0 then
 should read
 for j := 1 step 1 until n-1 do if a[r,j] < 0 then
 The following changes to Bauer's program were made to increase its efficiency and reduce storage requirements.
 Change the statement
 begin integer i, k, j, l, r;
 to read
 begin integer i, k, j, l, r, c, t;
 Change the statement
 real lambda;
 to read
 real lambda, lambda;
 Delete the statement
 integer array t[1:n-1], c[1:n];
 Before the statement
 for j := 1 step 1 until n-1 do if a[r,j] < 0 then
 insert the statement
 lambda := 1.0;
 Change the statement
 begin if a[0,l] ≠ 0 then t[j] := entier(a[0,j]/a[0,l])
 to read
 begin if a[0,l] ≠ 0 then t := entier(a[0,j]/a[0,l])

Change the statement
 else t[j] := 1
 to read
 else t := 1
 After the statement
 else t[j] := 1
 insert the statements
 $\lambda := -a[r,j]/t;$
 $\lambda := \text{if } \lambda < \lambda \text{ then } \lambda \text{ else } \lambda;$
 Delete the statements starting with
 $\lambda := \text{abs}(a[r,1]/t[1]);$
 up to and including
 $\lambda := \text{abs}(a[r,j]/t[j]) \text{ end};$
 Change the statement
 begin c[j] := entier(a[r,j]/lambda);
 to read
 begin c := entier(a[r,j]/lambda);
 Change the statement
 if c[j] ≠ 0 then
 to read
 if c ≠ 0 then
 Change the statement
 for i := 0 step 1 until m do a[i,j] := a[i,j] + c[j] ×
 to read
 for i := 0 step 1 until m do a[i,j] := a[i,j] + c ×
 The "tie-breaking" procedure embodied in the three statements beginning at

3: if a[i,j] < a[i,l] then l := j else

will fail if the two columns being compared are identical. Although this cannot happen on the first iteration, it may occur later. To test for this condition change the two statements beginning with

begin i := i + 1; go to 3 end

to read
 begin i := i + 1; if i > m then go to 31 else go to 3 end;
 31: end;

The revised algorithm yielded satisfactory answers on a ten equation-seven variable problem in 159 iterations and a 35-equation 14-variable problem in 447 iterations.

The following comments may be helpful for preparing a problem for GOMORY. The problem constraints must be stated in the form:

$$\sum_j a_{ij}x_j + s_i = b_i$$

where the s_i are slack variables. The columns representing these slack variables need not appear in the initial tableau-matrix a .

Since the only variables in the solution that will necessarily be non-negative are the s_i , any non-negativity constraints on the other variables must be among the above equations (e.g. the constraint $x_i \geq 0$ is represented by $-x_i + s_k = 0$).

The size of the integers in the b vector substantially affects the number of iterations.

The requirement that all but the last tableau-columns be lexicographically positive means that the first nonzero element in these columns must be positive.

EDITOR'S NOTE: Prof. Bauer wishes to indicate that for the Algorithm 153, GOMORY, credit is due to Ch. Witzgall, who wrote the draft.

ALGORITHM 154
COMBINATION IN LEXICOGRAPHICAL ORDER
CHARLES J. MIFSUD
Armour Research Foundation, ECAC Annapolis, Md.

procedure COMB1 (n, r, I); **integer** n, r ; **integer array** I ;
comment The distinct combinations of the first n integers taken r at a time are generated in I in lexicographical order starting with an initial combination of the r integers 1, 2, ..., r . Each call of the procedure, after the first, must have in I the previous generated combination. The Boolean variable *first* is nonlocal to COMB1 and must be **true** before the first call. Thereafter *first* remains **false** until all combinations have been generated. When calling COMB1 with I containing $n - r + 1, n - r + 2, \dots, n$, I is left unchanged and *first* is set **true**;
begin **integer** s, j ;
if *first* **then** **begin** **for** $j := 1$ **step** 1 **until** r **do**
 $I[j] := j$;
first := **false**; **go to** EXIT **end**;
begin **if** $I[r] < n$ **then** $I[r] := I[r] + 1$; **go to** EXIT **end**;
for $j := r$ **step** -1 **until** 2 **do**
if $I[j-1] < n - r + j - 1$ **then**
begin $I[j-1] := I[j-1] + 1$;
for $s := j$ **step** 1 **until** r **do**
 $I[s] := I[j-1] + s - (j-1)$; **go to** EXIT **end** **end**;
first := **true**;
EXIT : **end**

CERTIFICATION OF ALGORITHM 154
COMBINATION IN LEXICOGRAPHICAL ORDER
[Charles J. Mifsud, *Comm. ACM*, Mar. 1963]
K. M. BOSWORTH
I.C.T. Ltd., Hayes, Middlesex, England

This procedure was tested

for $r := 1$ **step** 1 **until** n **with** $n = 6$

with correct results.

ALGORITHM 155
COMBINATION IN ANY ORDER
CHARLES J. MIFSUD
Armour Research Foundation, ECAC Annapolis, Md.

procedure COMB2 ($m, M, n, r, s, S, TOTAL$); **integer array** m, M, S ; **integer** $n, r, s, TOTAL$;
comment Each call of COMB2 generates a distinct combination S , (if possible) of the n integer values of J taken r ($r > 1$) at a time if J consists of $m[1]$ integers each equal to $M[1]$, and $m[2]$ integers each equal to $M[2]$, and so on, there being s integers available. $TOTAL$ must be set to zero before the first call of COMB2 and thereafter $TOTAL$ is increased by one after each new combination is generated. To speedup the machine operation arrange the s integers in M such that $m[1] \geq m[2] \geq \dots \geq m[s]$;
begin **integer** i, j, t, p ; **own integer array** $J[1:n], I[1:r]$; **own Boolean** *first*;
if $TOTAL = 0$ **then** **begin**
 $t := 1$; $p := 0$;

for $j := 1$ **step** 1 **until** s **do**
begin $p := p + m[j]$;
for $i := t$ **step** 1 **until** p **do**
begin $J[i] := M[j]$;
 $t := t + 1$ **end** **end**;
first := **true** **end**;
1: COMB1 (n, r, I);
if *first* **then** **go to** EXIT;
if $I[1] = 1$ **then** **go to** 2 **else** **go to** 3;
2: **for** $j := 2$ **step** 1 **until** r **do**
if ($J[I[j]] = J[I[j]-1]$) $\wedge$ ($I[j] > I[j-1] + 1$) **then** **go to** 1;
go to 4;
3: **if** $J[I[1]] = J[I[1]-1]$ **then** **go to** 1 **else** **go to** 2;
4: **for** $j := 1$ **step** 1 **until** r **do**
 $S[j] := J[I[j]]$;
 $TOTAL := TOTAL + 1$;
EXIT: **end**

CERTIFICATION OF ALGORITHM 155
COMBINATION IN ANY ORDER [Charles J. Mifsud, *Comm. ACM*, Mar. 1963]
K. M. BOSWORTH
I.C.T. Ltd., Hayes, Middlesex, England

This procedure was tested using

$m[1] = 4 \quad m[2] = 3 \quad m[3] = 2 \quad m[4] = 2$
 $M[1] = 4 \quad M[2] = 7 \quad M[3] = 9 \quad M[4] = 16$

and for $r := 1$ **step** 1 **until** s

It is correctly generated for $r = 1$ the four combinations 4, 7, 9, 16, as well as the ten combinations for $r = 2$, the eighteen combinations for $r = 3$, and the twenty-six combinations for $r = 4$.

Changes made due to compiler limitations were (i) systematic changes of upper case letters where there was conflict due to having only one case of letters, (ii) transfer of **own** declared variables to non-local variables, and (iii) integer labels to identifiers.

ALGORITHM 156
ALGEBRA OF SETS
CHARLES J. MIFSUD
Armour Research Foundation, ECAC Annapolis, Md.

procedure INOUT (A, n, SUM); **real array** A ; **integer** n ; **real** SUM ;
comment $SUM = \sum_1 A_i - \sum_2 A_i A_j + \sum_3 A_i A_j A_k - \dots \pm A_1 A_2 \dots A_n$ is formed where the symbols $\sum_1, \sum_2, \sum_3, \dots, \sum_{n-1}$ stand for summation of the possible combinations of the numbers $A_1, A_2, \dots, A_n$ taken one, two, three, ..., ($n-1$) at a time;
begin **real** $j, part, T$; **integer** i, r ; **integer array** $I[1:n]$; **Boolean** *first*;
 $r := SUM := 0$; $j := -1$;
B: *first* := **true**; $r := r + 1$; $part := 0$;
A: COMB1 (n, r, I);
if *first* **then** **begin** $j := -1 \times j$; $part := j \times part$;
 $SUM := SUM + part$;
if $r < n$ **then** **go to** *B* **else** **go to** EXIT **end**;
 $T := 1$;
for $i := 1$ **step** 1 **until** r **do**
 $T := A[I[i]] \times T$;
 $part := part + T$; **go to** *A*;
EXIT: **end**

CERTIFICATION OF ALGORITHM 156
ALGEBRA OF SETS [Charles J. Mifsud, *Comm. ACM*,
Mar. 1963]

K. M. BOSWORTH
I.C.T. Ltd., Hayes, Middlesex, England

One correction required in this procedure is the systematic change of label *A* to avoid conflict with the formal parameter array *A*.

The procedure was then tested for $n = 9$ and $Ai = i$, $i = 1, \dots, n$, producing the correct answer $SUM = 1$.

Two other tests with arbitrary values of Ai and $n = 4$ were also correct.

ALGORITHM 157
FOURIER SERIES APPROXIMATION

CHARLES J. MIFSUD
Armour Research Foundation, ECAC Annapolis, Md.

procedure *FOURIER* (*N*, *f*, *a*, *b*); **real array** *f*, *a*, *b*; **integer** *N*;
comment *Fourier* determines $2N+1$ constants a_p ($p=0, 1, \dots, N$), b_p ($p=1, 2, \dots, N$) in such a way that the equations $f_n = 1/2a_0 + \sum_{p=1}^N (a_p \cos 2\pi np/(2N+1) + b_p \sin 2\pi np/(2N+1))$ are satisfied, where the f_n are given numbers. The f_n may be thought of as the $2N+1$ values of a function $f(x)$ at the points $x_n = 2\pi n/(2N+1)$. The method used to generate a_p , b_p was formulated by G. Goertzel in "Mathematical Methods for Digital Computers" (John Wiley and Sons, Inc., 1960);

begin real array *S*, *C*[1:2], *u*[0:2]; **real** *TEMP*, *pi*;
integer *p*, *i*;
pi := 3.14159265; *C*[2] := 1; *S*[2] := 0;
C[1] := $\cos(2 \times \pi i / (2 \times N + 1))$;
S[1] := $\sin(2 \times \pi i / (2 \times N + 1))$;
for *p* := 0 **step** 1 **until** *N* **do**
 begin *u*[1] := *u*[2] := 0;
 for *i* := 2 $\times$ *N* **step** -1 **until** 1 **do**
 begin *u*[0] := *f*[*i*] + 2 $\times$ *C*[2] $\times$ *u*[1] - *u*[2];
 u[2] := *u*[1]; *u*[1] := *u*[0] **end**;
 a[*p*] := $2 / (2 \times N + 1) \times (f[0] + u[1] \times C[2] - u[2])$;
 b[*p*] := $2 / (2 \times N + 1) \times u[1] \times S[2]$;
 TEMP := *C*[1] $\times$ *C*[2] - *S*[1] $\times$ *S*[2];
 S[2] := *C*[1] $\times$ *S*[2] + *S*[1] $\times$ *C*[2];
 C[2] := *TEMP* **end end**

REMARK ON ALGORITHM 157
FOURIER SERIES APPROXIMATION [C. J. Mifsud,
Comm. ACM, Mar. 1963]

RICHARD GEORGE*
Argonne National Laboratory, Argonne, Ill.

This algorithm was written in FAP language for the 32-K IBM 704. It was tested on a sawtooth curve, and the sawtooth was recreated by summing the expansion up through the $2N+1$ constants, with excellent results.

The arrays *S*, *C* and *u* are never referenced with a variable subscript. For a saving of time, I suggest that simple variables be used instead.

By declaring one additional real variable, one can bring the phrase

$$2 / (2 \times N + 1)$$

outside of the **for** loops, because *N* does not change through the procedure. This results in a saving of $4N+2$ mult-ops.

REMARK ON ALGORITHM 157
FOURIER SERIES APPROXIMATION [Charles J.
Mifsud, *Comm. ACM*, Mar. 1963]

GEORGE R. SCHUBERT*
University of Dayton, Dayton, Ohio

* Undergraduate research project, Computer Science Program, Univ. of Dayton.

Algorithm 157 has been modified to fit $2N$ data points and has run successfully on the Burroughs 220 using BALGOL. With the modifications, $2N$ constants a_p ($p=0, 1, \dots, N$) and b_p ($p=1, 2, \dots, N-1$) are determined such that the equation $f_n = a_0/2 + \sum_{p=1}^{N-1} (a_p \cos \pi np/N + b_p \sin \pi np/N) + a_N/2 \cos \pi n$ is satisfied.

In the modified procedure, the second and third lines after the integer declaration should read:

C[1] := $\cos(\pi i/N)$;

S[1] := $\sin(\pi i/N)$;

The second **for** statement should read:

for *i* := 2 $\times$ *N* - 1 **step** -1 **until** 1 **do**

The lines containing the *a* and *b* coefficients should read:

a[*p*] := $(f[0] + u[1] \times C[2] - u[2]) / N$;

b[*p*] := $(u[1] \times S[2]) / N$;

REFERENCE: R. W. Hamming, *Numerical Methods for Scientists and Engineers*, pp. 68-73 (McGraw-Hill, 1962).

ALGORITHM 158 (ALGORITHM 134, REVISED)
EXPONENTIATION OF SERIES

HENRY E. FETTIS
Aeronautical Research Laboratories, Wright-Patterson
Air Force Base, Ohio

procedure *SERIESPWR* (*A*, *B*, *P*, *N*); **value** *A*, *P*, *N*;
 array *A*, *B*; **integer** *N*;
comment This procedure calculates the first *N* coefficients *B*[*i*] of the series $g(x) = f(x) \uparrow P$ given the first *N* coefficients of the series

$$f(x) = 1 + \sum A[i] \times x \uparrow i \quad (i=1, 2, \dots, N).$$

P may be any real number. Setting *P* := 0 gives the coefficients for $LN(g(x))$;

begin integer *i*, *k*;

real *P*, *S*;

if *P* = 0 **then** *B*[1] = *A*[1];

else *B*[1] := *P* $\times$ *A*[1];

for *i* := 2 **step** 1 **until** *N* **do**

begin *S* := 0;

for *k* := 1 **step** 1 **until** *i* - 1 **do**

S := *S* + (*P* $\times$ (*N* - *k*) - *k*) $\times$ *B*[*k*] $\times$ *A*[*N* - *k*];

B[*i*] := *P* $\times$ *A*[*i*] + (*S* / *i*)

end for *i*;

end SERIESPWR

CERTIFICATION OF ALGORITHM 158
EXPONENTIATION OF SERIES [H. E. Fettis, *Comm.*
ACM, Mar. 1963]

J. DENNIS LAWRENCE
Lawrence Radiation Laboratory, Livermore, Calif.

This procedure was translated into FORTRAN and run on the Remington-Rand LARC Computer. Three changes are necessary.

- (1) The last line of the comment should read
for the natural logarithm of $f(x)$;

(2) The third line from the end should read

$$S := S + (P \times (i-k) - k) \times B[k] \times A[i-k];$$

(This line was given correctly in algorithm 134.)

(3) The second line from the end apparently should read

$$B[i] := A[i] := (S/i);$$

for the case $P = 0$ only. Probably the best way to incorporate this is by making two changes:

(a) Change the if clause to read

if $P = 0$ then $R := 1$ else $R := P$; $B[1] := R \times A[1]$;

(b) Change the second line from the end to read

$$B[i] := R \times A[i] + (S/i);$$

A large number of examples were run quite successfully; the following give representative samples.

(1) $(1+2x+3x^2+0.5x^3)^2 = 1+4x+10x^2+13x^3+11x^4+3x^5+0.25x^6$
(using $A[4] := A[5] := A[6] := 0$).

(2) Setting $P := 1$ gives $B[i] := A[i]$.

(3) Let $f(x) = e^x = 1 + \sum_{i=1}^n \frac{1}{i!} x^i$ and let $P = \ln 2 = .693147181$.

Then $g(x) = 2^x = 1 + \sum_{i=1}^n \frac{(\ln 2)^i}{i!} x^i$. (See Table 1.)

(4) Let $f(x) = e^x$ and $P = -1$. Then $g(x) = e^{-x}$. For $P=0$, apparently the constant term of $g(x)$ should be zero instead of one.

TABLE 1

	A[i]	B[i]
1	1.000000000	0.693147181
2	0.500000000	0.240226507
3	0.166666667	0.055504109
4	0.041666667	0.009618129
5	0.008333333	0.001333356
6	0.001388889	0.000154035
7	0.000198413	0.000015253
8	0.000024802	0.000001322
9	0.000002756	0.000000102
10	0.000000276	0.000000007

(5) Let $f(x) = e^x$ and $P = 0$. Then $g(x) = x$.

(6) Let $f(x) = \sum_{i=0}^n x^i$ and $P = 0$. Then $g(x) = \ln(1-x^n) - \ln(1-x) = \sum_{i=1}^n \frac{1}{i} x^i$. (See Table 2.)

TABLE 2

	A[i]	B[i]
1	1.0	1.000000000
2	1.0	0.500000000
3	1.0	0.333333340
4	1.0	0.250000000
5	1.0	0.200000000
6	1.0	0.166666670
7	1.0	0.142857140
8	1.0	0.125000000
9	1.0	0.111111110
10	1.0	0.100000000
11	1.0	0.090909100
12	1.0	0.083333330
13	1.0	0.076923080
14	1.0	0.071428580
15	1.0	0.066666660

ALGORITHM 159

DETERMINANT

DAVID W. DIGBY

Oregon State University, Corvallis, Ore.

```

real procedure Determinant (X,n);
value n; integer n; array X;
comment Determinant calculates the determinant of the n-by-
n square matrix X, using the combinatorial definition of the
determinant. This algorithm is intended as an example of a
recursive procedure which is somewhat less trivial than Factorial
(Algorithm 33);
begin real D; integer i; Boolean array B[1:n];
procedure Thread (P,e,i);
value P, e, i; real P; integer e, i;
if i > n then D := D + P × (-1) ↑ e else if P ≠ 0 then
begin integer j, f;
f := 0;
for j := n step -1 until 1 do
if B[j] then f := f + 1 else
begin
B[j] := true;
Thread (P×X[i,j],e+f,i+1);
B[j] := false;
end of loop;
end of Thread;
for i := 1 step 1 until n do
B[i] := false;
D := 0;
Thread (1,0,1);
Determinant := D;
end Determinant;

```

CERTIFICATION OF ALGORITHM 159

DETERMINANT [David W. Digby, *Comm. ACM*,
March 1963]

ARNOLD LAPIDUS

Courant Institute of Mathematical Sciences, New York
University, New York, N. Y.

Algorithm 159 was translated into FORTRAN II for the IBM 7090 as part of a test of FORTRAN subroutines designed to facilitate the implementation of recursive procedures. As expected, the numerical results were poor. For the Hilbert matrices $H_n = (a_{ij})$, $a_{ij} = 1/(i+j-1)$, results were as follows:

n	Det H_n (true)	Det H_n (computed by Algorithm 159)
2	8.333 333 3 (- 2)	8.333 333 2 (- 2)
3	4.629 629 6 (- 4)	4.629 623 1 (- 4)
4	1.653 439 2 (- 7)	1.651 933 4 (- 7)
5	3.749 295 1 (-12)	-2.910 383 0 (-11)

Determinants of order 4 and 6 with integer elements were also evaluated. The algorithm gave full accuracy for these.

ALGORITHM 160

COMBINATORIAL OF M THINGS

TAKEN N AT A TIME

M. L. WOLFSON AND H. V. WRIGHT

United States Steel Corp., Monroeville, Penn.

```

integer procedure combination (m, n);
value n; integer m, n;

```

comment calculates the number of combinations of m things taken n at a time. If n is less than half of m , then the program calculates the combinations of m things taken $m - n$ at a time which is the exact equivalent of m things taken n at a time;

```
begin integer p, r, i;
  p := m - n;
  if n < p then begin p := n; n := m - p end;
  if p = 0 then begin r := 1; go to exit end;
  r := n + 1;
  for i := 2 step 1 until p do r := (r × (n+i))/i;
exit: combination := r
end combination
```

CERTIFICATION OF ALGORITHM 160
COMBINATORIAL OF M THINGS TAKEN N AT
A TIME [M. L. Wolfson and H. V. Wright, *Comm. ACM*,
Apr. 1963]

DMITRI THORO
San Jose State College, San Jose, Calif.

Algorithm 160 was translated into FORTRAN II and FORGO for the IBM 1620. Correct results were obtained for values of m up to 20.

CERTIFICATION OF ALGORITHM 160
COMBINATORIAL OF M THINGS TAKEN N AT
A TIME [M. L. Wolfson and H. V. Wright, *Comm.*
ACM; April 1963]

ROBERT F. BLAKELY
Indiana Geological Survey, Bloomington, Ind.

Algorithm 160 was translated into ALGO, a compiler for the Control Data Corp. G-15 computer (formerly the Bendix G-15).

With the restriction that $m \geq n \geq 0$, correct results were obtained for all integer values of m and n , where $0 \leq m \leq 10$. Several other values were tested and all results were correct.

ALGORITHM 161
COMBINATORIAL OF M THINGS
TAKEN ONE AT A TIME, TWO AT A TIME,
UP TO N AT A TIME
H. V. WRIGHT AND M. L. WOLFSON
United States Steel Corp., Monroeville, Penn.

```
procedure combination vector (m, n, v);
integer m, n; integer array v;
comment calculates all combinations of m things taken from 1
to n at a time. The result is a vector, v, within which the first
element is the combination of m things taken 1 at a time, the
second element is the combinations of m things taken 2 at a time,
the third element taken 3 at a time, ..., and the nth element
taken n at a time.
begin integer i;
  v[1] := m;
  for i := 2 step 1 until n do
    v[i] := (v[i-1] × (m-i+1))/i;
end combination vector
```

CERTIFICATION OF ALGORITHM 161
COMBINATORIAL OF M THINGS TAKEN ONE AT
A TIME, TWO AT A TIME, UP TO N AT A TIME
[H. V. Wright and M. L. Wolfson, *Comm. ACM*, Apr.
1963]

DMITRI THORO
San Jose State College, San Jose, Calif.

Algorithm 161 was translated into FORTRAN II and FORGO for the IBM 1620. Correct results were obtained for values of m up to 20.

CERTIFICATION OF ALGORITHM 161
COMBINATORIAL OF M THINGS TAKEN ONE AT
A TIME, TWO AT A TIME, UP TO N AT A TIME
[H. V. Wright and M. L. Wolfson, *Comm. ACM*,
Apr. 1963]

DAVID H. COLLINS
Indiana Geological Survey, Bloomington, Ind.

Algorithm 161 was translated into ALGO, a compiler for the Control Data Corp. G-15 computer (formerly the Bendix G-15).

With the restriction that $m \geq n \geq 1$, correct results were obtained for all integer values of m and n , where $1 \leq m = n \leq 15$. Several other values were tested (including cases where $m \neq n$) and all results were correct.

ALGORITHM 162
XYMOVE PLOTTING
FRED G. STOCKTON
Shell Development Co., Emeryville, Calif.

```
procedure xymove (XZ, YZ, XN, YN); value XZ, YZ, XN, YN;
integer XZ, YZ, XN, YN;
```

comment xymove computes the code string required to move the pen of a digital incremental X,Y-plotter from an initial point (XZ, YZ) to a terminal point (XN, YN) by the "best" approximation to the straight line between the points. The permitted elemental pen movement is to an adjacent point in a plane Cartesian point lattice, diagonal moves permitted. The eight permitted pen movements are coded

1 = +Y, 2 = +X+Y, 3 = +X, 4 = +X-Y,
5 = -Y, 6 = -X-Y, 7 = -X, 8 = -X+Y.

The approximation is "best" in the sense that each point traversed is at least as near the true line as the other candidate point for the same move.

xymove does not use multiplication or division;

```
begin integer A, B, D, E, F, T, I, move;
```

comment code (J) is a procedure which returns a value of code according to the following table:

J	1	2	3	4	5	6	7	8
code	1	2	3	2	3	4	5	4
J	9	10	11	12	13	14	15	16
code	5	6	7	6	7	8	1	8

plot (move) is a procedure which sends move to the plotter as a plotter command;

if XZ = XN ^ YZ = YN then go to return;

```

A := XN - XZ; B := YN - YZ; D := A + B; T :=
B - A; I := 0;
if B ≥ 0 then I := 2;
if D ≥ 0 then I := I + 2;
if T ≥ 0 then I := I + 2;
if A ≥ 0 then I := 8 - I else I := I + 10;
A := abs(A); B := abs(B); F := A + B; D := B - A;
if D ≥ 0 then begin T := A; D := -D end else T := B;
E := 0;
repeat: A := D + E; B := T + E + A;
if B ≥ 0 then begin E := A; move := code(I);
F := F - 2 end
else begin E := E + T; F := F - 1;
move := code(I-1) end;
plot(move);
if F > 0 then go to repeat;
return:
end

```

CERTIFICATION OF ALGORITHM 162
XYMOVE PLOTTING [Fred G. Stockton, *Comm. ACM*,
Apr. 1963]

WILLIAM E. FLETCHER
Bolt, Beranek and Newman Inc., Los Angeles, Calif.

The line in the body of the procedure which read:

```
if D ≥ 0 then I := I + 2;
```

was corrected to read:

```
if D ≥ 0 then I := I + 2;
```

With this one change the body of the procedure was translated into DECAL-BBN and successfully run on a PDP-1 computer utilizing the cathode ray tube output to display the path of a simulated digital incremental plotter.

REMARK ON ALGORITHM 162 [J6]
XYMOVE PLOTTING [F. G. Stockton, *Comm. ACM* 6
(Apr. 1963), 161; 6 (Aug. 1963), 450]
D. K. CAVIN (Recd. 10 Feb. 1964)
Oak Ridge National Laboratory, Oak Ridge, Tenn.

The following modifications were made to Algorithm 162 to decrease the average execution time. The last nine lines of Algorithm 162 are replaced by the following:

```

move := code(I-1); I := code(I);
repeat: A := D + E; B := T + E + A;
if B ≥ 0 then begin E := A; F := F - 2; plot(I) end
else begin E := E + T; F := F - 1; plot(move) end;
if F > 0 then go to repeat;
return:
end

```

It is obvious that on any movement containing more than two elemental pen movements the use of the code procedure in the loop is redundant, since no more than two of the eight permitted pen movements are necessary for the approximation of any line. Therefore moving the call of the code procedure outside of the basic loop reduces the execution time whenever the X, Y movement requires more than two elemental pen movements. The procedures were coded in CODAP, the assembly language for the CDC 1604-A, and this modified version was approximately 40 percent faster in the loop than the original version. The timing comparisons used numbers in the range -2000 to 2000 with heavy emphasis on the subrange -150 to 150. The typographical error noted in the certification (*Comm. ACM*, August 1963) was corrected in both codes.

[A referee verifies that Algorithm 162 does indeed run, as changed.—G.E.F.]

ALGORITHM 163 MODIFIED HANKEL FUNCTION

HENRY E. FETTIS

Aeronautical Research Laboratories, Wright-Patterson
Air Force Base, Ohio

procedure *EXPK* (*P*, *X*, *E*); **real** *P*, *X*, *E*;
comment this procedure calculates the modified Hankel Function $e^x K_p(x)$ to within a given accuracy *E* from the integral representation:

$$e^x K_p(x) = \int_0^\infty e^{x(1-\cosh t)} \cosh(pt) dt;$$

```

begin real F, G, H, R, S, T, U, Y, Z, ZP;
R := 0.0;
H := 1.0;

```

```
iteration: begin
```

```

G := R;
T := .5 × H;
S := 0;
Z := exp(T);
U := Z × Z;

```

```
integration: begin
```

```

Y := X × (1 - .5 × (Z + 1/Z));
if P = 0 then ZP := 1
else ZP := Z ↑ P;
F := .5 × exp(Y) × (ZP + 1/ZP);
S := S + F;
Z := Z × U;
end;
if F ≥ E then go to integration
else R := H × S;
H := .5 × H;

```

```
end;
```

```

if abs(R - G) ≥ E then go to iteration
else EXPK := R

```

```
end EXPK
```

CERTIFICATION OF ALGORITHM 163
MODIFIED HANKEL FUNCTION [Henry E. Fettis,
Comm. ACM, Apr. 1963]

HENRY C. THACHER, JR.*

Argonne National Laboratory, Argonne, Ill.

Since this algorithm is a function declaration, the procedure declaration should be:

```
real procedure EXPK(D, X, E); ...
```

Otherwise, no syntactical errors were noticed.

The body of the procedure was translated and run on the LGP-30 computer, using the Dartmouth SCALP system. Results for $E = 0.0001$, $X = 0.1(0.1)1.0$, $P = 0, 0.3333333, 0.6666667$ and 1.000000 agreed with values tabulated in Jahnke-Emde-Losch to the 3-4D given in the tables, except for errors discovered in the table of $2/\pi K_{2/3}(x)$.

With $X = 0$, the program ended in floating-point overflow. The algorithm itself, or the call of the procedure, should include a test to insure that the variable is greater than *eps*, where *eps* is chosen to prevent exceeding machine capacity.

The algorithm was found to be excessively slow. Times on the LGP-30 were of the order of 6 minutes. A considerable saving in time could be realized by improving the quadrature formula, currently the simple midpoint formula, repeated completely for each iteration. A more effective method would be a modified Romberg algorithm. A procedure based on the latter approach is being developed in this division.

ALGORITHM 164 ORTHOGONAL POLYNOMIAL LEAST SQUARES SURFACE FIT

R. F. CLARK, R. N. KUBIK, L. P. PHILLIPS
The Babcock & Wilcox Co., Atomic Energy Div.,
Lynchburg, Va.

procedure surfacefit ($x, u, y, w, z, nmax, mmax, imax, jmax$)
result: (β , ϕ , $zcomp$, $minsqd$, $minsqdcomp$, $sumdifcomp$,
 $maxdifcomp$);
real array $x, u, y, w, z, \phi, \beta, zcomp$;
integer $nmax, mmax, imax, jmax$;
real $minsqd, minsqdcomp, sumdifcomp, maxdifcomp$;
comment this is a transliteration of an operating program written in Burroughs ALGOL for the B-220. It fits, in the least squares sense, a polynomial function of two independent variables to values of a dependent variable specified at points on a rectangular grid in the plane of the independent variables. The use of orthogonal polynomials leads to a particularly simple system of linear equations rather than the ill-conditioned system which arises from the usual normal equations. It also provides a measure of the improvements resulting from each new term included which further leads, in this algorithm, to an automatic selection of a "best" degree polynomial function as determined by Gauss' criterion. The initial normalization of the variables results in significant reduction of round off errors in many cases. This algorithm is developed more fully in BAW-182. For a very similar approach to this and related problems see Cadwell, J. H., "Least Squares Surface Fitting Program", *The Computer J.* 3 (1961), 266 and Cadwell, J. H., and Williams, D. E., "Some Orthogonal Methods of Curve and Surface Fitting," *The Computer J.* 4 (1961), 260. A further reference is Gauss, C. F., "Theoria Combinationis Observationum Erroribus Minimis Obnoxial," *Gauss Werke* 4 (Gottingen 1873), 3-93. $x[i]$ and $y[j]$ are the independent variables, $z[i, j]$ is the dependent variable. $u[i]$ and $w[j]$ represent the weights corresponding to $x[i]$ and $y[j]$, respectively. $nmax$ is one more than the maximum degree of x to be considered. $mmax$ is one more than the maximum degree of y to be considered. $imax$ is the number of x 's, and $jmax$ is the number of y 's. $\beta[n, m]$ is a measure of the improvement resulting from the inclusion of the $x^n y^m$ th term. $\phi[n, m]$ is the polynomial coefficient for the $x^n y^m$ th term. Note the degree of the resulting polynomial may be less than the maximum degree specified as a result of the application of Gauss' criterion. $zcomp$ is the computed dependent variable.

$$minsqd = \left(\frac{\sum_{i,j} u[i] \cdot w[j] \cdot z[i,j]^2 - \sum_{n,m} \beta[n,m]^2}{imax \cdot jmax} \right)^{1/2}$$

$$minsqdcomp = \left(\frac{\sum_{i,j} u[i] \cdot w[j] (z[i,j] - zcomp[i,j])^2}{imax \cdot jmax} \right)^{1/2}$$

$$sumdifcomp = \frac{\sum_{i,j} |z[i,j] - zcomp[i,j]|}{imax \cdot jmax}$$

$$maxdifcomp = \max |z(i, j) - zcomp(i, j)|$$

$minsqd$ and $minsqdcomp$ are equal if computation is exact. In practice they will not be equal due to the imprecise nature of calculation. A wide discrepancy indicates excessive errors in calculation;

begin

real array $a, b, denpa[1:nmax], c, d, denqa[1:mmax],$
 $\alpha[1:nmax, 1:mmax], p[1:nmax, 1:imax], q[1:mmax, 1:jmax],$
 $pc[1:nmax, 1:mmax], qc[1:mmax, 1:mmax];$

integer $n, m, i, j, s, t, r;$

real $sumx, sumy, sumz, meanx, meany, meanz, numa, dena, denb,$
 $numc, denc, dend, alph, sumzsq, gausscrit, trialgausscrit, betasum,$
 $rescomp, poly;$

comment normalization of variables;
 $sumx := sumy := sumz := 0.0;$
for $i := 1$ **step** 1 **until** $imax$ **do**
 $sumx := sumx + x[i];$
 $meanx := sumx/imax;$
for $i := 1$ **step** 1 **until** $imax$ **do**
 $x[i] := x[i] - meanx;$
for $j := 1$ **step** 1 **until** $jmax$ **do**
 $sumy := sumy + y[j];$
 $meany := sumy/jmax;$
for $j := 1$ **step** 1 **until** $jmax$ **do**
 $y[j] := y[j] - meany;$
for $i := 1$ **step** 1 **until** $imax$ **do begin**
 for $j := 1$ **step** 1 **until** $jmax$ **do**
 $sumz := sumz + z[i,j] \text{ end};$
 $meanz := sumz/(imax \times jmax);$
 for $i := 1$ **step** 1 **until** $imax$ **do begin**
 for $j := 1$ **step** 1 **until** $jmax$ **do**
 $z[i, j] := z[i, j] - meanz \text{ end};$
 comment evaluate orthogonal polynomials;
 $numa := dena := 0.0;$
 for $i := 1$ **step** 1 **until** $imax$ **do begin**
 $p[1, i] := 1.0;$
 $numa := numa + u[i] \times x[i];$
 $dena := dena + u[i] \text{ end};$
 $a[2] := numa/dena;$
 for $i := 1$ **step** 1 **until** $imax$ **do**
 $p[2, i] := x[i] - a[2];$
 for $n := 3$ **step** 1 **until** $nmax$ **do begin**
 $numa := dena := denb := 0.0;$
 for $i := 1$ **step** 1 **until** $imax$ **do begin**
 $numa := numa + u[i] \times x[i] \times p[n-1, i] \uparrow 2;$
 $dena := dena + u[i] \times p[n-1, i] \uparrow 2;$
 $denb := denb + u[i] \times p[n-2, i] \uparrow 2 \text{ end};$
 $a[n] := numa/dena; \quad b[n] := dena/denb;$
 for $i := 1$ **step** 1 **until** $imax$ **do**
 $p[n, i] := (x[i] - a[n]) \times p[n-1, i] - b[n] \times p[n-2, i] \text{ end};$
 $numc := denc := 0.0;$
 for $j := 1$ **step** 1 **until** $jmax$ **do begin**
 $q[1, j] := 1.0;$
 $numc := numc + w[j] \times y[j];$
 $denc := denc + w[j] \text{ end};$
 $c[2] := numc/denc;$
 for $j := 1$ **step** 1 **until** $jmax$ **do**
 $q[2, j] := y[j] - c[2];$
 for $m := 3$ **step** 1 **until** $mmax$ **do begin**
 $numc := denc := dend := 0.0;$
 for $j := 1$ **step** 1 **until** $jmax$ **do begin**
 $numc := numc + w[j] \times y[j] \times q[m-1, j] \uparrow 2;$
 $denc := denc + w[j] \times q[m-1, j] \uparrow 2;$
 $dend := dend + w[j] \times q[m-2, j] \uparrow 2 \text{ end};$
 $c[m] := numc/denc; \quad d[m] := denc/dend;$
 for $j := 1$ **step** 1 **until** $jmax$ **do**
 $q[m, j] := (y[j] - c[m]) \times q[m-1, j] - d[m] \times q[m-2, j] \text{ end};$
 comment evaluate contribution of each orthogonal polynomial to the minimization of the residuals;
 for $n := 1$ **step** 1 **until** $nmax$ **do begin**
 $denpa[n] := 0.0;$
 for $i := 1$ **step** 1 **until** $imax$ **do**
 $denpa[n] := denpa[n] + u[i] \times p[n, i] \uparrow 2 \text{ end};$
 for $m := 1$ **step** 1 **until** $mmax$ **do begin**
 $denqa[m] := 0.0;$
 for $j := 1$ **step** 1 **until** $jmax$ **do**
 $denqa[m] := denqa[m] + w[j] \times q[m, j] \uparrow 2 \text{ end};$
 for $n := 1$ **step** 1 **until** $nmax$ **do begin**
 for $m := 1$ **step** 1 **until** $mmax$ **do begin**
 $alph := 0.0;$

```

for i := 1 step 1 until imax do begin
  for j := 1 step 1 until jmax do
    alph := alph + u[i] × w[j] × z[i, j] × p[n, i] × q[m, j]
  end;
  alpha[n, m] := alph / (denpa[n] × denqa[m]);
  beta[n, m] := alpha[n, m] × alph; end end;
comment application of Gauss' criterion to determine the de-
gree polynomial which yields the closest fit to the given data.
Gauss' criterion is, strictly speaking, applicable only to cases
where the weights u[i] and w[j] are unity;
sumzsq := 0.0;
for i := 1 step 1 until imax do begin
  for j := 1 step 1 until jmax do
    sumzsq := sumzsq + u[i] × w[j] × z[i, j] ↑ 2 end;
  s := t := 1;
  for n := 1 step 1 until nmax do begin
    betasum := 0.0;
    for m := 1 step 1 until mmax do begin
      for r := 1 step 1 until n do
        betasum := betasum + beta[r, m];
      if betasum > sumzsq then trialgausscrit := 0.0
      else
        trialgausscrit := -(sumzsq - betasum) / (imax × jmax - n × m);
      if n = 1 ∧ m = 1 then gausscrit := trialgausscrit;
      if gausscrit = trialgausscrit then begin
        if n × m < s × t then begin
          s := n;
          t := m end end;
        if gausscrit > trialgausscrit then begin
          gausscrit := trialgausscrit;
          s := n;
          t := m end end end;
    end;
  nmax := s;
  mmax := t;
  minsqd := (gausscrit × (imax × jmax - nmax × mmax) / (imax × jmax))
  ↑ 1/2;
comment evaluation of orthogonal polynomial coefficients;
for n := 1 step 1 until nmax do begin
  pc[n, m] := 1.0;
  for s := 1 step 1 until n - 1 do begin
    pc[n, s] := -a[n] × pc[n-1, s];
    if s ≠ 1 then pc[n, s] := pc[n, s] + pc[n-1, s-1];
    if s ≠ n - 1 then pc[n, s] := pc[n, s] - b[n] × pc[n-2, s]
  end end;
  for m := 1 step 1 until mmax do begin
    qc[m, m] := 1.0;
    for t := 1 step 1 until m - 1 do begin
      qc[m, t] := -c[m] × qc[m-1, t];
      if t ≠ 1 then qc[m, t] := qc[m, t] + qc[m-1, t-1];
      if t ≠ m - 1 then qc[m, t] := qc[m, t] - d[m] × qc[m-2, t]
    end end;
comment evaluation of approximating polynomial coefficients;
for s := 1 step 1 until nmax do begin
  for t := 1 step 1 until mmax do begin
    phi[s, t] := 0.0;
    for n := s step 1 until nmax do begin
      for m := t step 1 until mmax do
        phi[s, t] := phi[s, t] + alpha[n, m] × pc[n, s] × qc[m, t]
      end end end;
comment evaluation of dependent variables using the approxi-
mating polynomial;
minsqdcomp := sumdifcomp := maxdifcomp := 0.0;
for i := 1 step 1 until imax do begin
  for j := 1 step 1 until jmax do begin
    zcomp[i, j] := 0.0;
    for s := nmax step -1 until 1 do begin
      poly := phi[s, mmax];

```

```

    for t := mmax - 1 step 1 until 1 do
      poly := poly × y[j] + phi[s, t];
      zcomp[i, j] := zcomp[i, j] × x[i] + poly end;
    rescomp := z[i, j] - zcomp[i, j];
    zcomp[i, j] := zcomp[i, j] + meanz;
    minsqdcomp := minsqdcomp + u[i] × w[j] × rescomp ↑ 2;
    sumdifcomp := sumdifcomp + abs(rescomp);
    if abs(rescomp) > maxdifcomp then
      maxdifcomp := abs(rescomp) end end;
    minsqdcomp := (minsqdcomp / (imax × jmax)) ↑ 1/2;
    sumdifcomp := sumdifcomp / (imax × jmax);
  end surfacefit

```

CERTIFICATION OF ALGORITHM 164 ORTHOGONAL POLYNOMIAL LEAST SQUARES SURFACE FIT [R. E. Clark, R. N. Kubik, L. P. Phillips, *Comm. ACM*, April 1963]

C. V. BITTERLI

Johns Hopkins Univ. Applied Physics Lab., Silver Spring,
 Md.

The SURFACEFIT algorithm was translated into FORTRAN
 and successfully run on an IBM 7094. It was necessary to make the
 following corrections:

(a) 12th line after

comment evaluate orthogonal polynomials;

should read

numa := numa + u[i] × x[i] × p[n-1, i] ↑ 2;

(b) 2nd line after

comment evaluation of orthogonal polynomial coefficients;

should read

pc[n, n] := 1.0;

(c) 12th line after

comment evaluation of orthogonal polynomial coefficients;

should read

if t ≠ 1 then qc[m, t] := qc[m, t] + qc[m-1, t-1];

(d) 8th line after

comment evaluation of dependent variables using the approxi-
 mating polynomial

should read

for t := mmax - 1 step -1 until 1 do

The following function was used to generate data for checking
 this algorithm:

$$z = 1 - x + y - xy + x^2 - y^2$$

for $x = 0, 1, 2, 3, 4$

and $y = 0, 1, 2, 3, 4$

The resulting polynomial was:

$$z = x - 5y - xy + x^2 - y^2$$

which is correct for the normalized variables.

It should be pointed out in the comment for this procedure
 that the resulting polynomial is in the normalized variables and
 not the original variables.

ALGORITHM 165

COMPLETE ELLIPTIC INTEGRALS

HENRY C. THACHER, JR.*

Reactor Eng. Div., Argonne National Lab., Argonne, Ill.

* Work supported by the U.S. Atomic Energy Commission.

```

procedure KANDE(m1, K, E, tol, alarm);
  value m1, tol;
  real m1, K, E, tol;
  label alarm;
  comment this procedure computes the complete elliptic integrals
 $K(m1) = \int_0^{\pi/2} (1 - (1 - m1) \sin^2 v)^{-1/2} dv$  and  $E(m1) = \int_0^{\pi/2} (1 - (1 - m1) \sin^2 v)^{1/2} dv$  by the arithmetic-geometric-mean process. The accuracy is limited only by the accuracy of the arithmetic.

```

Except for the provision of tests for pathological values of the parameter, the calculation of K is only a slight modification of the second procedure of Algorithm No. 149 (*Comm. ACM*, 5 (Dec. 1962), 605). These integrals may also be approximated to limited (6D) accuracy by Algorithms 55 and 56 (*Comm. ACM*, 4 (Apr. 1961), 180). Unless the square-root is exceptionally fast, the latter algorithms are probably more efficient for 6D-accuracy.

The complementary parameter, $m1$, is chosen as the independent variable, rather than the parameter, m , the modulus, k or the modular angle α , because of the possibility of serious loss of significance in generating $m1$ from the other possible independent variables when $m1$ is small and $dK/dm1$ is very large. These variables are related by $m1 = 1 - m = 1 - k^2 = \cos^2 \alpha$.

The formal parameter, tol , determines the relative accuracy of the result. To prevent entering a nonterminating loop, tol should not be less than twice the relative error in the square root routine. If $m1 \leq 0$ or if $m1 > 1$, the procedure exits to alarm. $K(0) = \infty$ while $E(0) = 1.00000000$.

The body of this procedure has been tested using the Dartmouth SCALP processor for the LGP-30. With $tol = 5_{10} - 7$, results agreed with tabulated values to within 3 in the seventh significant digit;

```

begin real a, b, c, sum, temp;
  integer fact;
  if m1 > 1 or m1 ≤ 0 then go to alarm;
  a := fact := 1;
  b := sqrt(m1);
  temp := 1 - m1;
  sum := 0;
  iter: sum := sum + temp;
  c := (a - b)/2;
  fact := fact + fact;
  temp := (a + b)/2;
  b := sqrt(a × b);
  a := temp;
  temp := fact × c × c;
  if abs(c) ≥ tol × a or temp > tol × sum then go to iter;
  sum := sum + temp;
  K := 3.141592654/(a + b);
  comment pi must be given to the full accuracy desired;
  E := K × (1 - sum/2)
end

```

ALGORITHM 166

MONTECARLO

R. D. RODMAN

Burroughs Corp., Pasadena, Calif.

```

procedure montecarlo (n, a, row, tol, mzm, inv, test, count);
  value n, row, tol, mzm; integer n, row, mzm, count;
  real tol; real array a, inv, test;
  comment this procedure will compute a single row of the inverse of a given matrix using a monte carlo technique. n is the size of the matrix, array a is the matrix, row indicates which inverse row is to be computed, tol is a tolerance factor and thus a criterion for terminating the process, mzm is 1000 times the maximum number of random walks to be taken, after which the process is terminated, array inv contains the inverse row, array test contains the innerproduct of inv with the rowth column of a, count is the number of random walks executed upon termination. real procedure RANDOM must be declared in the blockhead of procedure MONTE CARLO and generates a single random number between 0 and 1. If a is the matrix to be inverted, the absolute value of the largest eigenvalue of the matrix  $I - a$  ( $I$  is the unit matrix) must be less than one to assure convergence. This procedure is easily adapted to finding a single unknown from a set of simultaneous linear equations;
  begin integer i, j, k, nwk, lastwalk, walk; real res, p, g;
  real array sum[1:n], v[1:n, 1:n];
  start: p := (n-1)/n × n;
  for i := 1 step 1 until n do for j := 1 step 1 until n do
    v[i, j] := if i ≠ j then -a[i, j]/p else (1-a[i, j])/p;
    nwk := 1000;
    count := res := 0;
    for k := 1 step 1 until n do test [k] := sum [k] := 0;
  start1: lastwalk := row; g := 1;
  start2: walk := (RANDOM/p) + 1;
  if walk > n then go to stop;
  g := v[lastwalk, walk] × g; lastwalk := walk;
  go to start2;
  stop: count := count + 1; sum[lastwalk] := sum[lastwalk] + g;
  if count < nwk then go to start1;
  for k := 1 step 1 until n do inv[k] := n × sum[k]/count;
  for i := 1 step 1 until n do for k := 1 step 1 until n do
    test[i] := inv[k] × a[k, i] + test[i];
  for i := 1 step 1 until row-1, row+1 step 1 until n do
    res := abs(test[i]) + res; res := abs(test[row]-1) + res;
  if res < tol then go to exit;
  if count ≥ 1000 × mzm then go to exit;
  nwk := nwk + 1000; res := 0;
  for k := 1 step 1 until n do test [k] := 0;
  go to start1;
  exit: end of monte carlo inversion procedure

```

REMARK ON ALGORITHM 166

MONTECARLO INVERSE [R. D. Rodman, *Comm. ACM*, Apr. 1963]

R. D. RODMAN

Burroughs Corp., Pasadena, Calif.

The algorithm contained two errors:

(1) The line which reads

start: *p* := (*n*-1)/*n* × *n*;

should read

start: *p* := (*n*-1)/*n* ↑ 2;

(2) The line which reads
`start2: walk := (random/p) + 1;`
 should read

`start2: walk := entier ((random/p) + 1);`

After making the preceding corrections, procedure *montecarlo* was transliterated into EXTENDED ALGOL and run successfully on the Burroughs B-5000. Convergence occurred in all cases where the matrix satisfied the conditions set down in the comment statement of the algorithm. It was found that convergence was quickest and the routine most practical for matrices with eigenvalues small relative to one.

ALGORITHM 167 CALCULATION OF CONFLUENT DIVIDED DIFFERENCES

W. KAHAN AND I. FARKAS

Institute of Computer Science, University of Toronto,
 Canada

real procedure *DVDFC*(*n*, *X*, *V*, *B*, *W*); **integer** *n*;

real array *X*, *V*, *B*, *W*;

comment *DVDFC* calculates the forward divided difference $\Delta f(X_1, X_2, \dots, X_n)$. *n* is an integer which takes the values $n = 1, 2, 3, \dots$ in turn. *X* is a real array of dimension at least *n* in which $X[i] = X_i$ for $i = 1, 2, \dots, n$. The values X_i need not be distinct nor in any special order, but once the array *X* is chosen it will fix the interpretation of the arrays *B* and *V*. If $X[1], X[2], \dots, X[n]$ are in monotonic order, then the effect of roundoff upon any *n*th divided difference is no more than would be caused by perturbing each $f(X[i])$ by *n* units at most in its last significant place. But if the X 's are not in monotonic order, the error can be catastrophic if some of the divided differences are relatively large. *V* is a real array of dimension at least *n* containing the values of the function $f(X)$ and perhaps its derivatives at the point X_i . $V[i] = f^{(m_i)}(X_i)/m_i!$ and $m_i = m_i$ for $i = 1, 2, 3, \dots, n$. m_i is the number of times that the value of X_i has previously appeared in the array *X*. *B* is a real array of dimension at least *n* containing backward divided differences. Before a reference to *DVDFC* is executed one should have $B[i] = \Delta f(X_i, X_{i+1}, \dots, X_{n-1})$ for $i = 1, 2, \dots, n-1$. After that reference to *DVDFC* is executed one will find $B[i] = \Delta f(X_i, X_{i+1}, \dots, X_{n-1}, X_n)$ for $i = 1, 2, \dots, n-1, n$. When $n = 1$ the initial state of *B* is irrelevant. *W* is a real array of dimension $(2 + \bar{m})$ at least, where $\bar{m}$ is the maximum value of m_i for $i = 1, 2, \dots, n$. *W* is used for work space;

begin **real** *DENOM*; **integer** *i*, *j*, *NK*, *NIN*;

if $n = 1$ **then go to** *L1*;

NK := 1;

for $i := 1$ **step** 1 **until** *n* **do**

begin

if $X[i] = X[n]$ **then** **begin** *NK* := *NK* + 1;

W[*NK*] := *V*[*i*] **end**

end *i*;

for $i := n$ **step** -1 **until** 2 **do**

begin *W*[1] := *B*[*i* - 1]; *B*[*i*] := *W*[2];

NIN := **if** $n - i + 2 < NK$ **then** $n - i + 2$ **else** *NK*;

for $j := NIN$ **step** -1 **until** 2 **do**

begin

DENOM := $X[n] - X[i + j - 3]$;

if *DENOM* $\neq 0$ **then go to** *L2*;

W[*j*] := *W*[*j* + 1];

if $NK - j - 1 \neq 0$ **then go to** *Cont*;

NK := *NK* - 1;

go to *Cont*;

L2: *W*[*j*] := (*W*[*j*] - *W*[*j* - 1])/*DENOM*;

Cont: **end** *j*;

end *i*;

B[1] := *W*[2];

go to *L3*;

L1: *B*[1] := *V*[1];

L3: *DVDFC* := *B*[1]

end *DVDFC*

The following program segment is an example of how *DVDFC* can be used to construct a table of forward or backward differences.

for $n := 1$ **step** 1 **until** *N* **do**

begin

X[*n*] := $\dots$; *V*[*n*] := $\dots$; *F*[*n*] := *DVDFC*(*n*, *X*, *V*, *B*, *W*)

end;

The array *F* can be used in *FNEWT*(*z*, *N*, *X*, *F*, *R*, *D*, *E*) or the array *B* in *BNEWT*(*z*, *N*, *X*, *B*, *P*, *D*, *E*). See algorithms "Newton interpolation with forward (backward) divided differences."

DVDFC has been written as a FORTRAN II function and is available from I.C.S., University of Toronto;

SEE ALGORITHM 169

ALGORITHM 168 NEWTON INTERPOLATION WITH BACKWARD DIVIDED DIFFERENCES

W. KAHAN AND I. FARKAS

Institute of Computer Science, University of Toronto,
 Canada

procedure *BNEWT*(*z*, *N*, *X*, *B*, *P*, *D*, *E*); **value** *z*, *N*;

real *z*, *P*, *D*, *E*; **integer** *N*; **real array** *X*, *B*;

comment *X* is a real array of dimension at least *N* in which $X[i] = X_i$ for $i = 1, 2, 3, \dots, N$. The values X_i need not be distinct nor in any special order, but once the array *X* is chosen it will fix the interpretation of the array *B*. *B* is a real array of dimension at least *N* and contains the backward divided differences $B[i] = \Delta f(X_i, X_{i+1}, \dots, X_N)$ $i = 1, 2, \dots, N$. If two or more of the values X_i are equal then some of the *B*'s must be confluent divided differences, see algorithm: "Calculation of confluent divided differences." *P* is the value of the following polynomial in *z* of degree *N*-1 at most, $B(N) + (z - X_N) \cdot \{B(N-1) + (z - X_{N-1})\{B(N-2) + \dots + (z - X_2)B(1)\} \dots \}$. This polynomial is an interpolation polynomial which would, but for rounding errors, match values of the function $f(x)$ and any of its derivatives that *DVDFC* might have been given. *D* is the value of the derivative of *P*. *E* is the maximum error in *P* caused by roundoff during the execution of *BNEWT*. The error estimate is based upon the assumption that the result of each floating point arithmetic operation is truncated to 27 significant binary digits as is the case in FORTRAN programs on the 7090. *BNEWT* has been written as a FORTRAN II subroutine and is available from I.C.S., University of Toronto;

begin **real** *z1*; **integer** *i*;

P := *D* := *E* := 0;

for $i := 1$ **step** 1 **until** *N* **do**

begin

z1 := $z - X[i]$;

D := *P* + *z1* $\times$ *D*;

P := *B*[*i*] + *z1* $\times$ *P*;

E := *abs*(*P*) + *E* $\times$ *abs*(*z1*)

end;

E := $(1.5 \times E - \text{abs}(P)) \times 3_{10} - 8$

end *BNEWT*

ALGORITHM 169 NEWTON INTERPOLATION WITH FORWARD DIVIDED DIFFERENCES

W. KAHAN AND I. FARKAS

Institute of Computer Science, University of Toronto,
Canada

procedure *FNEWT*(*z*, *N*, *X*, *F*, *R*, *D*, *E*); **value** *z*, *N*;
real *z*, *R*, *D*, *E*; **integer** *N*; **real array** *X*, *F*;
comment *X* is a real array of dimension at least *N* in which
 $X[i] = X_i$ for $i = 1, 2, \dots, N$. The values X_i need not be distinct nor in any special order, but once the array *X* is chosen it will fix the interpretation of the array *F*. *F* is a real array of dimension at least *N* and contains the forward divided differences $F[i] = \Delta f(X_1, X_2, \dots, X_i)$ $i = 1, 2, \dots, N$. If two or more of the values X_i are equal then some of the *F*'s must be confluent divided differences, see algorithm: "Calculation of confluent divided differences." *R* is the value of the following polynomial in *z* of degree *N*-1 at most, $F(1) + (z-X_1)\{F(2) + (z-X_2)\{F(3) + \dots + (z-X_{N-1})F(N)\} \dots \}$. This polynomial is an interpolation polynomial which would, but for rounding errors, match values of the function *f*(*x*) and any of its derivatives that *DVDFC* might have been given. *D* is the value of the derivative of *R*. *E* is the maximum error in *R* caused by roundoff during the execution of *FNEWT*. The error estimate is based upon the assumption that the result of each floating-point arithmetic operation is truncated to 27 significant binary digits as is the case in FORTRAN programs on the 7090. *FNEWT* has been written as a FORTRAN II subroutine and is available from I.C.S., University of Toronto;

begin **real** *z1*; **integer** *i*;
R := *D* := *E* := 0;
for *i* := *N* **step** -1 **until** 1 **do**
begin
z1 := *z* - *X*[*i*];
D := *R* + *z1* × *D*;
R := *F*[*i*] + *z1* × *R*;
E := *abs*(*R*) + *abs*(*z1*) × *E*
end;
E := (1.5 × *E* - *abs*(*R*)) × 3₁₀ - 8
end *FNEWT*

CERTIFICATION OF ALGORITHM 167 CALCULATION OF CONFLUENT DIVIDED DIFFERENCES [W. Kahan and I. Farkas, *Comm. ACM*, Apr. 1963]

CERTIFICATION OF ALGORITHM 168 NEWTON INTERPOLATION WITH BACKWARD DIVIDED DIFFERENCES [W. Kahan and I. Farkas, *Comm. ACM*, Apr. 1963]

CERTIFICATION OF ALGORITHM 169 NEWTON INTERPOLATION WITH FORWARD DIVIDED DIFFERENCES [W. Kahan and I. Farkas, *Comm. ACM*, Apr. 1963.]

HENRY C. THACHER, JR.*
Argonne National Laboratory, Argonne, Ill.

The bodies of these procedures were tested on the LGP-30 computer using the Dartmouth SCALP compiler. Compilation and execution revealed no syntactical or mathematical errors.

It is to be noted that, although with Algorithm 169, reducing the value of *N* from that used to generate *F* leads to an interpolation polynomial based on fewer points, this is not true for Algorithm 168. This flexibility could be supplied by adding an additional formal parameter, *deg*, say, to the procedure, and by making the **for** statement read:

"**for** *i* := *N* - *deg* **step** 1 **until** *N* **do** ..."

The logic of the error estimate in Algorithms 168 and 169 is not entirely clear. However, it appears that the estimate can be adjusted for different precision of arithmetic by adjusting the constant 3₁₀-8 appropriately. For the SCALP arithmetic, this constant was changed to 1₁₀-7.

The algorithms were tested on the examples given by Milne-Thomson [*The Calculus of Finite Differences*, p. 4, Macmillan, 1951] and by Milne [*Numerical Calculus*, p. 204, Princeton, 1949]. In both examples, Algorithm 167 reproduced the divided difference table, and both Algorithms 168 and 169 reproduced the input values. As a check of the calculation of confluent divided differences, values of the exponential function of its first two derivatives at *x* = 5.0 and 6.0 were used. The difference table shown in Table A was obtained.

TABLE A

<i>n</i>	<i>X</i> [<i>n</i>]	<i>V</i> [<i>n</i>]	<i>B</i> [<i>n</i>]	<i>B</i> [<i>n</i> -1]	<i>B</i> [<i>n</i> -2]	<i>B</i> [<i>n</i> -3]	<i>B</i> [<i>n</i> -4]	<i>B</i> [<i>n</i> -5]
1	5.0	148.4132	148.4132					
2	5.0	148.4132	148.4132	148.4132				
3	6.0	403.4288	403.4287	255.0155	106.6023			
4	6.0	403.4288	403.4287	403.4287	148.4132	41.81091		
5	5.0	74.20658	148.4132	255.0155	148.4132	41.81091	9.415191	
6	6.0	201.7144	403.4287	255.0155	148.4132	53.30115	11.49023	2.075043

The forward differences lie along the top diagonal.

Use of these results with *BNEWT* and with *FNEWT* gave the following results, for *N* = 6.

<i>z</i>	<i>BNEWT</i>			<i>FNEWT</i>		
	<i>P</i>	<i>D</i>	<i>E</i>	<i>R</i>	<i>D</i>	<i>E</i>
5.000000	148.4132	148.4132	.4567298 × 10 ⁻⁴	148.4132	148.4132	.7420658 × 10 ⁻⁵
5.500000	244.6973	244.6924	.4173722 × 10 ⁻⁴	244.6973	244.6924	.3078276 × 10 ⁻⁴
6.000000	403.4287	403.4287	.2017143 × 10 ⁻⁴	403.4287	403.4287	.7441404 × 10 ⁻⁴

ALGORITHM 170 REDUCTION OF A MATRIX CONTAINING POLYNOMIAL ELEMENTS

PAUL E. HENNION

Giannini Controls Corp., Astromechanics Res. Div.,
Berwyn, Penn.

real procedure POLYMATRIX (*A*, *NCOL*, *N*, *COE*, *NP1*);
value *A*, *NCOL*, *N*; **real array** *A*; **integer** *NCOL*, *N*;
comment this procedure will expand a general determinant,
where each of the elements are polynomials in the Laplace com-
plex variable. This program is useful for the investigation of
dynamic stability problems when using the transfer function
approach. The process is one of triangularization of a poly-
nomial matrix with real coefficients whereupon multiplication
of the diagonal elements the determinant polynomial is formed.
The polynomial matrix as defined herein is a matrix whose
elements are polynomials of the form $\sum_{i=0}^N a_i x^i$. When such a
matrix is triangularized, all elements below the main diagonal
are nulled. Then upon expanding, the nonvanishing terms are
those formed by the product of these diagonal elements. Hence
stability criteria may be checked by evaluating the roots of the
characteristic equation thus formed using some suitable root
extracting routine.

Consider the polynomial matrix with quadratic elements
(*N* = 2). In this case the three-dimensional input matrix *A* is
size *A*[1:*NCOL*, 1:*M*], where *NCOL* is the order of
the matrix and *M* = *N* × *NCOL* + 1. Here the first subscript
of *A* refers to the row, the second to the column, and the third
to the polynomial coefficient. Therefore, prior to entry the con-
stant term of a general polynomial element is contained in
A[*i*, *j*, 1], the linear term is contained in *A*[*i*, *j*, 2], and the
quadratic term in *A*[*i*, *j*, 3]. Upon completion of the routine, the
coefficients of the determinant polynomial are contained in
COE [1:*M*]. The constant coefficient being in *COE* [1], the linear
coefficient in *COE* [2], the quadratic coefficient in *COE* [3], etc.
The variable *NP1* will specify the number of coefficients of the
determinant polynomial. In general *NP1* ≠ *M* since some terms
may vanish during the expansion.

If the polynomials comprising the matrix elements are not
all of equal degree, set *N* prior to entry equal to the degree of
the highest ordered polynomial;

begin **real** *sa*, *sb*; **integer** *i*, *j*, *k*, *j1*, *j2*, *j3*, *j4*, *j5*, *j6*, *j7*, *j8*, *j9*, *j10*,
j11, *NP1*, *M*; **array** *C1*[1:*M*], *C2*[1:*M*], *COE*[1:*M*];
integer array *MAT* [1:*NCOL*, 1:*NCOL*];
start: *M* := *N* × *NCOL* + 1; **for** *i* := 1 **step** 1 **until** 1 *NCOL* **do**
begin **for** *j* := 1 **step** 1 **until** *NCOL* **do** **begin** *MAT* [*i*, *j*] := 0;
for *k* := 1 **step** 1 **until** *M* **do** **begin**
if *A*[*i*, *j*, *k*] ≠ 0 **then** *MAT* [*i*, *j*] := *k*; **end** **end** **end**; *j1* := 1;
L0: *j9* := 0; **for** *i* := *j1* **step** 1 **until** *NCOL* **do** **begin**
if *MAT* [*i*, *j1*] < 0 **then** **go to** *exit*;
else if *MAT* [*i*, *j1*] = 0 **then** **go to** L1
else *j9* := *j9* + 1; *j3* := *i*;
L1: **end**; if (*j9* - 1) < 0 **then** **go to** *exit*
else if (*j9* - 1) > 0 **then** **go to** L2
else if (*j3* - *j1*) < 0 **then** **go to** *exit*
else if (*j3* - *j1*) = 0 **then** **go to** L12
else **for** *j* := *j1* **step** 1 **until** *NCOL* **do**
begin *j2* := MAX(*MAT* [*j3*, *j*], *MAT* [*j1*, *j*]); *j4* := *MAT* [*j3*, *j*];
MAT [*j3*, *j*] := *MAT* [*j1*, *j*]; *MAT* [*j1*, *j*] := *j4*;
for *k* := 1 **step** 1 **until** *j2* **do**
begin *sa* := *A* [*j3*, *j*, *k*]; *A* [*j3*, *j*, *k*] := *A* [*j1*, *j*, *k*];
A [*j1*, *j*, *k*] := -*sa*; **end** **end**; **go to** L12;
L2: *j3* := *j1* + 1; **for** *i* := *j3* **step** 1 **until** *NCOL* **do** **begin**
L3: if (*MAT* [*i*, *j1*] < 0 **then** **go to** *exit*
else if (*MAT* [*i*, *j1*] = 0 **then** **go to** L11
else if (*MAT* [*j1*, *j1*] < 0 **then** **go to** *exit*
else if (*MAT* [*j1*, *j1*] = 0 **then** **go to** L4
else if (*MAT* [*i*, *j1*] - *MAT* [*j1*, *j1*]) ≥ 0 **then** **go to** L5 else

L4: **for** *j* := *j1* **step** 1 **until** *NCOL* **do** **begin**
j2 := MAX(*MAT* [*j1*, *j*], *MAT* [*i*, *j*]); *j4* := *MAT* [*j1*, *j*];
MAT [*j1*, *j*] := *MAT* [*i*, *j*]; *MAT* [*i*, *j*] := *j4*;
for *k* := 1 **step** 1 **until** *j2* **do** **begin** *sa* := *A* [*i*, *j*, *k*];
A [*i*, *j*, *k*] := *A* [*j1*, *j*, *k*]; *A* [*j1*, *j*, *k*] := -*sa*;
end **end**; **go to** L3;
comment Interchange row *i* with *j1*;
L5: *j7* := *MAT* [*i*, *j1*]; *j5* := *MAT* [*j1*, *j1*]; *j6* := *j7* - *j5*;
sb := *A* [*i*, *j1*, *j7*] / *A* [*j1*, *j1*, *j5*];
if (*abs*(*sb*) - 4) < 0 **then** **go to** L6
else if (*j6*) < 0 **then** **go to** *exit*
else if (*j6*) = 0 **then** **go to** L4 else
L6: **for** *j* := *j1* **step** 1 **until** *NCOL* **do** **begin** *j5* := *MAT* [*j1*, *j*];
for *k* := 1 **step** 1 **until** *j5* **do** **begin** *j7* := *k* + *j6*;
if (*j7* - *M*) > 0 **then** **go to** L10 else
L7: if (*abs*(*A* [*i*, *j*, *j7*] - *sb* × *A* [*j1*, *j*, *k*]) - 210 - 8) ≤ 0 **then** **go to** L8
else *A* [*i*, *j*, *j7*] := *A* [*i*, *j*, *j7*] - *sb* × *A* [*j1*, *j*, *k*];
go to L9;
L8: *A* [*i*, *j*, *j7*] := 0;
L9: **end** **end**;
L10: **for** *j* := *j1* **step** 1 **until** *NCOL* **do** **begin**
j7 := MAX(*MAT* [*i*, *j*], *MAT* [*j1*, *j*] + *j6*); *MAT* [*i*, *j*] := 0;
for *k* := 1 **step** 1 **until** *M* **do** **begin** if (*A* [*i*, *j*, *k*] ≠ 0 **then**
MAT [*i*, *j*] := *k* **end** **end**;
L11: **end**; **go to** L0;
L12: *j1* := *j1* + 1; if (*j1* - *NCOL*) < 0 **then** **go to** L0 else
for *j* := 1 **step** 1 **until** *NCOL* **do** **begin**
j2 := *MAT* [*j*, *j*];
for *k* := 1 **step** 1 **until** *j2* **do** *C1*[*k*] := *A* [*j*, *j*, *k*];
L13: if (*j* - 1) < 0 **then** **go to** *exit*
else if (*j* - 1) = 0 **then** **go to** L14
else **for** *k* := 1 **step** 1 **until** *NP1* **do** *C2*[*k*] := *COE*[*k*];
for *k* := 1 **step** 1 **until** *M* **do** *COE*[*k*] := 0;
if (*j2*) < 0 **then** **go to** *exit*
else if (*j2*) = 0 **then** **go to** L15
else **for** *k* := 1 **step** 1 **until** *j2* **do** **begin**
for *j10* := 1 **step** 1 **until** *NP1* **do** **begin**
j11 := *k* + *j10* - 1;
COE[*j11*] := *COE*[*j11*] + *C1*[*k*] × *C2*[*j10*];
end **end**; *NP1* := *j11*; **go to** L15;
L14: **for** *k* := 1 **step** 1 **until** *j2* **do** *COE* [*k*] := *C1* [*k*];
NP1 := *j2*;
L15: **end**;
exit: **end** POLYMATRIX

CERTIFICATION OF ALGORITHM 170 [F3]
REDUCTION OF A MATRIX CONTAINING POLY-
NOMIAL ELEMENTS [P. E. Hennion, *Comm. ACM*
6 (April 1963), 165; 6 (Aug. 1963), 450]
KAREN B. PRIEBE (Recd. 18 Dec. 1963 and 18 Feb. 1964)
Woodward Governor Co., Rockford, Ill.

Algorithm 170 was translated into FAST for the NCR 315 and
gave satisfactory results with the following corrections:

1. **real procedure** ... **integer** *NCOL*, *N*; should be replaced
by

procedure POLYMATRIX (*A*, *NCOL*, *N*, *COE*, *NP1*);
value *NCOL*, *N*; **real array** *A*, *COE*;
integer *NCOL*, *N*, *NP1*;

2. At the end of the first comment add:

The global integer procedure MAX is assumed and furnishes the
maximum of two integers.

3. **integer** *i*, *j*, *k*, ... *COE*[1:*M*];

should be replaced by

integer *i*, *j*, *k*, *j1*, *j2*, *j3*, *j4*, *j5*, *j6*, *j7*, *j8*, *j9*, *j10*, *j11*, *M*;
array *C1*, *C2*[1:*N* × *NCOL* + 1];

4. Immediately after *start*: the statement

$NP1 := N + 1;$

should be added, and the third line after *start*: i.e.,

for $k := 1$ **step** 1 **until** M **do begin**

should be replaced by

for $k := 1$ **step** 1 **until** $NP1$ **do begin**

5. The third line after $L10$: i.e.,

for $k := 1$ **step** 1 **until** M **do ...**

should be replaced by

for $k := 1$ **step** 1 **until** $j7$ **do ...**

The last two changes simply shorten both of the indicated **for** statements.

[EDITOR'S NOTE. In addition to the above corrections, we have two comments on the Remark on Algorithm 170 by Hennion, *loc. cit.*, p. 450:

First, the semicolon at the end of the first line after $L0$ must be removed.

Second, correction (4) is irrelevant.

The referee confirms that a transcription into Burroughs Extended ALGOL of the program as corrected by Mrs. Priebe runs on the B5000.—G.E.F.]

REMARK ON ALGORITHM 170

REDUCTION OF A MATRIX CONTAINING POLYNOMIAL ELEMENTS [P. E. Hennion, *Comm. ACM*, Apr. 1963]

P. E. HENNION

Giannini Controls Corp., Berwyn, Penn.

Four typographical errors were found upon reviewing the procedure. The following corrections should be made:

- (1) The increment for the **for** statement of line *start*:, should be 1.
- (2) The colon at the end of the third line after line *start*:, should be replaced by a semicolon.
- (3) The semicolon at the end of the first line after line $L0$:, may be removed.
- (4) The last statement of the first column should read:

$MAT[i, j] := k; \text{ end end};$

ALGORITHM 173

ASSIGN

OTOMAR HÁJEK

Research Institute of Mathematical Machines, Prague, Czechoslovakia

procedure *assign* (*a*) the value of : (*b*) with dimension : (*dim*) indices : (*ind*) bounds : (*low*, *up*) tracer : (*j*);

value *dim*; **integer** *dim*, *ind*, *low*, *up*, *j*;

comment This procedure uses Jensen's device (cf. ALGOL Report, procedure Innerproduct) twice: the *a*, *b* may depend on *ind* and also *ind*, *low*, *up* may depend on *j*;

begin

$j := \text{dim};$

for *ind* := *low* **step** 1 **until** *up* **do**

if *dim* > 1

then

begin

assign (*a*, *b*, *dim*−1, *ind*, *low*, *up*, *j*);

$j := \text{dim}$

end

else $a := b$

end assign;

comment The obvious use of "assign" is in assigning the value of one array to another. The point here is that one procedure declaration serves for all the dimensions used. In fact, the dimension may even be a variable: thus a procedure essentially identical with "assign" was used by the author in implementing the recursive own process in an ALGOL compiler.

However, in addition to this, "assign" can have further functions, as illustrated below. The activation *assign* (*a*, (if $i=1$ then false else *a*) $\forall b_{i,1}, 1, i, 1, n, j$) will calculate the join-trace of a Boolean 2-dimensional array *b*.

assign ($a_{i,1}$, (if $i_1=1$ then 0 else $a_{i,1}$) + $b_{i,1} \times c_{i,1}$, 3, $i_j, 1$, if $j=1$ then *n* else if $j=2$ then *m* else *p*, *j*)

will assign to *a* the matrix product of *b*, *c*. It may be noticed that, more generally, "assign" will perform all the tensor operations, e.g. tensor multiplication, alternation, etc.

CERTIFICATION OF ALGORITHM 173

ASSIGN [Otomar Hájek, *Comm. ACM*, June 1963]

R. S. SCOWEN

English Electric Co. Ltd., Whetstone, Leicester, England

Algorithm 173 (ASSIGN) has been tested successfully using the DEUCE ALGOL 60 compiler. The only changes necessary were the addition of specifications for the formal parameters *a*, *b* (DEUCE ALGOL 60 compiler requires specifications for all formal parameters).

The author's example, *assign* ($a[i[1], i[2]]$, (if $i[3]=1$ then 0.0 else $a[i[1], i[2]]$) + $b[i[1], i[3]] \times c[i[3], i[2]]$, 3, $i[j], 1$, if $j=1$ then *n* else if $j=2$ then *m* else *p*, *j*); did form the matrix product $B \times C$ and store it in *A*.

The algorithm was also used to read a matrix into the computer using the procedure call

assign ($b[i[1], i[2]]$, *read*, 2, $i[j], 1$,

if $j=1$ **then** *n* **else** *p*, *j*);

(*read* is a real procedure which takes the value given by the next number on the input tape).

These examples took about three times as long to run as the simpler equivalent statements

for $i := 1$ **step** 1 **until** *n* **do**

for $j := 1$ **step** 1 **until** *m* **do**

begin

$a[i, j] := 0.0;$

for $k := 1$ **step** 1 **until** *p* **do**

$a[i, j] := a[i, j] + b[i, k] \times c[k, j]$

end;

and

for $j := 1$ **step** 1 **until** *p* **do**

for $i := 1$ **step** 1 **until** *n* **do**

$b[i, j] := \text{read};$

CERTIFICATION OF ALGORITHM 173

ASSIGN [O. Hájek, *Comm. ACM*, July 1963]

Z. FILSAK and L. VRCHOVECKÁ

Research Institute of Mathematical Machines, Prague, and Computing Center Kancelářské stroje, Prague

The algorithm was modified for input to the Elliott-ALGOL system as follows. In Elliott-ALGOL, name-called parameters in

recursive procedures are prescribed. Luckily, the only parameter which varies during the recursive call in the body of *Assign* is called by value (it is the parameter *dim* which determines depth of recursion). The body of *Assign* was replaced by (i) a procedure declaration *Ass(dim)*, whose body is that of the original *Assign*, but with the recursive call of *Assign* replaced by that of *Ass*, and (ii) a single statement, the activation of *Ass(dim)*.

The resulting procedure was tested (on the National-Elliott 803 in the Computing Center), on a rather large set of examples, including those described in the text following Algorithm 173. It was found that in the last example, matrix multiplication, indices i_1 and i_2 should be interchanged throughout.

No changes of the algorithm itself were necessary. It seems that the modification described above, motivated by limitations of Elliott-ALGOL, also improve efficiency, at least for large dimensions of the arrays concerned.

ALGORITHM 174 A POSTERIORI BOUNDS ON A ZERO OF A POLYNOMIAL*

ALLAN GIBB

University of Alberta, Calgary, Alberta, Canada

comment The procedures below make use of Algorithm 61, Procedures for Range Arithmetic [Comm. ACM 4 (1961)]. It is assumed that the procedures below and the range arithmetic procedures are contained in an outer block and, therefore, that the procedures are available as required. Together the procedures make possible an attempt to determine absolute bounds on a zero of a polynomial given an initial estimate of the zero. The procedures below are given for the complex case but may readily be adapted for the real case;

procedure *RngPlyC* (*N*, *A*, *Z*, *P*);

comment *RngPlyC* finds bounds $[P_1, P_2] + i[P_3, P_4]$ on the value of an n th degree polynomial $\sum_{k=0}^n \{a_{4k+1}, a_{4k+2}\} + i\{a_{4k+3}, a_{4k+4}\}z^k$ with complex range coefficients for a complex range argument $z = [Z_1, Z_2] + i[Z_3, Z_4]$;

integer *N*; **array** *A*, *Z*, *P*;

begin integer *K*, *J*; **array** *X*, *Y*[1:4];

P[1] := *P*[2] := *P*[3] := *P*[4] := 0;

for *K* := 4 × *N* **step** -4 **until** 0 **do**

begin for *J* := 1 **step** 1 **until** 4 **do** *X*[*J*] := *A*[*K*+*J*];

RNGMPYC (*P*[1], *P*[2], *P*[3], *P*[4], *Z*[1], *Z*[2], *Z*[3], *Z*[4], *Y*[1], *Y*[2], *Y*[3], *Y*[4]);

RNGSUMC (*Y*[1], *Y*[2], *Y*[3], *Y*[4], *X*[1], *X*[2], *X*[3], *X*[4], *P*[1], *P*[2], *P*[3], *P*[4])

end

end;

procedure *RngAbsC* (*A*, *C*);

comment *RngAbsC* produces the range absolute value [*C*₁, *C*₂] of the complex range number [*A*₁, *A*₂] + *i*[*A*₃, *A*₄];

array *A*, *C*;

begin array *B*[1:4];

RANGESQR (*A*[1], *A*[2], *B*[1], *B*[2]);

RANGESQR (*A*[3], *A*[4], *B*[3], *B*[4]);

RANGESUM (*B*[1], *B*[2], *B*[3], *B*[4], *C*[1], *C*[2]);

C[1] := *sqrt*(*C*[1]);

C[2] := *sqrt*(*C*[2]);

comment It is assumed that the accuracy of the *sqrt* routine used is known and that the maximum error in *sqrt*(*C*) is $\pm K \times \text{CORRECTION}(C)$. *K* is to be replaced below by its appropriate numerical value;

C[1] := *C*[1] - *K* × *CORRECTION* (*C*[1]);

C[2] := *C*[2] + *K* × *CORRECTION* (*C*[2])

end;

procedure *BndZrPlyC* (*N*, *ZOR*, *ZOJ*, *A*, *W*);

integer *N*; **real** *ZOR*, *ZOJ*; **array** *A*, *W*;

comment *BndZrPlyC* attempts to determine bounds [*W*₁, *W*₂]

+ [*W*₃, *W*₄] on a zero of an *N*-th degree polynomial in *z* with complex range coefficients. It is assumed that an estimate

ZO = *ZOR* + *iZOJ* of the zero is available. The following theorem is used. Assume *f* is regular at *z*₀ with *f*'(*z*₀) ≠ 0. Let

*h*₀ = -*f*(*z*₀)/*f*'(*z*₀), let Δ be the region $|z - z_0| \leq r |h_0|$, and assume that *f* is regular in Δ . If, for some $r > 0$, $|f'(z)| \geq (1/r)$.

$|f'(z_0)|$ for all $z \in \Delta$ then Δ contains a zero of *f* (see [1], pp. 29-31);

begin integer *I*, *J*; **array** *B*[1:4×*N*], *E*, *F*, *FP*, *D*[1:4], *AF*, *AFP*, *G*[1:2];

real *RH*, *RHS*, *NL*, *NR*, *R*, *RNL*, *RNR*;

for *I* := 1 **step** 1 **until** *N* **do**

begin *J* := 4 × *I*;

RANGEMPY (*I*, *I*, *A*[*J*+1], *A*[*J*+2], *B*[*J*-3], *B*[*J*-2]);

RANGEMPY (*I*, *I*, *A*[*J*+3], *A*[*J*+4], *B*[*J*-1], *B*[*J*])

end;

E[1] := *E*[2] := *ZOR*; *E*[3] := *E*[4] := *ZOJ*;

RngPlyC(*N*, *A*, *E*, *F*);

RngAbsC(*F*, *AF*);

RngPlyC(*N*-1, *B*, *E*, *FP*);

RngAbsC(*FP*, *AFP*);

RANGEDVD(*AF*[1], *AF*[2], *AFP*[1], *AFP*[2], *NL*, *NR*);

R := 2;

1: *RANGEMPY*(*R*, *R*, *NR*, *NR*, *RNL*, *RNR*);

RANGESUM(*ZOR*, *ZOR*, -*RNR*, *RNR*, *W*[1], *W*[2]);

RANGESUM(*ZOJ*, *ZOJ*, -*RNR*, *RNR*, *W*[3], *W*[4]);

comment We have replaced the disk of the theorem by a square;

RngRlyC(*N*-1, *B*, *W*, *D*);

RngAbsC(*D*, *G*);

if *G*[1] = 0 **then go to** *failure1*;

comment *failure1* and *failure2* are non-local labels;

RANGEDVD(*AFP*[2], *AFP*[2], *R*, *R*, *RH*, *RHS*);

if *G*[1] < *RHS* **then**

begin *R* := 2 × *R*;

if *R* > 1024 **then go to** *failure2*;

go to 1

end

end

comment The following procedure may replace *BndZrPlyC* above;

procedure *BndZrPlyC2* (*N*, *ZOR*, *ZOJ*, *A*, *W*);

integer *N*; **array** *A*, *W*; **real** *ZOR*, *ZOJ*;

comment *BndZrPlyC2* is similar to *BndZrPlyC* above. The theorem used here follows. If, in the disk $|z - z_0| \leq 2 |h_0|$ we have $|f''(z)| \leq |f'(z_0)|/(2 |h_0|)$, then there is a unique zero in the disk (see [2], pp. 43-50);

begin integer *I*, *J*; **array** *B*[1:4×*N*], *C*[1:4×*N*-4], *F*, *D*, *P*, *S*[1:4], *X*, *T*, *Q*, *Y*[1:2]; **real** *V*, *VP*, *R*, *RL*;

for *I* := 1 **step** 1 **until** *N* **do**

begin *J* := 4 × *I*;

RANGEMPY(*I*, *I*, *A*[*J*+1], *A*[*J*+2], *B*[*J*-3], *B*[*J*-2]);

RANGEMPY(*I*, *I*, *A*[*J*+3], *A*[*J*+4], *B*[*J*-1], *B*[*J*])

end;

for *I* := 1 **step** 1 **until** *N* - 1 **do**

begin *J* := 4 × *I*;

RANGEMPY(*I*, *I*, *B*[*J*+1], *B*[*J*+2], *C*[*J*-3], *C*[*J*-2]);

RANGEMPY(*I*, *I*, *B*[*J*+3], *B*[*J*+4], *C*[*J*-1], *C*[*J*])

end;

D[1] := *D*[2] := *ZOR*;

D[3] := *D*[4] := *ZOJ*;

RngPlyC(*N*, *A*, *D*, *F*);


```

RngPlyC(N-1, B, D, P);
RngAbsC(F, T);
RngAbsC(P, X);
if X[1] = 0 then go to failure1;
comment failure1 and failure2 are non-local labels;
RANGEDVD(T[1], T[2], X[1], X[2], Q[1], Q[2]);
RANGEMPY(2, 2, Q[2], Q[2], RL, R);
RNGSUMC(-R, R, -R, R, ZOR, ZOR, ZOJ, ZOJ, W[1], W[2],
W[3], W[4]);
RngPlyC(N-2, C, W, S);
RngAbsC(S, Y);
RANGEDVD(X[1], X[1], R, R, V, VP);
if Y[2] > V then go to failure2
end

```

References:

1. GIBB, ALLAN. ALGOL procedures for range arithmetic. Tech. Report No. 15, Appl. Math. and Statistics Laboratories, Stanford University (1961).
2. OSTROWSKI, A. M. *Solution of equations and systems of equations*. Academic Press, New York, 1960.

* These procedures were developed under Office of Naval Research Contract Nonr-225(37) at Stanford University. The author wishes to thank Professor George E. Forsythe for assistance with this work.

ALGORITHM 175³ SHUTTLE SORT

C. J. SHAW AND T. N. TRIMBLE

System Development Corporation, Santa Monica, Calif.

```

procedure shuttle sort (m, Temporary, N);
value m; integer m; array N[1:m];
comment This procedure sorts the list of numbers N[1] through
N[m] into numeric order, by exchanging out-of-order number
pairs. The procedure is simple, requires only Temporary as
extra storage, and is quite fast for short lists (say 25 numbers)
and fairly fast for slightly longer lists (say 100 numbers). For
still longer lists, though, other methods are much swifter. The
actual parameters for Temporary and N should, of course, be
similar in type;
begin integer i, j;
for i := 1 step 1 until m - 1 do
  begin
    for j := i step -1 until 1 do
      begin
        if N[j] ≤ N[j+1] then go to Test;
      Exchange: Temporary := N[j]; N[j] := N[j+1];
        N[j+1] := Temporary; end of j loop;
      Test: end of i loop
    end shuttle sort
  end

```

CERTIFICATION OF ALGORITHM 175

SHUTTLE SORT [C. J. Shaw and T. N. Trimble, *Comm.*
ACM, June 1963]

GEORGE R. SCHUBERT*

University of Dayton, Dayton, Ohio

* Undergraduate research project, Computer Science Program, Univ. of Dayton.

Algorithm 175 was translated into BALGOL and ran successfully

on the Burroughs 220. The following actual sorting times were observed:

Number of Items	Average Time (sec)
25	1.6
50	6.2
100	25.8
250	181
500	684

The algorithm can be extended so that the sort is made on one array, while retaining a one-to-one correspondence to a second array. This is done by inserting immediately before **end of the j loop** the following:

Temporary := Y[j]; Y[j] := Y[j+1]; Y[j+1] := Temporary; where Y[k] is the element to be associated with N[k]. Other variations are obviously possible.

REMARK ON ALGORITHM 175

SHUTTLE SORT [C. J. Shaw and T. N. Trimble, *Comm.*

ACM 6 (June 1963), 312; G. R. Schubert, *Comm.*

ACM 6 (Oct. 1963), 619; O. C. Juelich, *Comm. ACM*

6 (Dec. 1963), 739]

OTTO C. JUELICH (Recd. 18 Dec. 1963)

North American Aviation, 4300 E. Fifth Ave., Columbus, Ohio

The appearance of Schubert's certification has caused me to restudy the algorithm. What I supposed were errors amount to a rearrangement of the order in which the comparisons are carried out. The efficiency of the algorithm is not much affected by the rearrangement, since the number of executions of the statements labeled *Exchange* remains the same.

REMARK ON ALGORITHM 175

SHUTTLE SORT [C. J. Shaw and T. N. Trimble, *Comm.*

ACM 6, June 1963]

O. C. JUELICH

North American Aviation, Inc., Columbus, Ohio

The authors of this algorithm do well to remind the reader that "Shuttle Sort" is not an efficient procedure, except for lists of items so short that they do not justify the housekeeping apparatus needed by the usual sorting routines.

The algorithm as published is not free from errors. The statement

for j := i **step** - 1 **until** 1 **do**

should be replaced by either:

for j := m - 1 **step** - 1 **until** i **do**

or

for j := 1 **step** 1 **until** m - i **do**

In the former case the process can be visualized as placing the *i*th smallest element in place on the *i*th pass; in the latter the *i*th largest element is put in place on the *i*th pass.

The label "Test" should precede the delimiter "end of j loop" rather than the "end of i loop". The algorithm can be slightly accelerated by rewriting the body of the procedure:

begin integer i, j, j max;

i := m - 1;

loop: j max := 1;

for j := 1 **step** 1 **until** i **do**

begin

compare: **if** N[j] > N[j+1] **then**

begin Exchange: Temporary := N[j];

N[j] := N[j+1];

N[j+1] := Temporary;

```

        j max := j
    end Exchange;
end of j loop;
i := j max;
if i > 1 then go to loop;
end shuttle sort

```

The revised procedure body will eliminate redundant iterations when some of the data is already ordered.

It was studied in this form by R. L. Boyell and the writer on the ORDVAC at Ballistics Research Laboratories, Aberdeen Proving Ground, in 1955. For randomly ordered data the i -loop may be expected to be executed about $m - \sqrt{m}$ times.

ALGORITHM 176 LEAST SQUARES SURFACE FIT

T. D. ARTHURS

The Boeing Company, Transport Division, Renton, Wash.

```

procedure SURFIT ( $F, z, W, m, n$ ) answers: ( $a, e, rms$ );
integer  $m, n$ ; real  $rms$ ; array  $F, z, W, e$ ;
procedure Invert, sqrt;

```

comment Given a set of m ordinates and the corresponding values of n prescribed general functions, (f_i), of one or more linearly independent variables, this procedure fits the points, in the least squares sense, with a function of the form $a_1 f_1 + a_2 f_2 + \dots + a_n f_n$ where a_i are the unknown coefficients. Also computed are the vectors of residuals (e_i) and their lengths (rms). Provision is made for weighting the data points. Essentially, the matrix equation $F^T W F a = F^T W z$ is solved, where a is the vector of unknowns, W is an $m \times m$ diagonal matrix of data point weights, z is the vector of ordinate values and F is the $m \times n$ matrix of corresponding function values. The availability of a procedure *Invert*, which replaces a real matrix with its inverse, is assumed;

```

begin integer  $i, j, k$ ; real  $sqsum, g$ ; array  $G[1:n, 1:n]$ ;
comment  $G$  is working space for the inversion procedure;
 $sqsum := 0$ ;
for  $i := 1$  step 1 until  $n$  do
  for  $j := 1$  step 1 until  $n$  do
    begin  $G[i, j] := 0$ ;
      for  $k := 1$  step 1 until  $m$  do
         $G[i, j] := G[i, j] + F[k, i] \times F[k, j] \times W[k]$ 
      end  $k$ ;
    end  $j$ ;
  end  $i$ ;
end  $j$ ;
begin  $a[i] := 0$ ;
  for  $j := 1$  step 1 until  $m$  do
    begin  $g := 0$ ;
      for  $k := 1$  step 1 until  $n$  do
         $g := g + G[i, k] \times F[j, k]$ ;
       $a[i] := a[i] + g \times z[j] \times W[j]$ 
    end  $k$ ;
  end  $j$ ;
end  $i$ ;
for  $i := 1$  step 1 until  $m$  do
  begin  $e[i] := y[i]$ ;
    for  $j := 1$  step 1 until  $n$  do
       $e[i] := e[i] - a[j] \times F[i, j]$ ;
     $sqsum := sqsum + e[i]^2$ 
  end  $j$ ;
end  $i$ ;
 $rms := \text{sqrt}(sqsum/m)$ 
end SURFIT

```

ALGORITHM 177

LEAST SQUARES SOLUTION WITH CONSTRAINTS

M. J. SYNGE

The Boeing Company, Transport Division, Renton, Wash.

```

procedure CONLSQ ( $A, y, w, n, m, r$ ) results: ( $x$ ) residuals:
( $e, rms$ );

```

```

real  $rms$ ; integer  $n, m, r$ ; array  $A, y, w, x, e$ ; procedure
abs, SURFIT;

```

comment This procedure solves an overdetermined set of n simultaneous linear equations in m unknowns, $Ax = y$. The first r equations ($r \leq m$) are satisfied exactly and the remaining $n - r$ are satisfied as well as possible by the method of least squares. Each equation is assigned a weight from the vector w , although the first r weights have no relevance. This procedure may be used for curve or surface fitting when the approximating function or its derivatives are required to have fixed values at a number of points;

```

begin integer  $i, j, k, ii, ick$ ; integer array  $ic[1:m]$ ;
array  $B[1:n-r, 1:m-r]$ ; real  $Amax$ ;
for  $i := 1$  step 1 until  $r$  do
  begin  $k := 1$ ; for  $j := 2$  step 1 until  $m$  do
    begin if  $\text{abs}(A[i, j]) > \text{abs}(A[i, k])$  then  $k := j$ ; end;
     $ic[i] := k$ ;  $Amax := A[i, k]$ ; for  $j := 1$  step 1 until  $m$  do
       $A[i, j] := A[i, j] / Amax$ ;  $y[i] := y[i] / Amax$ ;
    for  $ii := 1$  step 1 until  $r$  do
      begin if  $ii = i$  then go to skip;  $Amax := A[ii, k]$ ;
        for  $j := 1$  step 1 until  $m$  do
           $A[ii, j] := A[ii, j] - A[i, j] \times Amax$ ;
           $y[ii] := y[ii] - y[i] \times Amax$ ;
        end  $j$ ;
      end  $ii$ ;
    end  $j$ ;
     $ick := r + 1$ ; for  $j := 1$  step 1 until  $m$  do
      begin  $k := 1$ ;
        repeat: if  $j = ic[k]$  then go to next;
           $k := k + 1$ ; if  $r \geq k$  then go to repeat;
           $ic[ick] := j$ ;  $ick := ick + 1$ ;
        next: end  $k$ ;
      for  $i := r + 1$  step 1 until  $n$  do
        begin for  $k := 1$  step 1 until  $r$  do
           $y[i] := y[i] - y[k] \times A[i, ic[k]]$ ;
          for  $j := r + 1$  step 1 until  $m$  do
            begin  $B[i, j] := A[i, ic[j]]$ ;
              for  $k := 1$  step 1 until  $r$  do
                 $B[i, j] := B[i, j] - A[i, ic[k]] \times A[k, ic[j]]$ 
              end  $k$ ;
            end  $j$ ;
          end  $k$ ;
           $SURFIT(B, y[r+1:n], w[r+1:n], n-r, m-r, x[r+1:m],$ 
             $e[r+1:n], rms)$ ;
        comment The procedure SURFIT is called to solve the reduced
          set of  $n - r$  simultaneous linear equations in  $m - r$  unknowns,
           $Bx_2 = y_2'$ , which have no constraints;
        for  $j := r + 1$  step 1 until  $m$  do  $x[ic[j]] := x[j]$ ;
        for  $j := 1$  step 1 until  $r$  do
          begin  $x[ic[j]] := y[j]$ ;
            for  $i := r + 1$  step 1 until  $m$  do
               $x[ic[j]] := x[ic[j]] - A[j, ic[i]] \times x[ic[i]]$ 
            end  $i$ ;
          end  $j$ ;
        end CONLSQ

```

REMARK ON ALGORITHM 177

LEAST SQUARES SOLUTION WITH CONSTRAINTS

[Michael J. Synge, Comm. ACM, June 63]

MICHAEL J. SYNGE

The Boeing Co., Transport Division, Renton, Wash.

In row-reducing the constraint equations, *CONLSQ* does not

use full pivoting nor does it detect redundancy or inconsistency of the constraints; it was felt that the constraints were likely to be few in number and well-conditioned. However, these omissions may be made good by replacing the statement

ick := *ick* + 1;

by

done: *ick* := *ick* + 1;

and substituting the lines below for the first seven lines of the first compound statement of CONLSQ. If inconsistency is found, the procedure exits to the nonlocal label *inconsistent*. A roundoff tolerance, *eps*, is used in checking consistency, and some numerical value (e.g. 10^{-6}) should be substituted for it.

```
begin integer i, j, k, ii, ick, mr; integer array ic[1:m];
      array B[1:n-r, 1:m-r];
      real Amax, Atemp;
      for i := 1 step 1 until r do
        begin k := 1; mr := i; Amax := A[i, 1];
          for ii := i step 1 until m do
            begin for j := 1 step 1 until m do
                  begin if abs(Amax ≥ abs(A[ii, j]) then go to nogo;
                        mr := ii; k := j; Amax := A[ii, j];
                    nogo: end j;
                  end ii;
                  if abs(Amax) ≥ eps then go to allswell; mr := i;
                test: if abs(y[mr]) ≥ eps then go to inconsistent else mr := mr + 1;
                  if r ≥ mr then go to test else r := i - 1;
                  go to done;
                allswell: for j := 1 step 1 until r do
                  begin Atemp := A[mr, j]; A[mr, j] := A[i, j];
                        A[i, j] := Atemp/Amax;
                  end j;
                  Atemp := y[mr]; y[mr] := y[i]; y[i] := Atemp/Amax;
                The Algorithm then continues with the line:
                  for ii := 1 step 1 until r do
```

ALGORITHM 178 DIRECT SEARCH

ARTHUR F. KAUPPE, JR.

Westinghouse Electric Corp., Pittsburgh, Penn.

```
procedure direct search (psi, X, DELTA, rho, delta, S);
value K, DELTA, rho, delta; integer K; array psi;
      real DELTA, rho, delta; real procedure S;
comment This procedure may be used to locate the minimum
of the function S of K variables. A discussion of the use of this
procedure may be found in: Robert Hooke and T. A. Jeeves,
'Direct Search' Solution of Numerical and Statistical Problems
[J. ACM 8, 2 (1961), 212-229]. The notation is essentially that
used in Appendix B of the cited paper. The exceptions being the
spelling of the Greek letters and the introduction of notation to
distinguish between the process of calculating a value of S and
the value itself—thus S(phi) and Sphi. A modified version of this
procedure acceptable to the BAC compiler for the Burroughs
205 and 220 computers has been prepared and run successfully;
begin real SS, Spsi, Sphi, theta; array phi[1:K]; integer K, k;
procedure E; for k := 1 step 1 until K do
  begin phi[k] := phi[k] + DELTA; Sphi := S(phi);
  if Sphi < SS then SS := Sphi else
    begin phi[k] := phi[k] - 2 × DELTA; Sphi := S(phi);
    if Sphi < SS then SS := Sphi else phi[k] := phi[k] + DELTA;
  end E;
```

```
Start: Spsi := S(psi);
1: SS := Spsi;
for k := 1 step 1 until K do phi[k] := psi[k]; E;
if SS < Spsi then begin
  2: for k := 1 step 1 until K do begin
      theta := psi[k];
      psi[k] := phi[k];
      phi[k] := 2 × phi[k] - theta end;
      Spsi := SS; SS := Sphi := S(phi); E;
      if SS < Spsi then go to 2 else go to 1 end;
  3: if DELTA ≥ delta then begin DELTA := rho × DELTA;
      go to 1 end end
```

ALGORITHM 179 INCOMPLETE BETA RATIO*

OLIVER G. LUDWIG

Mathematical Laboratory and Department of Theoretical Chemistry, University of Cambridge, England

*Based in part on work done at Carnegie Institute of Technology, Pittsburgh, Pennsylvania and supported by the Petroleum Research Fund of the American Chemical Society and by the National Science Foundation.

```
real procedure incompletebeta (x, p, q, epsilon);
value x, p, q; real x, p, q, epsilon;
begin real finsum, infsum, temp, temp1, term, term1, qrecur, index;
      Boolean alter;
comment This procedure evaluates the ratio  $B_x(p, q)/B_1(p, q)$ ,
where  $B_x(p, q) = \int_0^x t^{p-1}(1-t)^{q-1} dt$ , with  $0 \leq x \leq 1$  and  $p, q > 0$ ,
but not necessarily integers. It assumes the existence of a non-
local label, alarm, to which control is transferred upon entry to
the procedure with invalid arguments. Also assumed is a procedure
to evaluate  $\int_0^\infty t^p e^{-t} dt$  which is called factorial(p), (cf. e.g.
Algorithm 80, March, 1962);
if x > 1 ∨ x < 0 ∨ p ≤ 0 ∨ q ≤ 0 then go to alarm;
if x = 0 ∨ x = 1 then begin incompletebeta := x; go to End end;
comment This part interchanges arguments if necessary to obtain
better convergence in the power series below;
if x ≤ 0.5 then alter := false else
  begin alter := true; temp := p; p := q; q := temp; x :=
    1 - x end;
comment This part recurs on the (effective) q until the power
series below does not alternate;
finsum := 0; term := 1; temp := 1 - x; qrecur := index := q;
for index := index - 1 while index > 0 do
  begin qrecur := index;
    term := term × (qrecur+1)/(temp × (p+qrecur));
    finsum := finsum + term;
  end;
comment This part sums a power series for non-integral effective
q and yields unity for integer q;
infsum := term := 1; index := 0;
comment In the following statement the convergence criterion
might well be altered to term > epsilon, since infsum > 1 always,
thus saving one divide per cycle at the cost, perhaps, of a few
more cycles;
for index := index + 1 while (term/infsum) > epsilon do
  begin term := term × x × (index-qrecur) × (p+index-1)/
    (index × (p+index)); infsum := infsum + term;
  end;
comment This part evaluates most of the necessary factorial
functions, minimizing the number of entries into the factorial
procedure;
```

```

temp := temp 1 := factorial (qrecur-1);
term := term 1 := factorial (qrecur+p-1);
for index := qrecur step 1 until (q-0.5) do
  begin temp 1 := temp 1 × index;
    term 1 := term 1 × (index+p)
  end;
comment This part combines the partial results into the final
one;
temp := x ↑ p × (infsum×term/(p×temp)+finsum×term 1×
(1-x) ↑ q/(q×temp 1))/factorial (p-1);
incompletebeta := if alter then 1-temp else temp;
end: end incompletebeta

```

ALGORITHM 180 ERROR FUNCTION—LARGE X

HENRY C. THACHER, JR.*

Argonne National Laboratory, Argonne, Ill.

* Work supported by the U. S. Atomic Energy Commission.

real procedure *erfL*(*x*); **value** *x*; **real** *x*;
comment This procedure evaluates the error function of real

argument, $\text{erf}(x) = (2/\sqrt{\pi}) \int_0^x e^{-u^2} du$ by the Laplace continued

fraction for the complementary error function: $\text{erfc}(x) = 1 - (1/(1+v/(1+2v/(1+3v/(1+\dots)))))/(\sqrt{\pi}x e^{x^2})$ where $v = 1/(2x^2)$. Successive even convergents of the continued fraction are evaluated, using an algorithm suggested by Maehly, until the full accuracy of the arithmetic being used is attained.

The continued fraction converges for all $x > 0$. For small x , however, convergence may be excessively slow, and overflow may occur. In this region, the Taylor series converges satisfactorily, and algorithms such as No. 123 are suitable.

For $x \leq 0$, the procedure calls the global procedure alarm.

The body of this procedure has been checked on the LGP-30 computer, using the Dartmouth Self Contained Algol Processor. The program was used to tabulate *erf*(*x*) from 0.9(1)5.0. The maximum error was 2×10^{-6} , which is explainable by roundoff errors. The number of convergents calculated ranged from 36 for $x = 0.9$ to 2 for $x \geq 3.3$. Overflow occurred for $x = 0.87$;

begin integer *m*; **real** *B min 2*, *B min 3*, *P*, *R*, *T*, *v*, *v2*;
if $x \leq 0$ **then alarm**;
v := $x \times x$;
T := $-0.56418958/x/\exp(v)$;
comment The constant $0.56418958 \dots = \pi^{-1/2}$, and should
be given to the full accuracy required of the procedure;
v := $0.5/v$;

P := $v \times T$;
v2 := $v \times v$;
T := $T + 1$;
m := 0;
R := *B min 3* := *B min 2* := 1;
for $m := m + 1$ **while** $T \neq R$ **do**
 begin *R* := *T*;
 B min 3 := $v \times (m-1) \times B \text{ min } 3 + B \text{ min } 2$
 T := *B min 2*;
 B min 2 := $v \times m \times B \text{ min } 2 + B \text{ min } 3$;
 T := $R - P/B \text{ min } 2/T$;
 P := $m \times (m+1) \times v2 \times P$
 end while;
 erfL := *T*
end

ALGORITHM 181 COMPLEMENTARY ERROR FUNCTION— LARGE X

HENRY C. THACHER, JR.*

Argonne National Laboratory, Argonne, Ill.

* Work supported by the U. S. Atomic Energy Commission.

real procedure *erfcL*(*x*); **value** *x*; **real** *x*;
comment This procedure evaluates the complementary error
function, $\text{erfc}(x) = 1 - \text{erf}(x) = (2/\sqrt{\pi}) \int_x^\infty \exp(-u^2) du$ by
the Laplace continued fraction:

$\text{erfc}(x) = (1/(1+v/(1+2v/(1+3v/(1+\dots)))))/(\sqrt{\pi}x e^{x^2})$
where $v = 1/(2x^2)$. Successive even convergents of the continued
fraction are evaluated, using an algorithm suggested by Maehly,
until the full accuracy of the arithmetic being used is attained.

The continued fraction converges for all $x > 0$. For small x ,
however, convergence may be excessively slow, and overflow
and round-off accumulation may occur. In this region, the
Taylor series converges satisfactorily.

For $x \leq 0$, the procedure calls the global procedure alarm.

The body of this procedure has been checked on the LGP-30
Computer, using the Dartmouth Self Contained Algol Processor,
for $x = 1.2(0.1)5.0$. Results were generally correct to 1 in the
6th significant digit, although a few errors were as large as 6
in that digit. The errors are believed to be due to round-off
only. The number of convergents calculated ranged from 46
for $x = 1.2$ to 10 for $x = 5.0$.

Overflow occurred for $x = 1.183$;

begin integer *m*; **real** *B min 2*, *B min 3*, *P*, *R*, *T*, *v*, *v2*;
if $x \leq 0$ **then alarm**;
v := $x \times x$;
T := $0.56418958/x/\exp(v)$;
comment The constant $0.56418958 \dots = \pi^{-1/2}$, and should be
given to the full accuracy required of the procedure;
v := $0.5/v$;
v2 := $v \times v$;
P := $v \times T$;
m := *R* := 0;
B min 3 := *B min 2* := 1;
for $m := m + 2$ **while** $R \neq T$ **do**
 begin *R* := *T*;
 B min 3 := $v \times (m-1) \times B \text{ min } 3 + B \text{ min } 2$;
 T := *B min 2*;
 B min 2 := $v \times m \times B \text{ min } 2 + B \text{ min } 3$;
 T := $R - P/B \text{ min } 2/T$;
 P := $m \times (m+1) \times v2 \times P$
 end while;
 erfcL := *T*
end

CERTIFICATION OF ALGORITHM 181 [S15] COMPLEMENTARY ERROR FUNCTION—LARGE X [Henry C. Thacher, Jr., *Comm. ACM* 6 (June 1963), 315]

I. CLAUSEN AND L. HANSSON (Recd. 20 Aug. 1964)
DAEC, Risø, Denmark.

The procedure *erfcL* was tested in GIER-ALGOL with 29 signifi-
cant bits and the number-range $\text{abs}(x) < 2 \uparrow 512$ (approx. 1.3×10^{154}).
The statement $m := R := 0$; was corrected to $m := 0$; $R :=$
0; [Because *m* and *R* are of different type; cf. Sec. 4.2.4 of the
ALGOL Report, *Comm. ACM* 6 (Jan. 1963), 1-17.—Ed.] After this
the tests were successful. The procedure was checked a.o. for
 $x = 1.19$ (-0.01) 0.72 . The differences from table values increased
from 10^{-8} at $x = 1.1$ to 7×10^{-8} at $x = 0.75$. Overflow occurred at
 $x = 0.71$.

ALGORITHM 182

NONRECURSIVE ADAPTIVE INTEGRATION

W. M. McKEEMAN AND LARRY TESLER

Stanford University, Stanford, Calif.

```

real procedure Simpson(F) limits : (a, b) tolerance : (eps);
real procedure F; real a, b, eps; value a, b, eps;
begin comment A nonrecursive translation of Algorithm 145.
  Note that the device used here can be used to simulate recursion
  for a wide class of algorithms;
  integer lvl;
  switch return := r1, r2, r3;
  real array dx, epsp, x2, x3, F2, F3, F4, Fmp, Fbp,
    est2, est3 [1:30], pval [1:30, 1:3];
  integer array rtrn [1:30];
  real absarea, est, Fa, Fm, Fb, da, sx, est1, sum, F1;
  comment the parameter setup for the initial call;
  lvl := absarea := est := 0; da := b - a;
  Fa := F(a); Fm := 4.0 × F((a+b)/2.0); Fb := F(b);
  recur:
    lvl := lvl + 1; dx[lvl] := da/3.0;
    sx := dx[lvl]/6.0; F1 := 4.0 × F(a+dx[lvl]/2.0);
    x2[lvl] := a + dx[lvl]; F2[lvl] := F(x2[lvl]);
    x3[lvl] := x2[lvl] + dx[lvl]; F3[lvl] := F(x3[lvl]);
    epsp[lvl] := eps; F4[lvl] := 4.0 × F(x3[lvl]+dx[lvl]);
    Fmp[lvl] := Fm; est1 := (Fa+F1+F2[lvl]) × sx;
    Fbp[lvl] := Fb; est2[lvl] := (F2[lvl]+F3[lvl]+Fm) × sx;
    est3[lvl] := (F3[lvl]+F4[lvl]+Fb) × sx;
    sum := est1 + est2[lvl] + est3[lvl];
    absarea := absarea - abs(est) + abs(est1) + abs(est2[lvl]) +
      abs(est3[lvl]);
    if (abs(est-sum) ≤ epsp[lvl] × absarea) ∨ (lvl ≥ 30) then
      begin comment done on this level;
        up : lvl := lvl - 1;
        pval[lvl, rtrn[lvl]] := sum;
        go to return [rtrn[lvl]];
      end;
    rtrn[lvl] := 1; da := dx[lvl]; Fm := F1;
    Fb := F2[lvl]; eps := epsp[lvl]/1.7; est := est1;
    go to recur; r1:
    rtrn[lvl] := 2; da := dx[lvl]; Fa := F2[lvl];
    Fm := Fmp[lvl]; Fb := F3[lvl]; eps := epsp[lvl]/1.7;
    est := est2[lvl]; a := x2[lvl]; go to recur; r2:
    rtrn[lvl] := 3; da := dx[lvl]; Fa := F3[lvl];
    Fm := F4[lvl]; Fb := Fbp[lvl]; eps := epsp[lvl]/1.7;
    est := est3[lvl]; a := x3[lvl]; go to recur; r3:
    sum := pval[lvl, 1] + pval[lvl, 2] + pval[lvl, 3];
    if lvl > 1 then go to up;
  Simpson := sum
end Simpson

```

CERTIFICATION OF ALGORITHM 182

NONRECURSIVE ADAPTIVE INTEGRATION [W.

M. McKeeman and Larry Tesler, *Comm. ACM* 6 (June 1963), 315]

HAROLD S. BUTLER (Recd 8 Nov. 1963; rev. 6 Dec. 1963)
Stanford Linear Accelerator Center, Stanford, Calif.

A BALGOL transliteration of *Simpson* has been prepared at Stanford by its authors and it has been used in a number of problems involving numerical integration. Its value was most strikingly displayed when it was utilized in a triple integral in which the final integration was over a strongly peaked function that spanned seven orders of magnitude. *Simpson* effectively minimized the number of evaluations and completed the integration five times faster than alternate schemes to subdivide the region of

interest. The values of the integral agreed with independent calculations well within the required tolerance.

The following changes should be made to the published algorithm:

Line 13 should be changed to:

lvl := 0; *absarea* := *est* := 1.0; *da* := *b* - *a*;

Line 17 should read:

sx := *dx*[*lvl*]/6.0; *F1* := 4.0 × *F*(*a* + *dx*[*lvl*]/2.0);

Line 20 should read:

epsp[*lvl*] := *eps*; *F4*[*lvl*] := 4.0 × *F*(*x3*[*lvl*] + *dx*[*lvl*]/2.0);

The condition of line 27 should be changed to:

if ((*abs*(*est*-*sum*) ≤ *epsp*[*lvl*] × *absarea*) ∧ (*est* ≠ 1.0)) ∨ (*lvl* ≥ 30) **then**

ALGORITHM 183

REDUCTION OF A SYMMETRIC BANDMATRIX TO TRIPLE DIAGONAL FORM

H. R. SCHWARZ

Swiss Federal Institute of Technology, Zürich, Switzerland

procedure *bandred*(*a*, *n*, *m*);

value *n*, *m*; **integer** *n*, *m*; **array** *a*;

comment *bandred* reduces a real and symmetric matrix of band type (order *n*, *a*[*i*, *k*] = 0 for |*i* - *k*| > *m*) by a sequence of orthogonal similarity transformations to triple diagonal form. The procedure represents a generalization of the algorithm *m21* by H. Rutishauser. Due to symmetry only the upper part of the band matrix must be given and these elements are denoted for convenience in the following way: *a*[*i*, 0] (*i* = 1, 2, ..., *n*) represents the diagonal element in the *i*th row, and *a*[*i*, *k*] (*i* = 1, 2, ..., *n* - *k* and *k* = 1, 2, ..., *m*) represents the generally nonzero element in the *i*th row and the *k*th position to the right of the diagonal. After completion of the reduction, the elements of the symmetric triple diagonal matrix are given by *a*[*i*, 0] (*i* = 1, 2, ..., *n*) and *a*[*i*, 1] (*i* = 1, 2, ..., *n* - 1);

begin integer *r*, *k*, *i*, *j*, *p*, *rr*; **real** *b*, *g*, *c*, *s*, *c2*, *s2*, *cs*, *u*, *v*;

for *r* := *m* **step** -1 **until** 2 **do**

begin

for *k* := 1 **step** 1 **until** *n* - *r* **do**

begin

for *j* := *k* **step** *r* **until** *n* - *r* **do**

begin

comment This compound statement describes the rotation involving the *i*th and (*i*+1)st rows and columns in order to reduce either *a*[*j*, *r*] or the off-band element *g* to zero, respectively. This rotation produces a new off-band element *g* (in general different from zero) provided *i* + *r* < *n*;

if *j* = *k* **then**

begin if *a*[*j*, *r*] = 0 **then go to** *endk*;

b := -*a*[*j*, *r*-1]/*a*[*j*, *r*]

end

else

begin if *g* = 0 **then go to** *endk*;

b := -*a*[*j*-1, *r*]/*g*

end;

s := 1/sqrt(1 + *b* × *b*); *c* := *b* × *s*;

c2 := *c* × *c*; *s2* := *s* × *s*; *cs* := *c* × *s*;

i := *j* + *r* - 1;

cross elements:

u := *c2* × *a*[*i*, 0] - 2 × *cs* × *a*[*i*, 1] + *s2* × *a*[*i* + 1, 0];

```

v := s2 × a[i, 0] + 2 × cs × a[i, 1] + c2 × a[i+1, 0];
a[i, 1] := cs × (a[i, 0] - a[i+1, 0]) + (c2-s2) × a[i, 1];
a[i, 0] := u; a[i+1, 0] := v;
column rotation:
for p := j step 1 until i - 1 do
begin
u := c × a[p, i-p] - s × a[p, i-p+1];
a[p, i-p+1] := s × a[p, i-p] + c × a[p, i-p+1];
a[p, i-p] := u
end p;
if j ≠ k then
a[j-1, r] := c × a[j-1, r] - s × g;
row rotation:
rr := if r ≤ n - i then r else n - i;
for p := 2 step 1 until rr do
begin
u := c × a[i, p] - s × a[i+1, p-1];
a[i+1, p-1] := s × a[i, p] + c × a[i+1, p-1];
a[i, p] := u
end p;
if i + r < n then
new g: begin g := -s × a[i+1, r];
a[i+1, r] := c × a[i+1, r]
end
end j;
endk: end k
end r
end bandred

```

ALGORITHM 184

ERLANG PROBABILITY FOR CURVE FITTING

A. COLKER

U. S. Steel Applied Research Laboratory
Monroeville, Penn.

```

procedure ERLANG (X, XO, M, VARS, C, FACTORIAL, P);
value XO, M, VARS, C; integer C; real array X, P;
integer procedure FACTORIAL;
comment Computes the Erlang probability for the i-th interval
by  $\int_0^x f(x) dx - \int_0^{x_0} f(x) dx$  where  $f(x) = \frac{1}{(K\mu)^K} \frac{K^K}{(K-1)!} \cdot (x-x_0)^{K-1} e^{-K\mu(x-x_0)}$  where  $\mu = 1/M$ ,  $K = (M-X_0)^2/VARS$  is
the upper boundary for the class intervals,  $X_0$  is the lower
boundary of the first class interval,  $M$  is the mean of the Er-
lang,  $VARS$  is the variance corrected by Sheppard's correction,
 $C$  is the number of class intervals and  $P_i$  is the calculated
probability;

```

```

begin
integer I, J, K, F; real array XE[0 : C];
for I := 1 step 1 until C do
XE[I] := X[I] - XO;
XE[0] := 0;
ME := M - XO;
K := 0.5 + (ME^2)/VARS;
U := K/ME;
SP := 0;
for I := 1 step 1 until C do
begin
SUM1 := 0;
SUM2 := 0;
for J := 0 step 1 until K - 1 do
begin
F := FACTORIAL (J);

```

```

Z1 := U × XE[I-1];
SUM1 := SUM1 + (Z1^J)/F;
Z2 := U × XE[I];
SUM2 := SUM2 + (Z2^J)/F;
end J;
P[I] := SUM1 × (EXP(-U × XE[I-1])) - SUM2
× (EXP(-U × XE[I]));
SP := SP + P[I];
end I;
P[C+1] := 1.0 - SP;
end Erlang

```

ALGORITHM 185

NORMAL PROBABILITY FOR CURVE FITTING

A. COLKER

U. S. Steel Applied Research Laboratory
Monroeville, Penn.

```

procedure NORMAL (X, M, VARS, C, HASTINGS, P);
value M, VARS, C; integer C; real array X, P;
real procedure HASTINGS;
comment Computes the normal probabilities for the i-th interval
by  $\int_0^x f(x) dx - \int_0^{x_0} f(x) dx$  where  $f(x)$  is Hastings' approxi-
mation to the normal interval. Hastings' formula is

```

$$\phi(X_{ni}) = \frac{1}{2} [1 - (1 + a_1 X_{ni} + a_2 X_{ni}^2 + a_3 X_{ni}^3 + a_4 X_{ni}^4 + a_5 X_{ni}^5) e^{-X_{ni}^2}]$$

where $a_1 = 0.09979268$, $a_2 = 0.04432014$, $a_3 = 0.00969920$, $a_4 = -0.00009862$, and $a_5 = 0.00058155$. The X_{ni} are normalized boundary values of X_i where $X_{ni} = (X_i - M)/\sqrt{VARS}$, where M is the mean and $VARS$ is the variance corrected by Sheppard's correction, C is the number of class intervals and P_i the calculated probability;

```

begin
integer I; real array XN[1 : C];
for I := 1 step 1 until C do XN[I] := (X[I] - M)/SQRT(VARS);
P[1] := 0.5 - HASTINGS (ABS(XN[1]));
for I := 2 step 1 until C do
begin
if
XN[I] < 0 then
P[I] := HASTINGS (ABS(XN[I-1])) - HASTINGS
(ABS(XN[I])); else
begin
if (XN[I] > 0) ∧ (XN[I-1] < 0)
then P[I] := HASTINGS (XN[I]) + HASTINGS
(ABS(XN[I-1])); else
P[I] := HASTINGS (XN[I]) - HASTINGS (XN[I-1]);
end;
end I;
P[C+1] := 0.5 - HASTINGS (XN[C]);
end NORMAL

```

ALGORITHM 186 COMPLEX ARITHMETIC

R. P. VAN DE RIET
Mathematical Centre, Amsterdam, Holland

```

procedure Complex arithmetic (a, b, R, r); value a, b; array
a, b, R, r;
comment This procedure assigns the value  $a^2 + b^2$  to R and the
value  $(a+ib)/(a-ib)$  to r, where a, b, R and r are complex
numbers. These two arithmetic expressions are of course fully
arbitrary. They serve only to demonstrate the use of the pro-
cedures P, Q, S, T, J and U. With them one can build up any
arithmetic expression with complex variables, as easily as one
can form them with real variables in ALGOL 60 (As one sees
immediately these procedures can-easily be extended for use in
quaternion arithmetic or general vector and tensor calculus).
We focus attention to the value call of the procedure-parameters,
which is essential. Furthermore, we notice that the depth or
height of the accumulator H is the number of right-handed
brackets placed one after another not counting the brackets
which occur in parameter-delimiters. It is perhaps superfluous to
mention that this procedure was tested on the X1 computer of the
Mathematical Centre.;
begin integer i, k; array H[1:4,1:2];
integer procedure P(i, j); value i, j; integer i, j;
comment P forms the product of the ith and jth element of H;
begin real a; k := k - 1; a := H[i, 1] × H[j, 1] - H[i, 2]
× H[j, 2]; H[k, 2] := H[i, 1] × H[j, 2] + H[i, 2] ×
H[j, 1]; H[k, 1] := a; P := k
end;
integer procedure Q(i, j); value i, j; integer i, j;
comment Q forms the quotient of the ith and jth element of H;
begin real a, b; k := k - 1; b := H[j, 1] ↑ 2 + H[j, 2] ↑ 2;
a := (H[i, 1] × H[j, 1] + H[i, 2] × H[j, 2]) / b;
H[k, 2] := (H[i, 2] × H[j, 1] - H[i, 1] × H[j, 2]) / b;
H[k, 1] := a; Q := k
end;
integer procedure S(i, j); value i, j; integer i, j;
comment S forms the sum of the ith and jth element of H;
begin k := k - 1; H[k, 1] := H[i, 1] + H[j, 1];
H[k, 2] := H[i, 2] + H[j, 2]; S := k
end;
integer procedure T(a); array a;
comment T assigns to the k+1th element of H the complex
variable a;
begin k := k + 1; H[k, 1] := a[1]; H[k, 2] := a[2]; T := k
end;
integer procedure J(i, expi); integer i; real expi;
comment J assigns to the (k+1)th element of H a complex
variable which is decomposed in real and imaginary part;
begin k := k + 1; i := 1; H[k, 1] := expi; i := 2;
H[k, 2] := expi;
J := k
end;
procedure U(i, R); value i; integer i; array R;
comment U assigns to R the ith element of H;
begin R[1] := H[i, 1]; R[2] := H[i, 2]; k := 0 end;
k := 0; U(S(P(T(a)) times: (T(a))) plus: (P(T(b)) times:
(T(b))), R);
comment (a × a) + (b × b) =: R; U(Q(S(T(a)) plus:
(P(J(i, i-1)) times: (T(b)))) divided by: (S(T(a))
plus: (P(J(i, 1-i)) times: (T(b))))), r);
comment (a + (i × b)) / (a + (-i × b)) =: r;
end Complex Arithmetic;

```

The contents of this Algorithm are published in the Technical
Note TN 27, Mathematical Centre, Nov. 1962.

ALGORITHM 187 DIFFERENCES AND DERIVATIVES

R. P. VAN DE RIET
Mathematical Centre, Amsterdam, Holland

```

begin real h; integer i, k; array A[1:50];
comment This program calculates, only to demonstrate the
procedures DELTA and DER, the third derivative of the expo-
nential function with a sixth order difference scheme. We do
not propose to use these procedures in actual calculations, for
as we observed with the X1 computer of the Math. Centre, they
work, but very slowly as a consequence of the strong recursive-
ness of the procedures. In actual programming one has to take
the trouble to write out the well-known formula of Gregory, or
for higher derivatives to multiply this formula a number of
times by itself, then one has to collect the same function-values.
All this trouble is taken over by the computer if one uses the
procedures described below. My purpose, however, in publishing
these procedures lies not in the numerical use but in a demon-
stration of the flexibility of ALGOL 60, if one uses the recursive-
ness property of procedures.;
real procedure SUM(i, h, k, ti); value k; integer i, k, h;
real ti;
begin real s; s := 0; for i := h step 1 until k do s := s + ti;
SUM := s
end;
real procedure DELTA (N, k, k0, fk); value N, k0; real fk;
integer N, k, k0;
comment N is the order of the forward difference which is
calculated from a set of function-values with equidistant
parameter-values;
begin integer i;
DELTA := if N = 1
then SUM (k, k0, k0+1, (-1) ↑ (k+1-k0) × fk)
else DELTA (1, i, k0, DELTA (N-1, k, i, fk))
end;
real procedure DER (OR, N, h, k, k0, fk); value OR, N, h, k0;
real fk, h;
integer OR, N, k, k0;
comment OR is the order of the derivative, calculated from a
given set of function-values f(k), with equidistant parameter-
values, the error is of the order  $h \uparrow (N+1-OR)$ , where h is the
steplength. k0 is the point where the derivative is calculated;
begin integer i;
DER := if OR = 1
then SUM(i, 1, N, DELTA(i, k, k0, fk))
× (-1) ↑ (i+1)/i / h
else DER(1, N+1-OR, h, i, k0, DER(OR-1, N-1, h,
k, i, fk))
end;
for i := 1 step 1 until 50 do A[i] := exp(i/50);
for i := 1 step 1 until 25 do A[i] := DER(3, 6, .02, k, i, A[k])
end

```

The contents of this Algorithm are published in the Technical
Note TN 27, Mathematical Centre, Nov. 1962.

ALGORITHM 188

SMOOTHING 1.

F. RODRIGUEZ-GIL

Central University, Caracas, Venezuela

```

procedure Smooth 13(n, x);
integer n;
real array x;
comment This procedure uses Gram's first-degree three-point
  formulas, as described in Hildebrand's "Introduction to Nu-
  merical Analysis," Ch. 7, to smooth a series of n equally spaced
  values. If the procedure is entered with less than three points,
  control is transferred to a nonlocal label error;
begin real array xp[1 : n]; integer i;
  if n < 3 then go to error;
  for i := 1 step 1 until n do xp[i] := x[i];
  x[1] := 0.83333333 × xp[1] + 0.33333333 × xp[2] - 0.16666667
    × xp[3];
  for i := 2 step 1 until n - 1 do x[i] := (xp[i-1] + xp[i]
    + xp[i+1]) × 0.33333333;
  x[n] := -0.16666667 × xp[n-2] + 0.33333333 × xp[n-1]
    + 0.83333333 × xp[n];
end Smooth 13
  
```

ALGORITHM 189

SMOOTHING 2

F. RODRIGUEZ GIL

Central University, Caracas, Venezuela

```

procedure Smooth 35(n, x);
integer n;
real array x;
comment This procedure is similar to Smooth 13, except that
  Gram's third-degree five-point formulas are used, and that a
  minimum of five points is needed for a successful application;
begin real array xp[1 : n]; integer i;
  if n < 5 then go to error;
  for i := 1 step 1 until n do xp[i] := x[i];
  x[1] := 0.98571429 × xp[1] + 0.05714286 × (xp[2] + xp[4])
    - 0.08571429 × xp[3] - 0.01428571 × xp[5];
  x[2] := 0.05714286 × (xp[1] + xp[5]) + 0.77142857 × xp[2]
    + 0.34285714 × xp[3] - 0.22857143 × xp[4];
  for i := 3 step 1 until n - 2 do x[i] := -0.08571429 × (xp[i-2]
    + xp[i+2]) + 0.34285714 × (xp[i-1] + xp[i+1]) + 0.48571429
    × xp[i];
  x[n-1] := 0.05714286 × (xp[n-4] + xp[n]) - 0.22857143
    × xp[n-3] + 0.34285714 × xp[n-2] + 0.77142857 × xp[n-1];
  x[n] := -0.01428571 × xp[n-4] + 0.05714286 × (xp[n-3]
    + xp[n-1]) - 0.08571429 × xp[n-2] + 0.98571429 × xp[n];
end Smooth 35
  
```

ALGORITHM 190

COMPLEX POWER

A. P. RELPH

The English Electric Co. Ltd., Whetstone, England

```

procedure Complex power (a, b, c, d, n, x, y); value a, b, c, d, n;
real a, b, c, d, x, y; integer n;
comment This procedure calculates  $(x+iy) = (a+ib) \uparrow (c+id)$ 
  where i is the root of -1. In the complex plane, with a cut along
  the real axis from 0 to -∞, p is the sum of the principal value
  of the argument of (a+ib) and 2nπ (n is positive, negative or
  zero depending on the solution required). arctan is assumed to
  be in the range - $\pi/2$  to  $\pi/2$ . The case n = 0, d = 0 is given by
  Algorithm 106;
begin real p, r, v, w;
  if a = 0 then begin if b = 0 then begin x := y := 0;
    go to L end
  else p := 1.57079633 ×
    (sign(b) + 4 × n)
  end
  else begin p := 6.28318532 × n + arctan(b/a);
    if a < 0 then begin if b ≥ 0 then
      p := p + 3.14159265
    else
      p := p - 3.14159265
    end
  end;
  r := .5 × ln(a2 + b2); v := c × p + d × r;
  w := exp(c × r - d × p);
  x := w × cos(v); y := w × sin(v);
L: end
  
```

ALGORITHM 191

HYPERGEOMETRIC

A. P. RELPH

The English Electric Co. Ltd., Whetstone, England

```

procedure Hypergeometric (a1, a2, b1, b2, c1, c2, z1, z2) Results:
  (s1, s2); value a1, a2, b1, b2, c1, c2, z1, z2; real a1, a2, b1, b2,
  c1, c2, z1, z2, s1, s2;
begin comment calculates the hypergeometric function
   ${}_1F_2(a, b, c, z)$  with complex parameters (a = a1 + ia2,
  etc);
real d, y1, y2; integer n;
procedure comp mult (a1, a2, b1, b2, c1, c2); value a1,
  a2, b1, b2; real a1, a2, b1, b2, c1, c2;
  begin comment calculates the product of the two
  complex numbers (a1 + ia2) and (b1 + ib2)
  where i is the root of -1;
  c1 := a1 × b1 - a2 × b2; c2 := a2 × b1 +
  a1 × b2
  end;
  s1 := y1 := 1; s2 := y2 := 0;
  for n := 1 step 1 until 100 do
    begin d := n × ((c1 + n - 1)2 + c22);
      comp mult (a1 + n - 1, a2, y1/d, y2/d, y1, y2);
      comp mult (y1, y2, b1 + n - 1, b2, y1, y2);
      comp mult (y1, y2, c1 + n - 1, -c2, y1, y2);
      comp mult (y1, y2, z1, z2, y1, y2);
      if s1 = s1 + y1 ∧ s2 = s2 + y2 then go to L;
      s1 := s1 + y1; s2 := s2 + y2
    end;
L: end
  
```


CERTIFICATION OF ALGORITHM 191 AND 192 HYPERGEOMETRIC AND CONFLUENT HYPER- GEOMETRIC [A. P. Relph, *Comm. ACM* 6 (July 1963), 388]

HENRY C. THACHER, JR.* (Recd 2 Dec. 1963)

Argonne National Laboratory, Argonne, Ill.

* Work supported by the U.S. Atomic Energy Commission.

The bodies of these two procedures were transcribed for the Dartmouth SCALP processor for the LGP-30 computer. No syntactical errors were found, and the programs gave results agreeing within roundoff (7D) with tabulated values for the following special cases: ${}_2F_1(0.5, 0.5; 1; k^2) = (2/\pi) K(k)$; ${}_2F_1(0.5, -0.5; 1; k^2) = (2/\pi) E(k)$ where K and E are complete elliptic integrals of the first and second kinds; ${}_1F_1(.5; 1; iy) = J_0(x)$, and with ${}_1F_1(-1; 0.1; x)$; ${}_1F_1(-0.5; 0.1; x)$, and ${}_1F_1(-0.5; 0.5; x)$.

It should be observed that the function calculated by 191 is ${}_2F_1(a, b; c; z)$, not ${}_1F_2(a, b; c; z)$ as stated in the comment. These programs evaluate the functions by direct summation of the hypergeometric series. They are, therefore, relatively general, but inefficient. Precautions must also be taken against attempting to compute outside the range of effective convergence of the series.

ALGORITHM 192 CONFLUENT HYPERGEOMETRIC

A. P. RELPH

The English Electric Co. Inc., Whetstone, England

procedure *Confluent hypergeometric* (a1, a2, c1, c2, z1, z2)

Result: (s1, s2); **value** a1, a2, c1, c2, z1, z2;

real a1, a2, c1, c2, z1, z2, s1, s2;

begin **comment** calculates the confluent hypergeometric function ${}_1F_1(a, c, z)$ with complex parameters
($a = a1 + ia2$, etc);

real d, y1, y2; **integer** n;

procedure *comp mult* (a1, a2, b1, b2, c1, c2);

value a1, a2, b1, b2; **real** a1, a2, b1, b2, c1, c2;

begin **comment** calculates the product of the two complex numbers $(a1 + ia2)$ and $(b1 + ib2)$ where i is the root of -1 ;

c1 := a1 × b1 - a2 × b2;

c2 := a2 × b1 + a1 × b2

end;

s1 := y1 := 1; s2 := y2 := 0;

for n := **step** 1 **until** 100 **do**

begin d := n × ((c1 + n - 1)↑2 + c2↑2);

comp mult (a1 + n - 1, a2, y1/d, y2/d, y1, y2);

comp mult (y1, y2, c1 + n - 1, -c2, y1, y2);

comp mult (y1, y2, z1, z2, y1, y2);

if s1 = s1 + y1 $\wedge$ s2 = s2 + y2 **then go to** L;

s1 := s1 + y1; s2 := s2 + y2

end;

L: **end**

SEE ALGORITHM 191

ALGORITHM 193 REVERSION OF SERIES

HENRY E. FETTIS

Aeronautical Research Laboratories, Wright-Patterson Air
Force Base, Ohio

procedure *SERIESRVRT* (A, B, N);

value A, N; **array** A, B; **integer** N;

comment This procedure gives the coefficients $B[i]$ for the series $x = y + \sum B[i] \times y \uparrow i$ ($i=2, 3, \dots, n$) when the coefficients $A[i]$ of the series $y = x + \sum A[i] \times x \uparrow i$ are given. The procedure uses successive approximations after writing $y_{L+1} = x - \sum B[i] \times y_L \uparrow i$ ($i=2, 3, \dots, L+2$ and $L=0, 1, \dots, N-2$) starting with $y_0 = x$;

begin **integer** i, j, k, m;

array Q, R [0 : N];

real s;

A[1] := B[0] := 0;

B[1] := 1;

for k := 1 **step** 1 **until** N - 1 **do**

begin B[k+1] := 0;

for i := 0 **step** 1 **until** k + 1 **do**

R[i] := 0;

for j := k + 1 **step** -1 **until** 1 **do**

begin Q[0] := R[0] - A[j];

for i := 1 **step** 1 **until** k + 1 **do**

Q[i] := R[i];

for i := 0 **step** 1 **until** k + 1 **do**

begin s := 0;

for m := 0 **step** 1 **until** i **do**

s := s + B[m] × Q[i-m];

R[i] := s

end **for** i;

end **for** j;

for i := 2 **step** 1 **until** k + 1 **do** B[i] := R[i]

end **for** k;

end *SERIESRVRT*

CERTIFICATION OF ALGORITHM 193

REVERSION OF SERIES [Henry E. Fettis, *Comm.*

ACM 5, 1962]

HENRY C. THACHER, JR.*

Argonne National Laboratory, Argonne, Ill.

* Work supported by the U. S. Atomic Energy Commission

The body of Algorithm 193 was tested on the LGP-30 using the ALGOL 60 translator developed by the Dartmouth College Computer Center. No syntactical errors were found. The program successfully found the first four coefficients for the series for $\ln(1+y)$ from the first four coefficients of the series for $y = e^x - 1$.

ALGORITHM 194

ZERSOL

CARLOS DOMINGO

Universidad Central, Caracas, Venezuela

procedure *ZERSOL* (h, Y1, m, epsi, F, f, Z); **real** h, epsi, f;

array Y1, Z; **integer** m; **procedure** F;

comment *ZERSOL* finds the simple zeros of the solution $Y1(Y0)$ of the set of m first order differential equations $Y_j' = F_j(Y0, Y1, \dots, Ym)$. h is the step of integration, $epsi$ the error with

which the zeros are to be determined (assuming no error in the process of integration). $F(YS, j, v)$ is a procedure which calculates the functions F_j , taking the arguments from the array YS and leaving the results in v . The search for zeros stops when $Y0 > f$. The zeros are stored as elements of the array Z . MR is a 4×4 matrix with the coefficients of a Runge-Kutta method. For example MR may be row-wise $0.5, 1, 0.5, 0, 1 - a, 1 - a, 1 - a, 0.5, 1 + a, 1 + a, 1 + a, 0, \frac{1}{2}, \frac{1}{2}, 0.5, 0.5$, where $a = \sqrt{2}$;

```

begin real v, r, d; integer j, s, n, k; array Q[1:m], YS[0:m],
  YAL[0:m], YT[1:m], MR[1:4,1:4]; switch S := NOZ, ZER;
  n := 1;
for d := h while YI[0] ≤ f do
  begin s := 1;
    R1: for j := 1 step 1 until m do
      begin Q[j] := 0.0; YS[j] := YI[j]; YT[j] := YI[j] end;
      YS[0] := YI[0];
    R2: for k := 1 step 1 until 4 do
      begin YS[0] := YS[0] + MR[k, 4] × d;
        for j := 1 step 1 until m do
          begin F(YS, j, v); v := v × d;
            r := MR[k, 1] × v - MR[k, 2] × Q[j];
            YT[j] := YT[j] + r;
            Q[j] := Q[j] + 3.0 × r - MR[k, 3] × v
          end;
        for j := 1 step 1 until m do YS[j] := YT[j]
        end;
        go to S(s);
    NOZ: if sign(YI[1]) ≠ sign(YS[1]) then go to IT;
    TR: for j := 0 step 1 until m do YI[j] := YS[j]; go to R2;
    IT: s := 2;
        for j := 0 step 1 until m do YAL[j] := YS[j];
    ZER: d := d/2;
        if d ≤ epsi then go to STZ;
        if sign(YI[1]) = sign(YS[1]) then go to TR else go to R1;
    STZ: Z[n] := YI[0] := YI[0] + d; n := n + 1;
        for j := 0 step 1 until m do YI[j] := YAL[j]
      end;
end
end

```

ALGORITHM 195

BANDSOLVE

DONALD H. THURNAU

Marathon Oil Co., Littleton, Colo.

procedure BANDSOLVE (C, N, M, V); **value** N, M ; **integer** N, M ; **real array** C, V ;

comment *BANDSOLVE* is effective in solving the matrix equation $AX = B$ when the matrix A is of large order and sparse such that a narrow band centered on the main diagonal includes all the non-zero elements. Parameter N is the order of A , and M is the width of the band, necessarily an odd number of elements. *BANDSOLVE* is very efficient because it operates only on the band portion of the matrix A , given in the N by M array C . The band elements of a given row of A appear in the same row of C but shifted such that element $A[i, j]$ becomes $C[i, j - i + (M+1)/2]$. All band elements whether zero or non-zero must be given. The values of undefined elements of C , such as $C[1, 1]$ or $C[N, M]$, are irrelevant. The array V initially contains the vector B . After solution, the array V contains the answer vector X . The contents of array C are destroyed during solution which is done by Gauss elimination with row interchanges, followed by back substitution;

```

begin integer JM, LR, I, PIV, R, J; real T;
  LR := (M+1) ÷ 2;
  for R := 1 step 1 until LR - 1 do
    for I := 1 step 1 until LR - R do
      begin for J := 2 step 1 until M do
        C[R, J-1] := C[R, J];
        C[R, M] := C[N+1-R, M+1-I] := 0
      end of row shifting and zero placement;
    for I := 1 step 1 until N - 1 do
      begin PIV := I;
        for R := I + 1 step 1 until LR do
          if abs(C[R, 1]) > abs(C[PIV, 1]) then
            PIV := R;
          if PIV ≠ I then
            begin T := V[I];
              V[I] := V[PIV];
              V[PIV] := T;
            for J := 1 step 1 until M do
              begin T := C[I, J];
                C[I, J] := C[PIV, J];
                C[PIV, J] := T
              end J
            end of row interchange;
            V[I] := V[I]/C[I, 1];
          for J := 2 step 1 until M do
            C[I, J] := C[I, J]/C[I, 1];
          for R := I + 1 step 1 until LR do
            begin T := C[R, 1]
              V[R] := V[R] - T × V[I];
            for J := 2 step 1 until M do
              C[R, J-1] := C[R, J] - T × C[I, J];
              C[R, M] := 0
            end R;
            if LR ≠ N then LR := LR + 1
          end of triangularization;
          V[N] := V[N]/C[N, 1];
          JM := 2;
          for R := N - 1 step -1 until 1 do
            begin for J := 2 step 1 until JM do
              V[R] := V[R] - C[R, J] × V[R-1+J];
            if JM ≠ M then JM := JM + 1
            end of back solution
          end BANDSOLVE

```

ALGORITHM 196

MULLER'S METHOD FOR FINDING ROOTS OF AN ARBITRARY FUNCTION

ROBERT D. RODMAN

Burroughs Corp., Pasadena, Calif.

procedure MULLER ($p1, p2, p3, mxm, nrts, ep1, ep2, sw1, sw2, sw3, swr, rrt, irt$);

value $p1, p2, p3, mxm, nrts, ep1, ep2, sw1, sw2, sw3, swr$;

integer $mxm, nrts$; **boolean** $sw1, sw2, sw3, swr$;

real $p1, p2, p3, ep1, ep2$; **array** rrt, irt ;

begin comment *MULLER* finds real and complex roots of an arbitrary function. $p1, p2$, and $p3$ are starting values. Roots nearest these points are found first. mxm is the maximum number of iterations to be made in finding any one root. $ep1$ and $ep2$ are specified as tolerance parameters. If $ABS((X_{i+1} - X_i)/X_{i+1}) < ep1$ or if the function value and modified function value are both less than $ep2$, a root has been found. If $sw1$ is true,

```

then each iterant of each root is printed. If sw2 is true, the
value of each root found is printed. If sw3 is true, then, when
applicable, the complex conjugate of each root found is admitted
as a root. If swr is true, only real roots are found. rrt and irt
contain the real, and imaginary parts of each root found. Proce-
dure function is the function generator and procedure complex
performs necessary complex operations;
boolean bool; integer cl, rtc, i, itc; real rx1, rx2, rx3, ix1,
ix2, ix3, rroot, iroot, rdnr, idnr, t1, it1, frroot, firroot, rfx1, rfx2,
rfx3, ifx1, ifx2, ifx3, rh, ih, rlam, ilam, rdel, idel, t2, it2, t3, it3, t4,
it4, rg, ig, rden, iden, rfunc, ifunc;
switch j := m2, m3, m4, m7, m11;
procedure function (reale, imag, reval, ival);
value reale, imag; real reale, imag, reval, ival;
begin comment Coding for this procedure must be inserted at
compile time. reale and imag are the real and imaginary parts
of the dependent variable. reval and ival, the real and imaginary
parts of the function;
end function;
procedure complex (a, ia, b, ib, k, c, ic);
value a, ia, b, ib, k; integer k;
real a, ia, b, ib, c, ic;
begin real temp; switch j := mpy, dvd, sqt;
go to j[k];
mpy: c := a × b - ia × ib; ic := a × ib + ia × b; go to exit;
dvd: if (ib=0) ∧ (b=0) then begin ic := 0; c := 1;
go to exit end; temp := b ↑ 2 + ib ↑ 2;
c := (a×b+ia×ib)/temp; ic := (ia×b-a×ib)/temp;
go to exit;
sqt: if (ia=0) ∧ (a<0) then
begin c := 0; ic := sqrt(-a) end
else if ia = 0 then
begin c := sqrt(a); ic := 0 end
else begin temp := sqrt(a ↑ 2 + ia ↑ 2);
c := sqrt((temp + a)/2);
ic := if (temp - a) < 0 then 0
else sqrt((temp - a)/2) end;
if ((b+c) ↑ 2 + (ib+ic) ↑ 2) < ((b-c) ↑ 2 + (ib-ic) ↑ 2)
then begin c := b - c; ic := ib - ic end
else begin c := b + c; ic := ib + ic end;
exit: end of complex;
start: for i := 1 step 1 until nrts do rrt[i] := irt[i] := 0; rtc := 0;
m0: ix1 := ix2 := ix3 := c1; iroot := itc := 0;
rroot := p1; bool := false;
m1: cl := c1 + 1; rdnr := 1; idnr := 0;
for i := 1 step 1 until rtc do
begin
complex (rdnr, idnr, rroot-rrt[i], iroot-irt[i], 1, t1, it1);
rdnr := t1; idnr := it1
end;
function (rroot, iroot, t1, it1);
complex (t1, it1, rdnr, idnr, 2, frroot, firroot);
go to j[cl];
m2: rfx1 := frroot; ifx1 := firroot; rroot := p2;
go to m1;
m3: rfx2 := frroot; ifx2 := firroot; rroot := p3;
go to m1;
m4: rfx3 := frroot; ifx3 := firroot; rx1 := p1;
rx2 := p2; rx3 := p3; rh := rx3 - rx2;
ih := ix3 - ix2;
complex (rh, ih, rx2 - rx1, ix2 - ix1, 2, rlam, ilam);
rdel := rlam + 1; idel := ilam;
m9: if (rfx1=rfx2) ∧ (rfx2=rfx3) ∧ (ifx1=ifx2) ∧ (ifx2=ifx3)
then begin rlam := 1; ilam := 0; go to m8 end;
complex (rfx1, ifx1, rlam, ilam, 1, t1, it1);
complex (rfx2, ifx2, rdel, idel, 1, t2, it2);
t1 := t1 - t2 + rfx3; it1 := it1 - it2 + ifx3;

```

```

complex (rdel, idel, rlam, ilam, 1, t2, it2);
complex (t1, it1, t2, it2, 1, t3, it3);
complex (rfx3, ifx3, t3, it3, 1, t1, it1);
t1 := -4 × t1; it1 := -4 × it1;
complex (rfx3, ifx3, rlam+rdel, ilam+idel, 1, t2, it2);
complex (rdel ↑ 2 - idel ↑ 2, 2×rdel×idel, rfx2, ifx2, 1, t3, it3);
complex (rlam ↑ 2 - ilam ↑ 2, 2×rlam×ilam, rfx1, ifx1, 1,
t4, it4);
rg := t4 - t3 + t2; ig := it4 - it3 + it2;
if swr ∧ ((rg ↑ 2 + t1) < 0) then
begin rden := rg; iden := ig := 0 end
else complex (rg ↑ 2 - ig ↑ 2 + t1, 2×rg×ig+it1, rg, ig, 3,
rden, iden);
complex (-2×rfx3, -2×ifx3, rdel, idel, 1, t1, it1);
complex (t1, it1, rden, iden, 2, rlam, ilam);
m8: itc := itc + 1;
rx1 := rx2; rx2 := rx3; rfx1 := rfx2; rfx2 := rfx3;
ix1 := ix2; ix2 := ix3; ifx1 := ifx2; ifx2 := ifx3;
complex (rlam, ilam, rh, ih, 1, t1, it1);
rh := t1; ih := it1;
m6: rdel := rlam + 1; idel := ilam; rx3 := rx2 + rh;
ix3 := ix2 + ih; c1 := 3; rroot := rx3;
iroot := ix3; go to m1;
m7: rfx3 := frroot; ifx3 := firroot;
function (rx3, ix3, rfunc, ifunc);
complex (rfx3, ifx3, rfx2, ifx2, 2, t1, it1);
if (t1 ↑ 2 + it1 ↑ 2) > 100 then
begin rlam := rlam/2; rh := rh/2; ilam := ilam/2;
ih := ih/2; go to m6 end;
if sw1 then ...
comment option to output iterant and associated function
values;
t1 := rx3 - rx2; it1 := ix3 - ix2;
complex (t1, it1, rx2, ix2, 2, t2, it2);
if sqrt(t2 ↑ 2 + it2 ↑ 2) ≤ ep1 then go to fin1;
if (sqrt(rfx3 ↑ 2 + ifx3 ↑ 2) ≤ ep2) ∧
(sqrt(rfunc ↑ 2 + ifunc ↑ 2) ≤ ep2) then go to fin 2;
go to if itc ≥ mxm then fin3 else m9;
fin1: if sw2 then ...
comment option to output root; go to m12;
fin2: if sw2 then ...
comment option to output root; go to m12;
fin3: if sw2 then ...
comment no convergence, option to output last iterant;
bool := true;
m12: rtc := rtc + 1; rrt[rtc] := rx3; irt[rtc] := ix3;
if rtc ≥ nrts then go to exit;
if (ABS(ix3) > ep1) ∧ sw3 ∧ ¬ bool then
begin ix3 := -ix3; function (rx3, ix3, rfunc, ifunc);
rroot := rx3; iroot := ix3; c1 := 4;
go to m1;
m11: if sw2 then ...
comment the complex conjugate of the last root found is accept-
able. Option to output this root;
rtc := rtc + 1; rrt[rtc] := rx3; irt[rtc] := ix3
end else go to m0;
if rtc < nrts then go to m0;
exit: end of procedure MULLER

```

ALGORITHM 197 MATRIX DIVISION

M. WELLS

University of Leeds, Leeds, England

```

procedure Pos Div (b, c, m, n, solve);
value m, n, solve; array b, c; integer m, n; Boolean solve;
comment The matrix c, with m rows and n columns, is divided
  by the positive definite matrix b, of order m, by the square root
  method (see Fadeeva, V. N., Computational Methods of Linear
  Algebra, Chap 2, §10). The upper triangle of b is replaced by
  an upper triangular matrix N such that  $N^T N = b$ . The other
  elements of b are undisturbed. The matrix c is replaced by  $b^{-1}c$ .
  The Boolean solve is used as a switch. If its value is true, then
  it is assumed that an earlier entry to Pos Div has left the matrix
  N in place, and a further division of c by b takes place;

begin integer i, j, k;
real procedure dot (a, b, p, q);
value q; real a, b; integer p, q;
comment This is innerproduct, modified to define a function
  designator;
begin real s; s := 0;
for p := 1 step 1 until q do s := s + a × b;
dot := s end dot;
Start of program: if solve then go to back substitution;
for i := 1 step 1 until m do
begin b[i, i] := sqrt (b[i, i] - dot (b[j, i] ↑ 2, 1, j, i - 1));
for j := i + 1 step 1 until m do
  b[i, j] := (b[i, j] - dot (b[k, i], b[k, j], k, i - 1))/b[i, i]
end formation of upper triangular matrix;
back substitution: for i := 1 step 1 until n do
begin for j := 1 step 1 until m do
  c[i, j] := (c[i, j] - dot (b[k, j], c[i, k], k, j - 1))/b[j, j];
for j := m step -1 until 1 do
  c[i, j] := (c[i, j] - dot (b[j, m+1-k], c[i, m+1-k], k, m-j))/
    b[j, j]
end of double back substitution
end of Pos Div

```

CERTIFICATION OF ALGORITHM 197
MATRIX DIVISION [M. Wells, *Comm. ACM* 6 (Aug.
1963), 443]

M. WELLS (Recd 18 Nov. 63)

University of Leeds, Leeds, England

The procedure was tested on a Ferranti Pegasus, using the ALGOL compiler developed by the de Havilland Aircraft Company at Hatfield. The line after the one labelled 'start of program' should read

for i := 1 **step** 1 **until** m **do**

(the first 1 was omitted).

The statement labelled *back substitution* is incorrect, and should read

```

back substitution: for j := 1 step 1 until n do
begin for i := 1 step 1 until m do
  c[i, j] := (c[i, j] - dot (b[k, i], c[k, j], k, i - 1))/b[i, i];
for i := m step -1 until 1 do
  c[i, j] := (c[i, j] - dot (b[i, m+1-k], c[m+1-k, j], k, m-i))/b[i, i]
end of double back substitution

```

With these changes the program was operated successfully on a number of small test problems. The procedure is only applicable to symmetric positive definite matrices, and no systematic attempt has yet been made to assess the accuracy of the results.

The word 'symmetric' should be inserted before 'positive definite' in the comment.

It is interesting to note that the original, incorrect version of the procedure will divide one symmetric matrix by another, and so can be used for matrix inversion.

ALGORITHM 198 ADAPTIVE INTEGRATION AND MULTIPLE INTEGRATION

WILLIAM MARSHALL McKEEMAN

Stanford University, Stanford, Calif.

begin comment This program illustrates the declaration and call of a procedure used to numerically approximate definite integrals and multiple integrals. The integrand is an expression substituted for the first formal parameter and must be a function of the simple variable replacing the second formal parameter. Multiple integration is accomplished by substituting a complete call of *Integral* for the first formal parameter. Note that in this case that the limits of integration on the inside calls may be functions of the variable of integration on the outer call. The parameter *rule* selects a Newton-Cotes formula which matches a polynomial of degree = *rule* to the function in the interval of integration. (See Hamming, *Numerical Methods for Scientists and Engineers*, Sec. 12.2). In any case, the procedure *Integral* adapts its step size to the function in seeking to minimize the number of function evaluations. The program has been tested and run on a variety of functions using the ALGOL compiler on the Burroughs B-5000;

```

real procedure Integral (F) a function of the real variables: (x)
  between limits: (a,b) polynomial degree: (rule) tolerance: (eps);
value a, b, rule, eps; integer rule;
real F, x, a, b, eps;
begin comment set up the parameters for the recursion before
  calling the procedure NC;
switch nct := R1, R2, R3, R4, R5, R6, R7;
real array cf, fn [1:rule+1];
integer k; real da, ab;
real procedure NC(F, x, a, da, fn, k, cf, rule, eps, es, ab, lv1);
value a, da, rule, eps, es, lv1; real array cf;
integer k, rule, lv1; real F, x, a, da, fn, eps, es, ab;
begin comment NC is the adaptive heart of Integral;
  real array fc[1:rule+1, 1:rule+1], est, xx[1:rule+1];
  integer i, j; real dx, int, ep;
  real procedure SUM(term, index, upperlimit);
  real term; integer index, upperlimit;
  begin real t; t := 0;
  for index := 1 step 1 until upperlimit do
    t := t + term;
  SUM := t;
  end of SUM;
  comment begin the integration by evaluating F on the mesh
  points;
  for k := 1 step 1 until rule + 1 do fc[k, k] := fn;
  dx := da/(rule × (rule + 1));
  x := a;
  for i := 1 step 1 until rule + 1 do
    for j := 1 step 1 until rule do
      begin
        if j = 1 then xx[i] := x;
        if i ≠ j then fc[i, j] := cf[j] × F;
        x := x + dx;
      end having done all necessary function evaluations;
  for i := 1 step 1 until rule do
    fc[i, rule+1] := fc[i+1, 1];
  ep := eps/sqrt(rule+1);
  comment eps/(rule + 1) is the value to give an absolute
  error bound of eps in the final answer. It proves too strict in
  practice;
  dx := dx × rule;
  comment compute the integrals of the subintervals;
  for i := 1 step 1 until rule + 1 do
    est[i] := SUM(fc[i, j], j, rule+1) × dx;
  ab := ab - abs(es) + SUM(abs(est[i]), i, rule+1);

```

```

comment ab is the area under abs(F). It is used in computing
the relative error upon which to terminate;
int := SUM(est[i],i,rule+1);
if lvl ≥ 100/(rule+1) then go to error;
NC := if abs(es-int) ≤ eps × ab ∧ es ≠ 1.0 then int
else SUM(NC(F,x,xx[i],dx,fc[i,j],j,cf,rule,ep,est[i], ab,lvl+1),
i,rule+1);
go to return;
error; NC := int;
comment abs(es - int) is the approximate error caused by
terminating the recursion. In most cases, termination at
this level will not adversely affect the accuracy of the result;
return;
end of NC;
comment now initialize the Newton-Cotes coefficients;
go to nct [rule];
R1: cf[1] := cf[2] := 1.0/2.0; go to compute;
R2: cf[1] := cf[3] := 1.0/6.0; cf[2] := 4.0/6.0;
comment R1 is trapezoidal rule, R2 is Simpson's rule;
go to compute;
R3: cf[1] := cf[4] := 1.0/8.0;
cf[2] := cf[3] := 3.0/8.0; go to compute;
R4: cf[1] := cf[5] := 7.0/90.0;
cf[2] := cf[4] := 32.0/90.0;
cf[3] := 12.0/90.0; go to compute;
R5: cf[1] := cf[6] := 19.0/288.0;
cf[2] := cf[5] := 75.0/288.0;
cf[3] := cf[4] := 50.0/288.0; go to compute;
R6: cf[1] := cf[7] := 41.0/840.0;
cf[2] := cf[6] := 216.0/840.0;
cf[3] := cf[5] := 27.0/840.0;
cf[4] := 272.0/840.0; go to compute;
R7: cf[1] := cf[8] := 75.1/1728.0;
cf[2] := cf[7] := 357.7/1728.0;
cf[3] := cf[6] := 134.3/1728.0;
cf[4] := cf[5] := 298.9/1728.0;
compute: da := b - a;
for k := 0 step 1 until rule do
begin
x := a + k × da/rule;
fn[k+1] := F × cf[k+1];
end;
ab := 1.0;
Integral := NC(F,x,a,da,fn[k],k,cf,rule,eps,1.0,ab,0);
end of Integral;
comment Now evaluate the integral of 1.0/sqrt(abs(x+y))
on the unit disk in the x,y-plane;
real x, y, answer;
answer := Integral(Integral(1.0/sqrt(abs(x+y)), x,
-sqrt(1.0-y↑2), sqrt(1.0-y↑2), 7, 0.001),y, -1.0,1.0,3,0.001);
end of program;

```

ALGORITHM 199
CONVERSIONS BETWEEN CALENDAR DATE
AND JULIAN DAY NUMBER
ROBERT G. TANTZEN
Air Force Missile Development Center, Holloman AFB,
New Mex.

```

procedure JDAY (d,m,y,j);
integer d,m,y,j;

```

```

comment JDAY converts a calendar date, Gregorian calendar,
to the corresponding Julian day number j. From the given day
d, month m, and year y, the Julian day number j is computed
without using tables. The procedure is valid for any valid
Gregorian calendar date. When transcribing JDAY for other
compilers, be sure that integers of size 3 × 108 can be handled;
begin integer c, ya;
if m > 2 then m := m - 3
else begin m := m + 9; y := y - 1 end;
c := y ÷ 100; ya := y - 100 × c;
j := (146097 × c) ÷ 4 + (1461 × ya) ÷ 4 + (153 × m + 2) ÷ 5 + d + 1721119
end JDAY

```

```

procedure JDATE (j,d,m,y);
integer j,d,m,y;
comment JDATE converts a Julian day number j to the corre-
sponding calendar date, Gregorian calendar. Since j is an integer
for this procedure, it is correct astronomically for noon of the
day. JDATE computes the day d, month m, and year y, without
using tables. The procedure is valid for any valid Gregorian
calendar date. When transcribing JDATE for other compilers,
be sure that integers of size 3 × 108 can be handled;
begin j := j - 1721119;
y := (4 × j - 1) ÷ 146097; j := 4 × j - 1 - 146097 × y;
d := j ÷ 4;
j := (4 × d + 3) ÷ 1461; d := 4 × d + 3 - 1461 × j;
d := (d + 4) ÷ 4;
m := (5 × d - 3) ÷ 153; d := 5 × d - 3 - 153 × m;
d := (d + 5) ÷ 5;
y := 100 × y + j; if m < 10 then m := m + 3
else begin m := m - 9; y := y + 1 end;
end JDATE

```

```

procedure KDAY (d,m,ya,k);
integer d,m,ya,k;
comment KDAY converts a calendar date, Gregorian calendar,
to the corresponding serial day number k. From the given day
d, month m, and the last two decimals of the year, ya, the serial
day number k is computed without using tables. The procedure
is valid from 1 March 1900 (k=1) to 31 December 1999
(k = 36465). To obtain the Julian day number j (valid at noon)
use j = k + 2415079;
begin if m > 2 then m := m - 3
else begin m := m + 9; ya := ya - 1 end;
k := (1461 × ya) ÷ 4 + (153 × m + 2) ÷ 5 + d
end

```

```

procedure KDATE (k,d,m,ya);
integer k,d,m,ya;
comment KDATE converts a serial day number k to the corre-
sponding calendar date, Gregorian calendar. It computes day d,
month m, and the last two decimals of the year, ya, without
using tables. The procedure is valid from k = 1 (1 March 00) to
k = 36465 (31 December 99) for any one century. For the 20th
Century the relation between k and the Julian day number j
(at noon) is j = k + 2415079;
begin ya := (4 × k - 1) ÷ 1461; d := 4 × k - 1 - 1461 × ya;
d := (d + 4) ÷ 4; m := (5 × d - 3) ÷ 153;
d := 5 × d - 3 - 153 × m;
d := (d + 5) ÷ 5;
if m < 10 then m := m + 3
else begin m := m - 9; ya := ya + 1 end;
end KDATE

```

**CERTIFICATION OF ALGORITHM 199 [Z]
CONVERSIONS BETWEEN CALENDAR DATE AND
JULIAN DAY NUMBER [Robert G. Tartzen, *Comm.*
ACM 8 (Aug. 1963), 444].**

DAVID K. OPPENHEIM (Recd. 10 Jul. 64 and 27 Jul. 64)
System Development Corp., Santa Monica, Calif.

Algorithm 199 was translated into JOVIAL J3 and tested on the Philco 2000. Input was generated with a random number generator that produced uniformly distributed dates between the years 1583 and 2583. The results were checked for 50 different dates in that range.

The procedures as written place unnecessary restrictions on some of the parameters. Expressions cannot always be used as inputs to the procedures. Also, the original input to *JDAY*, *JDATE* and *KDAY* will be modified during the operation of the respective procedures. It should also be noted that in many implementations of ALGOL the use of parameters called by name may be more expensive than those called by value. The call by name is a far more powerful tool than is necessary for most of the parameters of these procedures. For these reasons the following changes are suggested:

1. In procedure *JDAY*
change: integer *d*, *m*, *y*, *j*;
to: value *d*, *m*, *y*; integer *d*, *m*, *y*, *j*;
2. In procedure *JDATE*
change: integer *j*, *d*, *m*, *y*; to: value *j*; integer *j*, *d*, *m*, *y*;
3. In procedure *KDAY*
change: integer *d*, *m*, *ya*, *k*;
to: value *d*, *m*, *ya*; integer *d*, *m*, *ya*, *k*;
4. In procedure *KDATE*
change: integer *k*, *d*, *m*, *ya*;
to: value *k*; integer *k*, *d*, *m*, *ya*;

**ALGORITHM 200
NORMAL RANDOM**

RICHARD GEORGE*

Argonne National Laboratory, Argonne, Ill.

* Work supported by United States Atomic Energy Commission.

real procedure NORMAL RANDOM (Mean, Sigma *n*);

procedure Random;

real Mean, Sigma;

integer *n*;

comment *Random* is assumed to be a real procedure which generates a random number uniform on the interval $(-1, +1)$. The value of *n* should be greater than 10, in order to approximate the normal distribution with accuracy. However, very large values of *n* will increase the running time. The use of Mean and Sigma should be obvious. Reference: R. W. Hamming, *Numerical Methods for Scientists and Engineers*;

begin

integer *i*; real sum;

sum := 0;

for *i* := step 1 until *n* do

sum := sum + Random;

NORMAL RANDOM := Mean + Sigma × sum × sqrt (3.0/*n*)

end NORMAL RANDOM

**ALGORITHM 201
SHELLSORT**

J. BOOTHROYD

English Electric-Leo Computers, Kids Grove, Staffs, England

procedure Shellsort (*a*, *n*); value *n*; real array *a*; integer *n*;
comment *a*[1] through *a*[*n*] of *a*[1:*n*] are rearranged in ascending order. The method is that of D. A. Shell, (A high-speed sorting procedure, *Comm. ACM* 2 (1959), 30-32) with subsequences chosen as suggested by T. N. Hibberd (An empirical study of minimal storage sorting, SDC Report SP-982). Subsequences depend on *m*₁ the first operative value of *m*. Here: $m_1 = 2^k - 1$ for $2^k \leq n < 2^{k+1}$. To implement Shell's original choice of $m_1 = \lfloor n/2 \rfloor$ change the first statement to *m* := *n*;
begin integer *i*, *j*, *k*, *m*; real *w*;
for *i* := 1 step *i* until *n* do *m* := 2 × *i* - 1;
for *m* := *m* ÷ 2 while *m* ≠ 0 do
begin *k* := *n* - *m*;
for *j* := 1 step 1 until *k* do
begin for *i* := *j* step -*m* until 1 do
begin if *a*[*i*+*m*] ≥ *a*[*i*] then go to 1;
***w* := *a*[*i*]; *a*[*i*] := *a*[*i*+*m*]; *a*[*i*+*m*] := *w*;**
end *i*;
end *j*;
end *m*;
end Shellsort;

**CERTIFICATION OF ALGORITHM 201
SHELLSORT [J. BOOTHROYD, *Comm. ACM* 6 (Aug. 1963), 445]**

M. A. BATTY (Recd 27 Jan. 1964)

English Electric Co., Whetstone, Nr. Leicester, England

This algorithm has been tested successfully using the DEUCE ALGOL Compiler. When the first statement of the algorithm was replaced by the statement

m := *n*;

to implement Shell's original choice of $m_1 = n/2$, a slight increase in sorting time was observed with most of the cases tested.

**ALGORITHM 202
GENERATION OF PERMUTATIONS IN LEXICOGRAPHICAL ORDER**

MOK-KONG SHEN

Postfach 74, München 34, Germany

procedure PERLE (*S*, *N*, *I*, *E*);

integer array *S*; integer *N*; Boolean *I*; label *E*;

comment If the array *S* contains a certain permutation of the *N* digits 1, 2, ..., *N* before call, the procedure will replace this with the lexicographically next permutation. If initialization is required set the Boolean variable *I* equal true, which will be changed automatically to false through the first call, otherwise set *I* equal false. If no further permutation can be generated, exit will be made to *E*. For reference see *BIT* 2 (1962), 228-231;

begin integer *j*, *u*, *w*;

if *I* then begin for *j* = 1 step 1 until *N* do *S*[*j*] := *j*;

I* := false; go to *Rose

end;

```

w := N;
Lilie: if S[w] < S[w-1] then
  begin if w = 2 then go to E;
        w := w - 1; go to Lilie
  end;
u := S[w-1];
for j := N step -1 until w do
  begin if S[j] > u then
    begin S[w-1] := S[j];
          -S[j] := u; go to Tulpe
    end
  end;
Tulpe: for j := 0 step 1 until (N-w-1)/2 + 0.1 do
  begin u := S[N-j];
        S[N-j] := S[w+j]; S[w+j] := u
  end;
Rose:
end PERLE

```

ALGORITHM 203

STEEP1

E. J. WASSCHER

Philips Research Laboratories

N. V. Philips' Gloeilampenfabrieken

Eindhoven-Netherlands

procedure STEEP1 (*lb, xs, ub, dx, xmin, fmin, n, eps, relax, dxmax,*
eta, psi, pmaz, zeta, FUNK);

value *dx, n, eps, relax, dxmax, eta, psi, pmaz, zeta;*

integer *n;*

real *fmin, eps, relax, dxmax, eta, psi, pmaz, zeta;*

array *lb, xs, ub, dx, xmin;* **real procedure** *FUNK;*

comment STEEP1 is a subroutine to find the minimum of a differentiable function of *n* variables, using the method of steepest descent. It mainly consists of three parts: (1) a subroutine *ACTIVE*, for computing the partial derivatives, (2) a subroutine *STEP*, for computing the components of an array *xstep[1:n]*, which is a new approximation of *xmin[1:n]*, (3) the compound tail of the procedure body. Both subroutines are only called for once, but by writing the program in this way it is quite easy to change the flow of the program.

Significance of the parameters: *lb(i)*, *ub(i)* are lower and upper bounds for the independent variables. *xs(i)* is the starting value for *xmin(i)*. *xmin(i)* is the computed *i*th component of the minimum, *fmin* the value of the function in *xmin*. *n* is the number of variables. *eps* is a small number which is a measure of the desired accuracy—rather of *fmin* than of *xmin(i)*. *FUNK* (*x*) is the function to be minimized. The other parameters are described in the comments on the three parts mentioned;

begin integer *j;* **real** *alpha, p;* **array** *xstep, dfdx, dfpr[1:n];*
procedure *ACTIVE;*

begin real *beta, gamma, lambda;* **Boolean** *A, B;*

comment 1. A useful estimate for the derivative is $\frac{f(x+dx)-f(x-dx)}{2dx}$, where *dx* should be small, but not so small

that roundoff noise dominates. This may be achieved by taking *dx* such that $\eta < \left| \frac{f(x+dx)-f(x-dx)}{f(x)} \right| < 100 \eta$, where η is a measure for the relative roundoff error. When $|f(x)| < 1$ it is better to replace the denominator by a constant. In the program the parameter *psi* is used for this purpose. The components *dx(i)* are used as a first guess. When the derivative is 0, the program enlarges *dx* until *dx* > *dxmax*.

ACTIVE computes *dfdx[1:n]* in *xmin*. The previously computed partial derivatives *dfpr[1:n]* as well as *relax* are used for relaxation purposes. See comment 3. The Boolean *A* is used when *x+dx* or *x-dx* crosses the boundary *ub* or *lb*. In that case *fmin* has to be recomputed afterwards. The Boolean *B* is of a somewhat complicated nature. It may be seen that *dx* has the character of an own array for *ACTIVE*. In the neighborhood of the minimum this may have the following effect: A step in one variable is taken such that *f(x+dx)* becomes equal to *f(x-dx)*. Then in the next call for *ACTIVE* *dx* has to be doubled, etc. By using the Boolean *B* it is possible to keep *dx* constant near the minimum.

A similar effect may occur in the large. When *f(x)* tends to a constant for *x* tending to $+\infty$ and $-\infty$, then for $|x|$ large *dx* has to be taken large. It is only possible to make *dx* smaller in the neighborhood of the minimum by reducing *dx* after each call of *ACTIVE*.

From the last two remarks one may deduce that the first guess for *dx(i)* should be made with considerable care. Tabulating the function near the starting point may be very helpful;

```

begin ACTIVE: lambda := 0;
for j := 1 step 1 until n do
  begin
    large: A := B := false; if xmin[j] + dx[j] > ub[j]
      then begin xmin[j] := ub[j] - dx[j]; A := true end
      else if xmin[j] - dx[j] < lb[j]
      then begin xmin[j] := lb[j] + dx[j]; A := true end;
    small: xmin[j] := xmin[j] + dx[j]; alpha := FUNK(xmin);
           xmin[j] := xmin[j] - 2 × dx[j]; beta := FUNK(xmin);
           xmin[j] := xmin[j] + dx[j]; if A then fmin := FUNK
           (xmin);
           A := false;
           if alpha - fmin > 0 ∧ beta - fmin > 0
           then begin B := true; go to comp end;
           gamma := abs((alpha-beta)/(if abs(fmin) < psi then
           psi else fmin)));
           if gamma > 100 × eta then
             begin dx[j] := .2 × dx[j]; go to small end;
           if gamma < eta then
             begin dx[j] := 2 × dx[j]; if dx[j] < dxmax then
             go to large else dx[j] := dxmax end
           comp: dfdx[j] := (alpha-beta)/(2 × dx[j]);
           lambda := lambda + dfdx[j] ↑ 2;
           if  $\neg B$  then dx[j] := .5 × dx[j]
           end for; lambda := sqrt(lambda);
           for j := 1 step 1 until n do
             dfdx[j] := dfdx[j]/lambda
           end procedure ACTIVE;

```

procedure *STEP;*

comment 2. A step is taken in all variables at the same time.

The order of magnitude of the step in one variable should be of the order of magnitude of this variable. To accomplish this three weighting factors are given to the partial derivatives:

$$1) \lambda = \left(\sum_{i=1}^n \left(\frac{\partial f}{\partial x_i} \right)^2 \right)^{-1} \quad (\text{see subroutine } ACTIVE),$$

2) $|x_i|$, or when small, *zeta*,

3) a number *p*, which is put equal to 1 at the beginning of the program and which tends to 0 at the minimum.

After a decrease of the function the step is accepted and *p* is multiplied by 1.5. After an increase *p* is divided by 2. *pmaz* replaces *p* when *p* becomes greater than *pmaz*;

```

begin for j := 1 step 1 until n do
  begin alpha := (1-relax) × dfdx[j] + relax × dfpr[j];
       xstep[j] := xmin[j] - p × alpha ×
       (if abs(xmin[j]) < zeta then zeta else abs(xmin[j]));
       dfpr[j] := alpha;
       if xstep[j] > ub[j] then xstep[j] := ub[j]

```

else if $xstep[j] < lb[j]$ then $xstep[j] := lb[j]$
 end for
 end STEP;
 comment 3. In the next part—the compound tail—the calls for *ACTIVE* and *STEP* are organized. The values 1.5 and .5 of the factors of p are not very important. During the iteration p gets an optimal value, which slowly varies. Only at the end p rapidly tends to 0. The programme was tested on the functions $\frac{y^2+1}{x^2+1}$

and $\frac{(x-y)^2-2}{(x+y)^2+2}$, the latter being the first one except for a rotation of the xy -plane over $\pi/4$ radians. In the first case a “gutter” coincides with the x -axis, while for $x > 0$ and $|y| \geq 1 \frac{dy}{dx} \leq 0$.

In the second case, where the gutter is along the line $x=y$, the relaxation is especially interesting, because with $relax = 0$ (and $pmax=100$) the iteration follows the gutter in an unstable way. With starting values $x=-14$ and $y=21$ from $x=y=26$ about 300 steps were taken along the gutter with p about .01. With $relax = .35$ and $pmax = .5$ we had about 150 steps from $x=y=23$. In the gutter itself $relax = .85$ gave the best results, but in that case the gutter was reached at $x=y=63$.

Other parameter values were: $zeta = psi = 1$, $dmax=100$, $eta = 10^{-7}$ with $eps = 10^{-8}$ gave $fmin$ in 10 figures correctly and $xmin[i]$ in 4 to 6 figures for various starting values of $xs[i]$;

```
p := 1;
for j := 1 step 1 until n do
begin xmin[j] := xs[j]; dfpr[j] := 0 end; fmin := FUNK(xmin);
deriv: ACTIVE;
next: STEP;
  alpha := FUNK(xstep);
if alpha < fmin then
  begin fmin := alpha; p := 1.5 × p;
    if p > pmax then p := pmax;
    for j := 1 step 1 until n do xmin[j] := xstep[j];
    go to deriv end;
```

```
p := .5 × p;
if p > eps then go to next;
```

comment As p has become smaller than eps this is the end of *STEEP1*. The program *ACTIVE* takes up rather a lot of computer time by the way it chooses a value for $dx(i)$. A thorough simplification is obtained by taking $dx(i)$ as $10 \uparrow - 3 \times abs(xmin[i])$, where again $xmin[i]$ may be replaced by $zeta$. Further, at the cost of some loss of accuracy, computing time is saved by taking $\frac{f(x+h)-f(x)}{h}$ as an estimate for the derivative. This program, as far as it differs from *STEEP1*, is described in algorithm 204, *STEEP2*. An interesting compromise between the two methods is obtained by interchanging the computation of dx and $dfdx$ in *ACTIVE* of *STEEP1* and omitting the iteration on dx . This routine *ACTIVE*, which has to be used in *STEEP1*, is given by J. G. A. Haubrich in algorithm 205;

end *STEEP1*

CERTIFICATION OF ALGORITHM 203 [E4] STEEP1 [E. J. Wasscher, *Comm. ACM* 9 (Sept. 1963), 517]

PHILIP WALLACK (Recd. 25 May 1964)
 Republic Aviation Corp., Farmingdale, L. I., N. Y.

STEEP1 was translated into FORTRAN IV and run on the IBM 7094. The program was tested on the function $x^4 + y^4 - 1$, with starting values $x = y = 1.5$. Other parameter values were those suggested in the body of the algorithm. After 17 steps the values of the variables were $x = .0180$, $y = .0191$, and the function value $fmin = -.9999999$.

I feel that good programming practice requires that a count be kept of the number of steps taken in *STEEP1* and the number of iterations in *ACTIVE*, with running checks on both these quantities to control looping. Counters were set up for this purpose in the version of the program I ran.

ALGORITHM 204

STEEP2

E. J. WASSCHER

Philips Research Laboratories
 N. V. Philips' Gloeilampenfabrieken
 Eindhoven-Netherlands

```
procedure STEEP2 (lb, xs, ub, dx, xmin, fmin, n, eps, relax,
  dmax, pmax, zeta, FUNK);
value dx, n, eps, relax, dmax, pmax, zeta;
integer n;
real dx, fmin, eps, relax, dmax, pmax, zeta;
array lb, xs, ub, xmin; real procedure FUNK;
comment dx should now be taken about  $10 \uparrow - 3$ , dmax could
  be taken equal to 1. As the program is equal to STEEP1 after
  the declaration of the procedure ACTIVE, the ALGOL description
  is cut off there;
begin integer j; real alpha, p;
  array xstep, dfdx, dfpr [1:n];
  procedure ACTIVE;
  begin real beta, lambda; lambda := 0;
    for j := 1 step 1 until n do
      begin alpha := dx × (if abs(xmin[j]) < dmax
        then dmax else abs(xmin[j]));
        if xmin[j] + alpha > ub[j] then alpha := -alpha;
        xmin[j] := xmin[j] + alpha; beta := FUNK(xmin);
        xmin[j] := xmin[j] - alpha;
        dfdx[j] := (beta - fmin)/alpha;
        lambda := lambda + dfdx[j] ↑ 2
      end for; lambda := sqrt(lambda);
      for j := 1 step 1 until n do dfdx[j] := dfdx[j]/lambda;
    end procedure ACTIVE
```

ALGORITHM 205

ACTIVE

J. G. A. HAUBRICH

Philips Research Laboratories
 N. V. Philips' Gloeilampenfabrieken
 Eindhoven-Netherlands

```
procedure ACTIVE;
begin real beta, lambda; Boolean A;
comment This routine may replace ACTIVE in STEEP1. The
  significance of eta has slightly changed;
lambda := 0;
for j := 1 step 1 until n do
  begin A := false; alpha := dx[j];
    if xmin[j] + alpha > ub[j] then
      begin xmin[j] := ub[j] - alpha; A := true end
    else if xmin[j] - alpha < lb[j] then
      begin xmin[j] := lb[j] + alpha; A := true end;
    xmin[j] := xmin[j] + dx[j]; alpha := FUNK(xmin);
    xmin[j] := xmin[j] - 2 × dx[j]; beta := FUNK(xmin);
    xmin[j] := xmin[j] + dx[j]; if A then fmin := FUNK(xmin);
    dfdx[j] := (alpha - beta)/(2 × dx[j]);
    lambda := lambda + dfdx[j] ↑ 2;
    if alpha - fmin > 0 ∧ beta - fmin > 0 then go to end;
    beta := abs((alpha - beta)/(if abs(fmin) < psi then psi else fmin));
    if beta > eta then dx[j] := 3 × dx[j] else
      begin dx[j] := × d3x[j]; if dx[j] > dmax then dx[j] := dmax end;
    end; end for;
    lambda := sqrt(lambda);
    for j := 1 step 1 until n do dfdx[j] := dfdx[j]/lambda
  end procedure ACTIVE
```


ALGORITHM 206

ARCCOSSIN

MISAKO KONDA

Japan Atomic Energy Research Institute, Tokai, Ibaraki, Japan

```

procedure ARCCOSSIN(x) Result:(arccos, arcsin);
value x;
real x, arccos, arcsin;
comment This procedure computes arccos(x) and arcsin(x) for
-1 ≤ x ≤ 1. The constant 2-n depends on the word length and
relative machine precision, and may be replaced by a variable
identifier. Alarm is the procedure which messages that x is in-
valid.
The approximation formula used here was coded for MUSA-
SINO-1 in its own language at the Electrical Communication
Laboratory Tokyo. This algorithm was translated into FAP and
successfully ran on an IBM 7090;
begin real A, x1, x2, a; integer r;
if abs(x) > 1
then go to Alarm
else if abs(x) > 2 ↑ (-27)
then go to L1
else begin arccos := 1.5707963; go to L3
end;
L1: if x = 1
then begin arccos := 0; go to L3
end
else if x = -1
then begin arccos := 3.1415926; go to L3
end
else begin A := 0; x1 := x;
for r := 0 step 1 until 26 do
begin if x1 < 0
then begin a := 1; x2 := 1 - 2 × x1 ↑ 2 end
else begin a := 0; x2 := 2 × x1 ↑ 2 - 1 end;
A := A + a × 2 ↑ (-r - 1);
x1 := x2
end;
arccos := 3.1415926 × A;
end;
L3: arcsin := 1.570963 - arccos;
end ARCCOSSIN
  
```

ALGORITHM 207

STRINGSORT

J. BOOTHROYD

English Electric-Leo Computers, Ltd.
Staffordshire, England

```

procedure stringsort (a, n); comment elements a[1] ... a[n]
of a[1:2n] are sorted into ascending sequence using a[n+1] ...
a[2n] as auxiliary storage. Von Neumann extended string logic
is employed to merge input strings from both ends of a sending
area into output strings which are sent alternately to either
end of a receiving area. The procedure takes advantage of
naturally occurring ascending or descending order in the origi-
nal data;
value n; integer n; array a;
begin integer d, i, j, m, u, v, z; integer array c[-1:1];
switch p := jz1, str i; switch q := merge, jz2;
oddpass: i := 1; j := n; c[-1] := n + 1; c[1] := 2 × n;
  
```

```

allpass: d := 1; go to firststring;
merge: if a[i] ≥ a[z]
then begin go to p[v];
jz1: if a[j] ≥ a[z]
then if a[i] ≥ a[j]
then str j: begin a[m] := a[j];
j := j - 1 end
else str i: begin a[m] := a[i];
i := i + 1 end
end
else begin v := 2; go to str i end
end
else begin u := 2;
jz2: if a[j] ≥ a[z]
then go to str j
else begin d := -d; c[d] := m;
firststring: m := c[-d];
v := u := 1;
go to ij
end
end;
z := m; m := m + d; if j ≥ i then go to q[u];
if m > n + 1 then begin comment evenpass; i := n + 1;
j := 2 × n; c[-1] := 1; c[1] := n; go to
allpass end
else if m < n + 1 then go to oddpass
end stringsort;
  
```

CERTIFICATION OF ALGORITHM 207 [M1]

STRINGSORT [J. Boothroyd, *Comm. ACM* 6 (Oct. 1963), 615]

CHARLES R. BLAIR (Recd. 31 Jul. 1964)

Department of Defense, Washington 25, D. C.

STRINGSORT compiled and ran successfully without correction on the ALDAP translator for the CDC 1604A. The following sorting times were observed.

Number of Items	Time in Seconds
10	0.03
20	0.05
50	0.20
100	0.38
200	1.03
500	3.22
1000	6.43
2000	12.85
5000	38.72
10000	90.72

ALGORITHM 208

DISCRETE CONVOLUTION

WILLIAM T. FOREMAN, JR.

Collins Radio Co.

Newport Beach, Calif.

```

procedure Discrete Convolution (m, n, prs) result: (Conv);
integer m, n; real procedure prs; real array conv;
comment This procedure finds the probability distribution of
the sum of m independent variables, each with a known distribu-
tion over the nonnegative integers. A real procedure prs with
results pr[k] is assumed to find each probability distribution in
  
```

succession. The maximum sum for which probabilities are computed must be fixed by the user. The number of iterations is roughly $m^2n/2$. The procedure *prs* will in general depend on additional parameters and should include the read-in of the parameters for that distribution. It may include the selection of one function from a set;

```
begin integer i, j, k, ix1, ix2;
real array prob [1:2, 0:m], pr [0:m];
i := 1; ix1 := 1; ix2 := 2; prs (m) result: (pr);
for j := 0 step 1 until m do prob[ix1, j] := pr[j];
for i := 2 step 1 until n do
begin
if ix1 = 1 then begin ix2 := 1; ix1 := 2 end
else begin ix2 := 2; ix1 := 1 end
prs (m) result: (pr);
for j := 0 step 1 until m do
begin
prob[ix1, j] := 0;
for k := 0 step 1 until j do
prob[ix1, j] := prob[ix1, j] + pr[k] × prob[ix2, j-k]
end j
end i;
for j := 0 step 1 until m do conv[j] := prob[ix1, j]
end Discrete Convolution
comment The convolution of discrete probability series is
isomorphic to the multiplication of polynomials. A useful variation
is to omit the parameters i, n and have prs recognize
the end of input. A FORTRAN program using this procedure has
been run on the IBM 7090 to find the sum of queue lengths in a
teletype switching center, where messages arrived according
to the Poisson distribution and message lengths were distributed
negative-exponentially. The following was used as the probability
procedure;
procedure prs (m) result: (pr);
value m; procedure read;
real array pr; integer m;
begin real trafficrate, linespeed, rho; integer j;
read (trafficrate, linespeed);
rho := trafficrate/linespeed;
pr[0] := 1 - rho;
for j := 1 step 1 until m do pr[j] := rho × pr[j-1]
end prs
```

ALGORITHM 209

GAUSS

D. IBBETSON,

Elliott Brothers (London) Ltd.,

Elstree Way, Borehamwood, Herts., England

real procedure Gauss(x); value x; real x;
comment Gauss calculates $(1/\sqrt{2\pi}) \int_{-\infty}^x \exp(-\frac{1}{2}u^2) du$ by means of polynomial approximations due to A. M. Murray of Aberdeen University;

```
begin real y, z, w;
if x = 0 then z := 0
else
begin y := abs(x)/2;
if y ≥ 3 then z := 1
else if y < 1 then
begin w := y × y;
z := (((((((0.000124818987 × w
- 0.001075204047) × w + 0.005198775019) × w
```

```
- 0.019198292004) × w + 0.059054035642) × w
- 0.151968751364) × w + 0.319152932694) × w
- 0.531923007300) × w + 0.797884560593) × y × 2
```

end

else

begin y := y - 2;

```
z := ((((((((((((-0.000045255659 × y
+ 0.000152529290) × y - 0.000019538132) × y
- 0.000676904986) × y + 0.001390604284) × y
- 0.000794620820) × y - 0.002034254874) × y
+ 0.006549791214) × y - 0.010557625006) × y
+ 0.011630447319) × y - 0.009279453341) × y
+ 0.005353579108) × y - 0.002141268741) × y
+ 0.000535310849) × y + 0.999936657524
```

end

end;

Gauss := if x > 0 then (z+1)/2 else (1-z)/2

end Gauss;

CERTIFICATION OF ALGORITHM 209

GAUSS [D. Ibbetson, *Comm. ACM* 6 (Oct. 1963), 616]

(Pvt.) G. W. GLADFELTER (Recd 4 Nov. 63)

RA17667701, 1st Inf. Battle Group U.S. Military Academy (9822), West Point, N.Y.

The algorithm was translated into FORTRAN for the GE 225 and used to publish a table of the error function. No errors were found in the algorithm and the table produced agreed with the published tables at hand (6 significant figures).

CERTIFICATION OF ALGORITHM 209 [S15]

GAUSS [D. Ibbetson, *Comm. ACM* 6, Oct. 1963, 616]

M. C. PIKE

Statistical Research Unit of the Medical Research Council, University College Hospital Medical School, London, England

This procedure was tested on an Elliott 803 computer using the standard Elliott ALGOL compiler. The expression

$$2 \times \text{Gauss}(x) - 1$$

was evaluated for $x = 0.016$ and the answers checked with those given in *Tables of Probability Functions*, vol. II, U.S. National Bureau of Standards, Washington, D.C., 1942, where they are given to 15 decimal places. There was a maximum error of 1 in the 8th decimal place.

ALGORITHM 210

LAGRANGIAN INTERPOLATION

GEORGE R. SCHUBERT*

University of Dayton, Dayton, Ohio

* Undergraduate research project, Computer Science Program, Univ. of Dayton.

procedure LAGRANGE (N, u, X, Y, ANS); real array X, Y;
integer N; real u, ANS;

comment This procedure evaluates an Nth degree Lagrange polynomial, given N + 1 data coordinates, and u the value where interpolation is desired. X is the abscissa array and Y the ordinate array. ANS is the resultant value of the function

at u . The notation is that used in R. W. Hamming, *Numerical Methods for Scientists and Engineers*, pp. 94-95 (McGraw-Hill Book Company, Inc., 1962);

```
begin integer i, j; real L;
  ANS := 0.0;
  for j := step 1 until N+1 do
    begin L := 1.0;
      for i := step 1 until N+1 do
        begin if i ≠ j then L := L × (u-X[i])/(X[j]-X[i])
        end;
        ANS := ANS + L × Y[j]
      end end
```

CERTIFICATION OF ALGORITHM 210 HERMITE INTERPOLATION [George R. Schubert, Comm. ACM, Oct. 1963]

THOMAS A. DWYER

Argonne National Laboratory, Argonne, Ill.

The body of *HERMITE* was transcribed for the Dartmouth SCALP processor for the LGP-30 computer and ran successfully without corrections. It was tested using the error function and its derivatives. Roundoff error in the LGP-30 began to appear for values of n greater than 3. For n equal to 2 (third degree polynomial) the interpolated value agreed with the function within machine limitations (six significant figures) for steps in the argument data of 0.005.

ALGORITHM 211 HERMITE INTERPOLATION

GEORGE R. SCHUBERT*

University of Dayton, Dayton, Ohio

* Undergraduate research project, Computer Science Program, Univ. of Dayton.

```
procedure HERMITE (n, u, X, Y, Y1, ANS); real array X, Y,
  Y1;
```

```
integer n; real u, ANS;
comment This procedure evaluates a(2n+1)th degree Hermite
polynomial, given the value of the function and its first deriva-
tive at each of n + 1 points. X is the abscissa array, Y the
ordinate array, and Y1 the derivative array. ANS is the interpo-
lated value of the function at u. REFERENCE: R. W. Hamming,
Numerical Methods for Scientists and Engineers, pp. 96-97 (Mc-
Graw-Hill Book Company, Inc., 1962);
```

```
begin integer i, j; real h, a;
  ANS := 0.0;
  for j := 1 step 1 until n + 1 do
    begin h := 1.0; a := 0.0;
      for i := 1 step 1 until n + 1 do
        begin if i = j then go to out;
          h := h × (u-X[i])↑2/(X[j]-X[i])↑2;
          a := a + 1.0/(X[j]-X[i]);
        end;
        ANS := ANS + h × ((X[j]-u) × (2×a×Y[j]-Y1[j]) + Y[j])
      end end
```

ALGORITHM 212 FREQUENCY DISTRIBUTION

MALCOLM D. GRAY

The Boeing Co., Seattle, Wash.

```
procedure FREQUENCY (N, A, B, IUL, K, X, KA);
integer N, IUL; integer array KA; real A, B, K;
real array X;
```

comment Given a set X of variables in some interval $I = [a, b]$ such that $a \leq \min x, \max x \leq b$, *FREQUENCY* determines the frequency distribution of X over k equal, half open subintervals of I . The interval I is transformed to the interval $J = [0, k]$ with unit subintervals by $x' = (x-a)/(b-a)/k$, $i = 1, 2, \dots, n$, and considering $x' = L \times M$, L and M integers. The value L then immediately determines the subinterval and M is used for boundary points. If $IUL = 0$, the subintervals are open on the upper end, except the k th. On entry, the array KA is assumed identically zero; on return, $KA[i]$ contains the frequency of X in the i th subinterval;

```
begin integer i, L; real BAK, XP;
  BAK := (B-A)/K;
  for i := 1 step 1 until N do begin
    XP := (X[i]-A)/BAK;
    L := entier (XP);
    if XP = L then go to p2 else L := L + 1; go to p5;
  p2: if IUL = 0 then go to p3 else if L = 0 then L := L + 1;
    go to p5;
  p3: if XP ≠ K then L := L + 1;
  p5: KA[L] := KA[L] + 1;
  end;
end FREQUENCY
```

ALGORITHM 213 FRESNEL INTEGRALS

MALCOLM D. GRAY

The Boeing Co., Seattle, Wash.

```
real procedure FRESNEL (w, S, C); value w; real S, C;
comment FRESNEL computes the Fresnel sine and cosine in-
tegrals  $S(w) = \int_0^w \sin [(\pi/2)t^2] dt$  and  $C(w) = \int_0^w \cos [(\pi/2)t^2] dt$ 
using the series expansions
```

$$S(w) = w \sum_{i=1}^{\infty} \frac{(-1)^{i+1} w^{2i-1}}{(4i-1)(2i-1)!} \quad \text{and}$$

$$C(w) = w \sum_{i=1}^{\infty} \frac{(-1)^{i+1} w^{2i-2}}{(4i-3)(2i-2)!}$$

for $|w| < \sqrt{22/\pi}$ and $x \equiv \pi w^2/2$, and using the asymptotic series

$$S(w) = \alpha - \frac{1}{\pi w} [P(x) \sin(x) + Q(x) \cos(x)],$$

$$C(w) = \alpha - \frac{1}{\pi w} [P(x) \cos(x) - Q(x) \sin(x)]$$

where $|w| \geq \sqrt{22/\pi}$, $x \equiv \pi w^2/2$,

$$Q(x) = 1 - \sum_{i=2}^{\infty} \frac{(-1)^i (4i-5)!!}{(2x)^{2i-2}}, \quad P(x) = \sum_{i=1}^{\infty} \frac{(-i)^{i+1} (4i-3)!!}{(2x)^{2i-1}},$$

and $n!! \equiv n(n-2)(n-4) \dots 1$. If $w \geq 0$, then $\alpha = \frac{1}{2}$, or if $w < 0$, then $\alpha = -\frac{1}{2}$.

This algorithm is a translation of a FAP coded subroutine currently in use on the IBM 7094 at the Boeing Company. The FAP program yields the following errors when tested at 0.05 increments of x :

x	ΔS	ΔC
0.00, 1.00	$<1 \times 10^{-7}$	$<1 \times 10^{-7}$
1.05, 8.65	$<1 \times 10^{-6}$	$<1 \times 10^{-6}$
8.70, 10.30	3×10^{-6}	2×10^{-6}
10.35, 11.00	5×10^{-6}	4×10^{-6}
11.05, 12.15	$<1 \times 10^{-6}$	3×10^{-6}
12.20, 15.00	$<1 \times 10^{-6}$	$<1 \times 10^{-6}$

where ΔS and ΔC are the approximate average absolute deviations (over the range) from the reference. The user must supply $S(w) = C(w) = \pm \frac{1}{2}$ if $w \rightarrow \pm \infty$. REFERENCES: ALGORITHMS 88-90, J. L. Cundiff, *Comm. ACM*, May 1962; Born, M. and Wolf, E., *Principles of Optics*, Pergamon Press (1958), pp. 369-431;

```
begin real x, x2, eps, term; integer n; eps := 0.000001;
x := w × w/0.6366198;
x2 := -x × x; if x ≥ 11.0 then go to asympt;
begin real frs, frsi;
frs := x/3; n := 5; term := x × x2/6;
frsi := frs + term/7;
loops: if abs(frs-frsi) ≤ eps then go to send; frs := frsi;
term := term × x2/n/(n-1); frsi := frs + term/(n+n+1);
n := n + 2; go to loops;
send: S := frsi × w; end;
begin real frc, frci;
frc := 1; n := 4; term := x2/2; frci := 1 + term/5;
loopc: if abs(frc-frci) ≤ eps then go to cend; frc := frci;
term := term × x2/n/(n-1); frci := frc + term/(n+n+1);
n := n + 2; go to loopc;
cend: C := frci × w; end; go to aend;
asympt: begin real S1, S2, half, temp; integer i;
x2 := 4 × x2; term := 3/x2; S1 := 1 + term; n := 8;
for i := 1 step 1 until 5 do begin n := n + 4;
term := term × (n-7) × (n-5)/x2; S1 := S1 + term;
if abs(term) ≤ eps then go to next; end i;
next: for i := 1 step 1 until 5 do begin n := n + 4;
term := term × (n-5) × (n-3)/x2; S2 := S2 + term;
if abs(term) ≤ eps then go to final; end i;
final: if w < 0 then half := -0.5 else half := 0.5; term := cos(x);
temp := sin(x); x2 := 3.1415927 × w;
C := half + (temp × S1 - term × S2)/x2;
S := half - (term × S1 + temp × S2)/x2;
end;
aend: end FRESNEL
```

CERTIFICATION OF ALGORITHM 213 [S20]
FRESNEL INTEGRALS [M.D. Gray, *Comm. ACM* 6
(Oct. 1963), 617]

Malcolm Gray (Recd. 29 May 1964 and, revised, 11 June 1964)

Computer Science Div., Stanford U., Stanford, Calif.
(now at The Boeing Company, Seattle, Wash.)

Necessary changes to the algorithm are:

- (1) in the first line, replace
real S, C ; with real w, S, C ;
- (2) in the formula for $P(x)$, replace $(-i)^{i+1}$ with $(-1)^{i+1}$
- (3) the statement beginning
loopc: if abs(frc-frci)
should read
loopc: if abs(frc-frci)

(4) in the body, replace the line

next: for i := 1 step 1 until 5 do begin n := n + 4;
with the lines

next: term := S2 := 0.5/x; n := 4;

for i := 1 step 1 until 5 do begin n := n + 4;

The procedure (with the above changes) was executed on the Burroughs B5000 at Stanford University and gave results as indicated in the algorithm.

Communications from Helmut Lotsch of the W. W. Hansen Laboratories, Stanford University, and from Harold Butler of the Los Alamos Scientific Laboratory, Los Alamos, New Mexico, state that they found these same errors, and after the corrections were made, similar results were obtained. Mr. Lotsch's work was done on the B5000 and Dr. Butler's work was done on the IBM 7090.

ALGORITHM 214

q-BESSEL FUNCTIONS $I_n(t)$

J. M. S. SIMÕES PEREIRA

Gulbenkian Scientific Computing Center, Lisbon, Portugal

procedure qBessel (t, q, n, j, s); integer n, j; real t, q, s;
array s;

comment This procedure computes values of any q-Bessel function $I_n(t)$ for n integer (positive, negative or zero) by the use of the well-known expansion

$$I_n(t) = \sum_{k=0}^{\infty} \frac{q^{k(k-1)/2 + (n+k)(n+k-1)/2} t^{n+k}}{(q)_k (q)_{n+k}}$$

where $|q| < 1$, $(q)_n = (1-q)(1-q^2) \cdots (1-q^n)$, $(q)_0 = 1$ and $1/(q)_{-n} = 0$ ($n=1, 2, 3, \dots$). (See L. Carlitz, The product of q-Bessel functions, *Port. Math.* 21 (1962), 5-9.) Moreover, j denotes the number of terms (at least 2) retained in the summation, and s[i] stands for the sum of the first i+1 terms of the expansion. This procedure has been translated into FORTRAN for the IBM 1620 and run successfully;

```
begin integer k, m, p; real c, u; m := abs(n); c := 1; if
n = 0 then go to A;
for p := 1 step 1 until m do c := c × (1-q↑p); if n < 0 then
go to B;
A: u := q ↑ (n × (n-1)/2) × (t↑n)/c; s[0] := u;
for k := 1 step 1 until j do
begin u := u × q ↑ (n+2 × k-2) × (t↑2)/((1-q↑k) × (1-q↑(n+k)));
s[k] := s[k-1] + u end;
B: u := q ↑ ((m-1) × m/2) × t ↑ (n+2 × m)/c; s[m] := u;
for k := m+1 step 1 until j do
begin u := u × q ↑ (n+2 × k-2) × (t↑2)/((1-q↑k) × (1-q↑(n+k)));
s[k] := s[k-1] + u end
end
```

REMARK ON ALGORITHM 214

q-BESSEL FUNCTIONS $I_n(t)$ [J. M. S. Simões Pereira,
Comm. ACM 6 (Nov. 1963), 662]

J. M. S. SIMÕES PEREIRA (Recd 6 Jan 1964)

Gulbenkian Scientific Computing Center, Lisbon, Portugal

Corrections:

1. Insert a dummy statement labeled C just before the final end.
2. Add a statement go to C just before the label B.
3. Add a colon in the clause for k := 1 step 1 until j do ...

ALGORITHM 215

SHANKS

HENRY C. THACHER, JR.*

Argonne National Laboratory, Argonne, Ill.

* Work supported by the U. S. Atomic Energy Commission

procedure Shanks (nmin, nmax, kmax, S);

value nmin, nmax, kmax;

integer nmin, nmax, kmax;

array S;

comment This procedure replaces the elements $S[nmin]$ through $S[nmax-2 \times kmax]$ of the array S by the $e[kmax]$ transform of the sequence S . The elements $S[nmax-2 \times kmax+1]$ through $S[nmax-1]$ are destroyed. The $e[k]$ transforms were discovered by D. Shanks (*J. Math. Phys.* 34 (1955), 1-42). $e[1]$ is equivalent to the $(\delta) \uparrow 2$ transformation. The $e[k]$ transforms are particularly valuable in estimating B in sequences which may be written in the form $S[n] = B + \sum a[i] \times q[i] \uparrow n$ ($i=1, 2, \dots, k$).

The transformation is carried out by the epsilon algorithm (Wynn, P., *M.T.A.C* 10 (1956), 91-96). ALGOL procedures for applying the algorithm to series of complex terms are given by Wynn (*BIT* 2 (1962), 232-255).

The body of this procedure has been tested using the Dartmouth Self-Contained ALGOL Processor for the LGP-30 computer. It gave the following results on the sequence for the smaller zero of the Laguerre polynomial, $L[2](x)$:

n	S(n)	e(1)(S(n))	e(2)(S(n))	e(1/2)(S(n))
0	0.0000000	0.5714285	0.5857432	0.5857616
1	0.5000000	0.5851059	0.5857854	0.5857859
2	0.5625000	0.5857318	0.5857861	0.5857861
3	0.5791016	0.5857816		
4	0.5838396	0.5857859		
5	0.5852172			
6	0.5856198	True Value	0.5857864375	

These results are in satisfactory agreement with those given by Wynn (1956);

begin integer j, k, limj, link, two kmax;

real T0, T1;

two kmax := kmax + kmax;

limj := nmax;

for j := nmin **step** 1 **until** limj **do**

begin T0 := 0;

lim := j - nmin;

if link > two kmax **then** link := two kmax **link** := link - 1;

for k := 0 **step** 1 **until** link **do**

begin T1 := S[j-k] - S[j-k-1];

if T1 ≠ 0 **then** T1 := T0 + 1/T1 **else**

if S[j-k] = 1099 **then** T1 := T0 **else**

T1 := 1099;

comment 1099 may be replaced by the largest number representable in the computer;

T0 := S[j-k-1];

S [j-k-1] := T1

end for k

end for j

end Shanks

CERTIFICATION OF ALGORITHM 215

SHANKS [H. C. Thacher, Jr., *Comm. ACM* 6 (Nov. 1963), 662]

LARRY SCHUMAKER (Recd. 16 Dec. 63)

Computation Ctr., Stanford U., Stanford, Calif.

Algorithm 215 was coded in Extended ALGOL for the Burroughs B-5000 and was tested on a large number of sequences. One ap-

parent typographical error was noted. The statement $lim := j - nmin$ should have read $link := j - nmin$. The following tables were reproduced exactly: (a) tables on p. 5 and p. 33 of [1]; (b) Table I on p. 95 of [2]; (c) Tables III and IV on p. 28 of [3].

REFERENCES:

1. SHANKS, D. Non-linear transformations of divergent and slowly convergent sequences. *J. Math. Phys.* 34 (1955), 1-42.
2. WYNN, P. On a device for computing the $e_m(S_n)$ transformation. *MTAC* 10 (1956), 91-96.
3. WYNN, P. On repeated application of the ϵ -algorithm. *Chiffres* 4 (1961), 19-22.

ALGORITHM 216

SMOOTH

RICHARD GEORGE*

Argonne National Laboratory, Argonne, Ill.

* Work supported by the U. S. Atomic Energy Commission.

procedure SMOOTH (Data) which is a list of length: (n);

integer n; **real** array Data;

begin

comment This procedure accomplishes fourth-order smoothing of a list using the method given by Lanczos, *Applied Analysis* (Prentice-Hall, 1956). This algorithm requires only one additional list for temporary storage;

real Factor, Top; **integer** Max I, I, J; **array** Delta [1 : n];

Factor := 3.0/35.0;

Max I := n - 1;

for I := 1 **step** 1 **until** Max I **do**

Delta [I] := Data [I+1] - Data [I];

for J := 1 **step** 1 **until** 3 **do**

begin

Top := Delta [1];

Max I := Max I - 1;

for I := 1 **step** 1 **until** Max I **do**

Delta [I] := Delta [I+1] - Delta [I]

end;

Max I := n - 2;

for I := 3 **step** 1 **until** Max I **do**

Data [I] := Data [I] - Delta [I-2] × Factor;

Data [1] := Data [1] + Top/5.0 + Delta [1] × Factor;

Data [2] := Data [2] - Top × 0.4 - Delta [1]/7.0;

Data [n] := Data [n] - Delta [n-3]/5.0 + Delta [n-4] × Factor;

Data [n-1] := Data [n-1] + Delta [n-3] × 0.4 - Delta [n-4]/7.0

end;

ALGORITHM 217

MINIMUM EXCESS COST CURVE

WILLIAM A. BRIGGS

Marathon Oil Co., Findlay, Ohio

procedure MINIMUM EXCESS COST CURVE (nodes, links, source, sink, I, J, crash, normal, slope, node, lij, ERROR);

value nodes, links, source, sink;

integer nodes, links, source, sink;

integer array I, J, crash, normal, slope, node, lij;

comment This procedure utilizes a network-type description of

a project to compute the minimum cost involved in expedition of the project completion date. Project tasks are identified and completion order specified by the vector pair I, J , which contain node numbers of the events starting and ending each task. The tasks are parameterized within the vectors *crash*, *normal*, and *slope*—which contain the crash or minimum task completion times, the normal task completion times, and the increased cost per unit decrease in task duration (the slope of the time-cost curve), which must be a nonzero integer. The procedure initially determines the normal-duration critical path, then successively reduces the durations of the tasks with the flattest cost slope, adjusting the critical path, until minimum durations are reached. The FORD-FULKERSON labeling technique is utilized. Each task must proceed from a lower-numbered node to a higher-numbered one—if not, exit to the nonlocal label *ERROR* is made. Nodes should be numbered sequentially, starting at the initial event (*source*) and continuing to the final event (*sink*). The maximum node number is equivalent to the value *nodes*, while the value *links* denotes the total number of tasks. The arrays are of dimensions $I, J, \text{crash}, \text{normal}, \text{slope}, \text{lij}[1:\text{links}]$ and $\text{node}[1:\text{nodes}]$;

```

begin integer m, n, lb, nji, nij, lex, kf, nj, ni, ntv, ord, infinity,
temp;
integer array labl[1: nodes, 1: 3], f[1: links, 1: 2];
comment infinity is herein used to represent the largest available integer;
for m := 1 step 1 until links-1 do
  if  $I[m] \geq J[m] \vee I[m] > I[m+1] \vee J[m] > J[m+1]$  then go to ERROR;
  if  $I[\text{links}] \geq J[\text{links}]$  then go to ERROR;
  for n := 1 step 1 until nodes do labl[n, 1] := labl[n, 2] := labl[n, 3] := node[n] := 0;
  for m := 1 step 1 until links do
    begin f[m, 1] := f[m, 2] := 0;
    temp := node[I[m]] + normal[m];
    if node[J[m]] < temp then node[J[m]] := temp
    end;
  ntv := ord := 0; lb := node[sink];
A: labl[source, 1] := source; labl[source, 3] := infinity;
  for m := 1 step 1 until links do
    begin if labl[I[m], 1] = 0 then go to B;
    if labl[J[m], 1]  $\neq$  0 then go to C;
    nji := node[J[m]] - node[I[m]];
    if nji  $\neq$  normal[m] then go to A1;
    lex := slope[m] - f[m, 1];
    if lex  $\leq$  0 then go to A1;
    kf := 1; go to A2;
A1: if nji  $\neq$  crash[m] then go to C;
    lex := infinity; kf := 2;
A2: labl[J[m], 1] := I[m]; labl[J[m], 2] := kf;
    if labl[I[m], 3] > lex then go to A3;
    labl[J[m], 3] := labl[I[m], 3]; go to A4;
A3: labl[J[m], 2] := lex;
A4: if J[m] = sink then go to D else go to C;
B: if labl[J[m], 1] = 0 then go to C;
    nij := node[I[m]] - node[J[m]];
    if nij  $\neq$  normal[m]  $\vee$  f[m, 1] = 0 then go to B1;
    lex := f[m, 1]; kf := -1; go to B2;
B1: if nij  $\neq$  normal[m]  $\vee$  f[m, 2] = 0 then go to C;
    lex := f[m, 2]; kf := -2;
B2: labl[I[m], 1] := J[m]; labl[I[m], 2] := kf;
    if labl[J[m], 3] > lex then go to B3;
    labl[I[m], 3] := labl[J[m], 3]; go to B4;
B3: labl[I[m], 3] := lex;
B4: if I[m] = sink then go to D;
C: end;
  for n := 1 step 1 until nodes do if labl[n, 1] = 0 then

```

```

    node[n] := node[n] - 1;
F: for n := 1 step 1 until nodes do labl[n, 1] := labl[n, 2] := labl[n, 3] := 0;
  go to A;
D: if labl[sink, 3] = infinity then go to OUT;
  ntv := ntv + labl[sink, 3]; nj := sink;
G: ni := labl[nj, 1];
  if labl[nj, 2] > 0 then go to G1;
  for m := 1 step 1 until links do if  $I[m] = nj \wedge J[m] = ni$  then  $f[m, -\text{labl}[nj, 2]] := f[m, -\text{labl}[nj, 2]] + \text{labl}[\text{sink}, 3]$ ;
G1: for m := 1 step 1 until links do if  $I[m] = ni \wedge J[m] = nj$  then  $f[m, \text{labl}[nj, 2]] := f[m, \text{labl}[nj, 2]] + \text{labl}[\text{sink}, 3]$ ;
  if ni = source then go to OUT;
  nj := ni; go to G;
OUT: for m := 1 step 1 until links do
  begin lij[m] := node[J[m]] - node[I[m]];
  if lij[m] > normal[m] then lij[m] := normal[m]
  end;
  ord := (lb - node[sink])  $\times$  ntv; lb := node[sink];
  if labl[sink, 3] = infinity then ntv := infinity;
ANS: comment as control passes through here—
  ord is the ordinate of the minimum project excess cost curve at a total project duration of node[sink], successive values of ord plotted versus node[sink] generate the minimum project excess cost curve.
  node[1: nodes] contains the event times at each node
  lij[1: links] contains the durations of each task
  ntv is the slope of the cost curve back in time from total duration node[sink].
  these values should be printed in some readable form;
  if ntv < infinity then go to F;
end MINIMUM EXCESS COST CURVE;

```

ALGORITHM 218

KUTTA MERSON

PHYLLIS M. LUKEHART*

Argonne National Laboratory, Argonne, Ill.

procedure KuttaMerson ($n, t, y, \text{eps}, h, \text{fct}, \text{first}$);

value n, eps ;

integer n ;

real t, eps, h ;

real array y ;

Boolean first;

procedure fct;

comment This procedure integrates the system of ordinary first-order differential equations $y[i] = f[i](t, y[1], y[2], \dots, y[n])$ from $t = t$ to $t = t + h$ by the Kutta-Merson method (L. Fox, *Numerical Solution of Ordinary and Partial Differential Equations*, p. 24, Pergamon Press, 1962). The working interval of calculation is adjusted by the procedure so that the maximum absolute error of the dependent variables is less than *eps*. For optimum error control, the equations should be scaled so that all dependent variables have approximately the same magnitude. Input variables for the procedure are n , the number of equations, t , initial value of the independent variable, y , array of initial values of dependent variables, *eps*, allowable error, h , the total interval, *fct*, a procedure evaluating the derivatives, and *first*, a Boolean variable which indicates whether the working interval has been adjusted to secure the desired accuracy. On the initial call of the procedure for a given system, *first*

should be true. It will be set false by the procedure, and the proper working interval determined. The procedure *fct* has as formal parameters the simple real variable *t*, and the real arrays *y* and *f*. For $i = 1, 2, 3, \dots, n$ it must assign to *f*[*i*] the value of the first derivative of *y*[*i*] appropriate to the values of *t* and *y*. The body of this procedure has been tested using the Dartmouth SCALP compiler for the LGP-30 computer. For the equation $dy/dt = -2ty^2$ and input data $t = 1, y = .5, h = 1, eps = .0001$, the average error was .000003 and the time was 30 min. For the linear boundary value problem $d^2y/dt^2 = -1 - (t^2+1)y$, $y(\pm 1) = 0$, the maximum error was .0000024 (L. Collatz, *The Numerical Treatment of Differential Equations*, pp. 145, 225, Springer-Verlag, Berlin, 1960) and the time, 90 min. More accuracy may be achieved by using a smaller value of *eps*;

```

begin integer i, loc;
real error;
array y0, y1, y2, f0, f1, f2[1:n];
own integer ploc;
own real hc;
Boolean increase;
if first then begin hc := h; ploc := 1; first := false end;
loc := 0;
next: fct(t, y0, f0);
for i := 1 step 1 until n do
y1[i] := y0[i] + hc/3 × f0[i];
fct(t + hc/3, y1, f1);
for i := 1 step 1 until n do
y1[i] := y0[i] + hc/6 × f0[i] + hc/6 × f1[i];
fct(t + hc/3, y1, f1);
for i := 1 step 1 until n do
y1[i] := y0[i] + hc/8 × f0[i] + 3 × hc/8 × f1[i];
fct(t + hc/2, y1, f2);
for i := 1 step 1 until n do
y1[i] := y0[i] + hc/2 × f0[i] - 3 × hc/2 × f1[i] + 2 × hc × f2[i];
fct(t + hc, y1, f1);
for i := 1 step 1 until n do
y2[i] := y0[i] + hc/6 × f0[i] + 2 × hc/3 × f2[i] + hc/6 × f1[i];
increase := true;
for i := 1 step 1 until n do
begin error := abs(.2 × (y1[i] - y2[i]));
comment To test on relative error change this expression to
abs(.2 - .2 × y2[i]/y1[i]);
if error > eps then
begin hc := hc/2;
ploc := 2 × ploc;
loc := 2 × loc;
go to next
end;
if error × 64 > eps then increase := false
end i;
t := t + hc;
for i := 1 step 1 until n do
y0[i] := y2[i];
loc := loc + 1;
if loc < ploc ∧ increase ∧ loc = loc ÷ 2 × 2 ∧ ploc > 1 then
begin hc := 2 × hc;
loc := loc ÷ 2;
ploc := ploc ÷ 2
end;
go to next
end KuttaMerson

```

CERTIFICATION OF ALGORITHM 218 [D2] KUTTA MERSON [Phyllis M. Lukehart, *Comm. ACM* 6 (Dec. 1963), 737]

KAREN BORMAN PRIEBE (Recd. 10 Feb. 1964)
Woodward Governor Company, Rockford, Illinois

Algorithm 218 was translated into FAST for the NCR 315 and gave satisfactory results with the following corrections, if the equations were scaled as recommended in the comment of the original algorithm. Ignoring this scaling can lead to results that do not satisfy the intended error criterion.

1. procedure *KuttaMerson* (*n, t, y, eps, h, fct, first, x*);
instead of
procedure *KuttaMerson* (*n, t, y, eps, h, fct, first*);
2. real array *y, x*;
instead of
real array *y*;
3. if first then begin for $i := 1$ step 1 until *n* do *y0*[*i*] := *y*[*i*];
hc := *h*;
instead of
if first then begin hc := *h*; ...
4. if loc < ploc then
begin
if increase ∧ loc = (loc ÷ 2) × 2 ∧ ploc > 1 then
begin
hc := 2 × hc;
loc := loc ÷ 2;
ploc := ploc ÷ 2
end;
go to next
end;
for $i := 1$ step 1 until *n* do *x*[*i*] := *y0*[*i*];
end *KuttaMerson*
instead of
if loc < ploc ∧ increase ...
end *KuttaMerson*
5. The following sentences should be added to the initial comment of the procedure:
The values of the dependent variables at $t + h$ are placed in the array *x*. Note that the values of *t* and *first* are changed as side-effects of the procedure. (As originally written, *KuttaMerson* seemed unable to obtain the values of the solution at *t* or to transmit the values of the solution at $t + h$ to the outside program!—Ed.)
6. Change array to array in the body of the procedure.
7. Insert after own integer ploc;
own array *y0*[1:n];

Delete *y0* from the existing array declaration.

ALGORITHM 219 TOPOLOGICAL ORDERING FOR PERT NETWORKS

ROBERT H. KASE
Atlantic Refining Co., Philadelphia, Penn.

procedure *Topological Ordering* (*i, j, tri, n, ne*);
integer *n, ne*; integer array *i, j, tri*;
comment Nodal points *i* and *j* represent activities in a PERT network. *n* is the number of activities. *tri* is a tape record index

```

vector locating where additional data for each activity is stored.;
begin integer a, b; integer array ni, nj, event[1:n];
comment An event vector is set up containing ne events.
New nodal numbers ni and nj are assigned for all activities.;
ne := ni[1] := 1; event[1] := i[1];
begin for a := 2 step 1 until n do
begin for b := 1 step 1 until ne do
if i[a] = event[b] then begin ni[a] := b;
go to repeat 1 end;
end;
ni[a] := ne := ne + 1; event[ne] := i[a];
repeat 1: end;
begin for a := 1 step 1 until n do
begin for b := 1 step 1 until ne do
if j[a] = event[b] then begin nj[a] := b;
go to repeat 2 end;
end;
nj := ne := ne + 1; event[ne] := j[a];
repeat 2: end;
begin integer t, bigtal; integer array rank, con[1:ne];
comment Event ranking (topological ordering);
for a := 1 step 1 until ne do
begin rank[a] := 1; con[a] := 0 end;
bigtal := 1;
pass: t := 0;
for a := 1 step 1 until n do
begin if rank[nj[a]] ≤ rank[ni[a]] then
rank[nj[a]] := rank[ni[a]] + 1 else go to fill;
if rank[nj[a]] > bigtal then
bigtal := rank[nj[a]]; t := 1
fill: con[rank[ni[a]]] := con[rank[nj[a]]] := 1
end;
if t ≤ 0 then go to new;
for a := 1 step 1 until bigtal do
begin if con[a] = 0 then go to Loop end;
comment Loop should be a label of a procedure statement
which calls a subroutine to detect those events which may
be in a loop in the PERT network or the label of a print out
indicating that loop(s) exist in the network. In any case
a loop exists and further problem processing is impossible.;
for a := 1 step 1 until bigtal do con[a] := 0;
go to pass;
comment Reassignment of a new nodal number, ni, to all
activities;
new: t := 1;
for a := 1 step 1 until bigtal do
begin for b := 1 step 1 until ne do
if rank[b] = a then begin event[b] := t; t := t + 1 end
end;
for a := 1 step 1 until n do ni[a] := event[ni[a]]
end;
comment Using the new nodal number, ni, activities (i and j)
and their corresponding tri may now be arranged in topological
sequence with conventional sort routines. Sorting should be
done on ni.;
end

```

ALGORITHM 220

GAUSS-SEIDEL

PETER W. SHANTZ

University of Waterloo, Waterloo, Ontario, Canada

```

procedure GAUSS-SEIDEL (n, A, B, tol);
value n, tol; array A, B; real tol; integer n;
comment GAUSS-SEIDEL solves a system,  $Ax = B$ , of  $n$ 
simultaneous linear equations in  $n$  unknowns.  $A$  is the matrix of
coefficients,  $B$  an inhomogeneous vector. The standard Gauss-
Seidel iterative technique is employed until  $|x_K^{(i)} - x_K^{(i-1)}| < tol$ 
for all  $K$ , where  $x_K^{(i)}$  denotes the  $i$ th iterant of the unknown  $x_K$ .
(Cf. Ralph G. Stanton, Numerical Methods for Science and Engi-
neering, Ch. 8);
begin array X, Y[1:n]; integer i, j, K;
for i := 1 step 1 until n do X[i] := Y[i] := 0;
START: for i := 1 step 1 until n do
begin Y[i] := B[i];
for j := 1 step 1 until n do
Y[i] := if i = j then y[i] else
Y[i] - A[i, j] × Y[j];
Y[i] := Y[i]/A[i, i]
end i;
comment Now test for convergence;
for K := 1 step 1 until n do
if abs(Y[K] - X[K]) ≥ tol then
begin for i := 1 step 1 until n do
X[i] := Y[i]; go to START
end convergence test;
end GAUSS-SEIDEL

```

CERTIFICATION OF AND REMARK ON ALGORITHM 220

GAUSS-SEIDEL [P. W. Shantz, *Comm. ACM* 6 (Dec. 1963), 739]

A. P. BATSON (Recd 6 Jan. 1964)

University of Virginia, Charlottesville, Va.

NIKLAUS WIRTH (Recd 6 Jan. 1964)

Computer Science Div., Stanford U., Stanford, Calif.

[EDITOR'S NOTE. Two substantially equivalent contributions were received on the same day, and so the editor has merged them.—G.E.F.]

The following errors were detected.

1. The procedure cannot communicate the solution to the outside block unless X (or Y) is made a parameter of the procedure.
2. The identifier *GAUSS-SEIDEL* may not contain a hyphen.
3. In the fourth line after the label *START* change $y[i]$ to $Y[i]$.

With the above errors corrected, *GAUSS SEIDEL* was successfully run on the Stanford 7090 computer in Wirth's Extended ALGOL, and on the Virginia ALGOL compiler for the Burroughs 205.

The following improvements would be desirable.

1. Avoid repeated reference to the subscripted variable $Y[i]$ inside the j loop.
2. Permit the user to initialize the array X to an appropriate value at the start of the iteration.
3. Modify tol to be a relative error, rather than an absolute error.
4. Incorporate a guard against nonconvergence.

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