MASTER

METHODS IN PROBABILITY AND
STATISTICAL INFERENCE

Progress Report
for Period June 15, 1975 — June 14, 1976

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ABSTRACT

I. Statistical Computing; Approximations to Statistical Tables and Functions.

David L. Wallace is developing efficient methods for approximating percentage points of the largest characteristic root of a Wishart matrix, and other statistical quantities of interest. He is also working on fitting non-additive models to two-way and higher-way tables, and the further development of the SNAP statistical computing system.

II. Numerical Computation of Boundary-Crossing Probabilities for Brownian Motion and Related Stochastic Processes.

Michael J. Wichura has implemented numerical procedures for computing boundary-crossing probabilities for Brownian motion and other stochastic processes, such as Bessel diffusions.

III. Probabilistic Methods in Statistical Mechanics.

Sandy Zabell and R. R. Bahadur have applied mathematical techniques from statistical mechanics to obtain a unified treatment of probabilities of large deviations of the sample mean, in the setting of general topological vector spaces. Zabell is studying the application of the Martin boundary to questions about infinite particle systems.

IV. Combining Independent Tests of Significance.

Michael D. Perlman and his co-author James A. Koziol have completed a comparative study of classical "omnibus" and Bayes procedures for combining several independent noncentral chi-square test statistics. Work proceeds on the related problem of combining noncentral F-tests.

V. Small-Sample Efficiencies of Tests and Estimates.

R. R. Bahadur and David L. Wallace, together with James A. Koziol, are engaged in a numerical study of the small-sample powers of the Pearson chi-square and likelihood ratio tests for multinomial goodness-of-fit. They are also studying the relationship between asymptotic (large-sample) efficiency of test statistics, as measured by Bahadur's concept of exact slope, and actual small-sample efficiency.

VI. Improved Procedures for Simultaneous Estimation and Testing of Many Correlations.

Michael D. Perlman and a graduate student S. P. Lin have developed a promising new technique for the simultaneous estimation of all correlation coefficients in a multivariate population. Their method adapts the James-Stein "shrinking" estimator (for location parameters) to the estimating of correlations.

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A. INTRODUCTION

This report describes the research activities of the Department of Statistics, University of Chicago, carried out or in progress under the auspices of ERDA Contract No. E(11-1)-2751, during the period 15 June 1975 to 14 June 1976. Six research projects are described in Part B of this report; the first five were originally proposed and described in our proposal of 19 May 1975, while the sixth was conceived during the summer of 1975. Part C contains a description of the statistical consultation activities of the Department which may be of interest to ERDA. Attention is especially directed to the series of scientific interactions between the Department and the scientists at Argonne National Laboratories. It is felt that this interaction is particularly germane to the purposes of this Contract.

Approximate percentage efforts devoted to the research projects supported by this Contract are as follows: Bahadur 10%, Perlman 20%, Wallace 25%, Wichura 25%, Zabell 20%. These percentages are expected to continue through the duration of the current term. There has been complete compliance with all requirements of the Contract.

B. RESEARCH PROGRESS REPORT: 15 June 1975 -- 14 June 1976

I. Statistical Computing; Approximations to Statistical Tables and Functions.

Investigator: David L. Wallace

- (a) Approximating percentage points of the largest characteristic root of a Wishart matrix.

Attention has been directed mainly to the distribution of the largest root of a Wishart matrix from a spherical normal sample. (Table 51 of Biometrika Tables for Statisticians, Volume II.) This two-parameter distribution is the limiting distribution for the three-parameter distribution of the first-root test in multivariate regression. Separately obtaining improved approximations to the limiting distribution and to the approach to the limit appears to be better than directly approximating the three-parameter distribution. Additionally, the first root for a spherical normal sample arises also in an important univariate fitting procedure described elsewhere in this report.

Among several approximations to the distribution of the first root for a matrix of dimension p , and degrees of freedom q , two approximations to the square root of the upper percent points are:

$$y_1(p, q) = x(p) + x(q) - x(1)$$

and

$$y_2(p, q) = y_1(p, q) - u(p)u(q)$$

where

$$u(p) = c \cdot \frac{x(p) - x(1)}{(a + x(p))}$$

$$a = \frac{6.5}{x(1)} - 2.4, \quad c = .94 - \frac{1}{x(1)}$$

and $x(p)$ denotes the square root of the percent point of chi-square on p degrees of freedom. All dependence on the probability level is

through the chi-square percent points.

The second approximation is a very good one, providing much better than .03% precision on the square root scale for a wide range of p , q , and for probability levels .95 to .995.

The first approximation is of interest as a base for building the second, and for its interpretation. As an approximation, it is no better than several others easier to use. It is simple -- apart from the choice of square root, its content is forced by the exact, elementary results for margins $p = 1$ or $q = 1$. For all probabilities more extreme than .90, y_1 is an overestimate of the true percent point. Its absolute error increases with p , with q , and with the probability level. For level .90, the approximation is quite good, with error of better than .3%, provided $\min(p, q) \leq 20$. At higher levels, the quality is poorer, with maximum percent error of .7% for .95, and increasing to 1.2% at .995.

Were the objective to develop an additive approximation, better results could be obtained for level .95 by replacing the square roots throughout by power .515 (and other powers for .99, etc.). But the square root is especially important, corresponding to the original scale of data being analyzed. In particular, the square root y of the 95% point of the first root is the required multiple of standard error of a contrast to set 95% simultaneous confidence statements on all contrasts of rank q and dimension p when the degrees of freedom for estimating standard errors is large. A useful interpretation of approximation y_1 is that the adjustment in width of confidence statement to allow for increasing the dimension p or increasing the rank q of the family of

contrasts is very nearly an additive adjustment to the critical multiplier of the standard error.

If degrees of freedom are not essentially infinite, critical values must be obtained from the null distribution of the first root θ_1 of one Wishart matrix relative to a second. Two improvements to the Marriott-Bartlett approximation

$$-n_B \ln(1 - \theta_1) \sim \chi^2(v_M)$$

are worth making. Replace the right-hand side chi-square by any superior approximation to the limiting distribution discussed above. (y_2^2 would be much superior; y_1^2 would not.) Secondly, make a second order adjustment to the Bartlett multiplier n_B to extend the applicability of the asymptotic result.

$$n_B = \frac{(p + q - c)^2}{10 n_B}$$

provides such an improvement, with $c = 1$ for 95%, $c = 2$ for 99%. This decomposition of the distribution into the part depending on the degrees of freedom and the limiting part helps to explain, if not simplify, the effect of degrees of freedom on simultaneous confidence intervals.

(b) Fitting non-additive models to two-way and higher-way tables.

Fitting two-way tables by forms like

$$\hat{y}_{ij} = a_i + b_j + \sum_{e=1}^r u_i^{(e)} v_j^{(e)}$$

with small r can be effective for precision and interpretation. Among others, Mandel (1971) and Gollob (1968) have proposed, studied, and used these techniques. Least squares fitting is just the singular value decom-

position applied to the residuals from an additive fit. Testing significance of the factor terms leads to distributions of the first few roots of central and noncentral Wishart matrices for spherical normal populations. The distribution of the simplest test statistic has been approximated by Johnson and Graybill (1972), but other distributions are open, all related to the class of distribution whose approximations are discussed elsewhere in this proposal.

If the fitting problem is modified to handle unbalanced tables or unbalanced weighted least squares or to criteria other than least squares or to multi-way tables, then the singular-value decomposition no longer provides a closed-form fitting procedure, and both computational and distributional problems are open. If a usable algorithm for fitting a factor model to minimize (unbalanced) weighted least squares and some approximations to the associated distribution theory were available, they would be directly useful. More importantly, they would provide a basis for handling outliers, non-Gaussian errors, and building a robust-fitting procedure by adopting the usual iterative reweighting techniques.

The need for robustness is likely greater here than in linear least squares, because of the sensitivity of first roots and factors to single bad values.

In extension to three-way tables, the fitting of the several two-way faces is reasonably straightforward, but the three-factor terms present new difficulties.

The overall objective is development of more effective tools for representing complex tables of data, physical measurements, mathematical

constants, to forms that are easily represented in digital computers, that are helpful in interpreting and understanding the structure of the tables, and that are potentially extrapolable to more complex situations.

(c) The SNAP statistical computing system.

Wallace's development of flexible computer systems for data analysis continued during the year. The SNAP statistical system that he has developed over the past seven years continued in heavy use at the University by students in Statistics courses, and by students and faculty doing research in theoretical statistics, sociology, physical anthropology, etc., where more flexibility and control over choice of analysis is wanted than SPSS or other packages provide. Developments during the year included incorporation of programs for maximum likelihood estimation of missing values, means and covariances in multivariate linear models, and for a variety of quantal analyses in bioassay. These illustrate the open-ended nature of the system whereby various new operations can easily be added on with the writer not required to have systems knowledge of the SNAP system. This open-endedness also enables general users with special requirements to construct private versions. The system is now usable interchangeably by batch mode or in interactive mode (through TSO). Inasmuch as the logical design of the system was inherently interactive, the conversion to the interactive mode was simple, with effort mostly concerned with the control over output at terminals as opposed to high-speed printers. Chief efforts now planned are the incorporation of enough graphic capabilities to enable users with graphics terminals incorporation of parts of the Tektronix software to enable effective graphics use in SNAP.

(d) Use of the Tektronix 4013.

The Tektronix terminal with associated hard copy unit and software packages was installed by pieces from October through February. As a character terminal, the terminal is fully usable. The graphics capability is still inactive pending completion by the University Computation Center systems programming staff of changes in their Telecommunications system to enable the transmittal to and from the Tektronix of the required full ASCII code. That change is expected to be completed by April 1976. The software packages are all ready for operation once the system change is made, and several applications programs such as to facilitate contour plotting are now being completed.

The system and programming packages have been tested on the Biomedical Computation Facility's Xerox Sigma-5 computer. The Tektronix can (and has) been used with that computer, but its size and system limitations make effective use of the Tektronix software impractical without major programming effort.

(e) Doctoral dissertations directed by David L. Wallace.

The dissertation "On Transformations of Multivariate Data" by S. G. Machado will be completed by April 1976. The dissertation "Linear Functional and Structural Relationships" by A. G. de Wet is expected to be completed by November 1976. Abstracts of these studies were included in the proposal of 19 May 1975.

References

Gollob, H. F. (1968). "A statistical model which combines features of factor analytic and analysis of variance techniques," Psychometrika 33, 73-116.

Johnson, D. E. and Graybill, F. A. (1972). "An analysis of a two-way model with interactions and no replications," J. Amer. Statist. Assoc. 67, 862-868.

Mandel, J. (1971). "A new analysis of variance table for non-additive data," Technometrics 13, 1-18.

II. Numerical Computation of Boundary-Crossing Probabilities for Brownian Motion and Related Stochastic Processes.

Investigator: Michael J. Wichura

The "Anderssen-deHoog-Weiss" computational procedure for boundary-crossing probabilities for Brownian motion and Brownian bridge, as mentioned in the May 1975 proposal, has been implemented and is working properly. At present, emphasis is being placed on developing flexible input and output procedures, which will allow the user considerable freedom in setting up the problem and outputting the results of the computation. For example, in a single run the user will be able to reference several parametrized families of moving boundaries. The output routines will allow the user to determine the amount of information printed and to store results for future analysis, such as display on the Tektronix 4013 Graphics and Display Terminal.

Upon completion (in the near future) of these input/output routines, a technical report will be prepared describing the operation and use of the program. Several members of the University community have expressed interest in utilizing the program in their own research. For example, Professor Luigi Ricciardi of the Department of Biophysics and Mathematical Biology intends to use the program to study a first passage problem involving the Ornstein-Uhlenbeck process (which is easily transformed into Brownian Motion).

The program has been written in such a way that extensions to other stochastic processes, such as Bessel diffusions, can be carried out fairly easily. We propose to make such extensions, as well as to study ways of

improving the efficiency of the computation, as discussed in the original proposal.

III. Probabilistic Methods in Statistical Mechanics.

Investigators: R. R. Bahadur and Sandy Zabell

As the first phase in his program of investigating interconnections between probability theory and statistical mechanics, Zabell is working with R. R. Bahadur on applying techniques from statistical mechanics (developed by O. Lanford [2]) to the theory of large deviations, a field of interest to both mathematical statisticians and probabilists. Results obtained so far substantially extend work of Sanov [3] and Hoadley [1], as well as considerably shorten the proofs in the literature. A technical report in preparation describes results so far obtained.

Zabell is also investigating the application of the Martin boundary, a tool in the theory of Markov chains, to questions about infinite particle systems; this work is still in the exploratory stage.

References

- [1] Hoadley, A. B. (1967). "On the probability of large deviations of functions of several empirical c.d.f.'s." Ann. Math. Statist. 38, 360-381.
- [2] Lanford, O. E. (1971). "Entropy and equilibrium states in classical statistical mechanics." Lecture Notes in Physics: Statistical Mechanics and Mathematical Problems, J. Ehlers et al., eds. (Berlin: Springer Verlag), pp. 1-113.
- [3] Sanov, I. N. (1957). "On the probability of large deviations of random variables." (Russian) Mat. Sbornik (N.S.), 42, 11-44; English translation in Select. Transl. Math. Statist. Prob., 1 (1961), 213-244.

IV. Combining Independent Tests of Significance.

Investigators: James A. Koziol and Michael D. Perlman

Koziol and Perlman have recently completed an extensive study ("Combining independent chi-square tests," Technical Report No. 19) of procedures for combining independent noncentral chi-square statistics. Among the main findings are the following. First, if no prior information is available to the statistician concerning the relative sensitivities of the test statistics to be combined, then Fisher's omnibus procedure is preferable to all competitors on minimax grounds, provided that the degrees of freedom of each chi-square statistic exceeds one. If each degree of freedom is one, then the simple sum test is preferable. Second, when prior information is available about the relative magnitudes of the noncentrality parameters expected if the null hypothesis is false, weighted linear combinations of the chi-square statistics are proposed and accurate approximations to their null distributions are presented. These linear combinations are obtained as Bayes test statistics for gamma prior distributions selected to approximate the prior information. (If all degrees of freedom are one, however, weighted Fisher procedures are found to incorporate the prior information more effectively.) Both numerical integration by quadrature and Monte Carlo have been used to evaluate the power functions of combination procedures under consideration. This work has been submitted for publication.

Koziol and Perlman are currently engaged in a study of the more complex problem of combining independent noncentral F-statistics, such as arise in the Analysis of Variance (ANOVA). As in the chi-square problem, they will consider two situations, where prior information is either absent or present.

For the latter situation they have constructed families of prior distributions richer than the gamma family, in order to approximate prior information about the several noncentrality parameters as closely as possible. Therefore, several different classes of Bayes statistics have been derived, and their power functions must be compared numerically to those of the standard "omnibus" procedures such as Fisher's. Some computation has been carried out, and more will be required.

V. Small-Sample Efficiencies of Tests and Estimates.

Investigators: R. R. Bahadur, James A. Koziol, and David L. Wallace.

The first topic under study under this heading is a comparison of the small-sample powers of the Pearson chi-square and likelihood ratio statistics for testing multinomial goodness-of-fit. Active investigation of this problem, which will require extensive numerical computation, will begin in May 1976 and will be carried forward during June and July when James Koziol will be in residence at the Department of Statistics.

A second topic under this heading concerns the relationship between the asymptotic and actual small-sample efficiency of a given test statistic. One way of defining the asymptotic efficiency of a test statistic is in terms of its stochastic exact slope [cf. Bahadur (1971)]. The problem of just how close this is to the actual stochastic efficiency in samples of a finite size involves difficult mathematical problems, but is amenable to computer-simulation studies. Bahadur has done some preliminary work on these questions for his 1974 Wald lectures and plans to do more. The particular statistics he is studying are the usual t-test or mean-test for a univariate normal mean versus the sign test for the same problem. The

t-test or mean-test is superior on all counts, but it is not known how soon the exact slope efficiency of the sign test becomes a reliable

numeric value $\left[\begin{array}{ll} \doteq 64\% & \text{near } \frac{\mu}{\sigma} \doteq 0; \\ \doteq 60\% & \text{for } \frac{\mu}{\sigma} = 0.5 \end{array} \right]$ as the sample size increases.

References

Bahadur, R. R. (1971). Some Limit Theorems in Statistics. NSF-CBMS Monograph, No. 4, (SIAM).

VI. Improved Procedures for Simultaneous Estimation and Testing of Many Correlations.

Investigator: Michael D. Perlman

This is a new project, not having been included in the original proposal of 19 May 1975. The problem of simultaneously estimating all correlations among the components of a multivariate population is extremely important, yet difficult if the dimension is not small and if accurate estimates are required. The reason for this is quite simple: if the multivariate observations are vectors of dimension p , then there are $p(p-1)/2 \doteq p^2/2$ correlations to be estimated (by contrast, there are only p means). Thus, much larger sample sizes are required to obtain accurate estimates of the population correlation matrix as compared to estimates of the population mean vector. It is customary to warn students in introductory statistics courses about the expected inaccuracies of estimates of correlations, especially if the dimension p is large and the sample size n is not. In particular, estimates of correlation coefficients are often too large in magnitude.

Therefore, it would seem essential to develop improved techniques for obtaining simultaneous estimates of correlation coefficients. In the past twenty years, improved techniques for estimating multivariate

location parameters (e.g., the population mean vector) have been developed and studied in detail. Notable contributions to this problem have been made by Charles Stein (cf. James and Stein (1961)), Efron and Morris (1975 and earlier), and others. It has occurred to Perlman and a doctoral student S. P. Lin that these techniques might be applied to the problem of simultaneous estimation of correlation coefficients. Their idea is to reduce the latter problem to the former by applying the Fisher z-transformation to each of the $p(p-1)/2$ sample correlation coefficients. This transforms the population correlation coefficients into location parameters for large sample sizes, and does so approximately for smaller sample sizes, so that the James-Stein and Efron-Morris estimation techniques may be applied to the transformed statistics. The transformation is then reversed, yielding estimates of the population correlations. Preliminary numerical studies indicate that this method yields estimates more accurate than the maximum likelihood estimates, both for large and small sample sizes. S. P. Lin is currently carrying out an extensive numerical investigation as part of his doctoral research.

The technique just described should be expected to lead to an improved estimate (relative to the maximum likelihood estimate) of the entire covariance matrix and in particular of its characteristic roots. Charles Stein, in the 1975 Rietz Lecture presented in Atlanta to the Institute of Mathematical Statistics, presented an alternate technique for obtaining improved estimates of these population roots. As part of their investigations Lin and Perlman also plan to compare these two techniques for estimating characteristic roots.

It should be pointed out that the techniques here described have another potential application. Consider the ordinary linear regression model $Y = X\beta + e$, where X is the design matrix and β the vector of unknown regression coefficients. The ordinary least squares estimator is $\hat{\beta} = (X'X)^{-1}X'Y$. When the matrix $X'X$ is nearly singular the estimator $\hat{\beta}$ is known to be relatively unstable. Recently much attention has been paid to "ridge regression" techniques wherein $X'X$ is replaced by $X'X + kI$ for some $k > 0$, hopefully reducing this instability. Lin and Perlman speculate that their technique (and that of Stein) for estimating covariance or correlation matrices, when applied to the matrix $X'X$ or its correlation matrix, may be preferable to the ridge regression method.

References

- Efron, B. and Morris, C. (1975). "Data analysis using Stein's estimator and its generalizations." J. Amer. Statist. Assoc. 70, 311-319.
(See also the earlier papers by Efron and Morris listed therein.)
- James, W. and Stein, C. (1961). "Estimation with quadratic loss." Proc. Fourth Berk. Symp. Prob. Math. Statist., Vol. I, 361-379.

C. CONSULTATION AND COOPERATIVE RESEARCH WITH OTHER SCIENTISTS AT
THE UNIVERSITY OF CHICAGO AND ARGONNE NATIONAL LABORATORIES

Through its consultation program the Department of Statistics participates in other research projects at the University of Chicago and Argonne National Laboratories which are of interest to ERDA. Roderick Little has served as the coordinator of the consultation program during 1975-76; he will be succeeded by Alan Izenman in 1976-77. All members of the Department of Statistics, as well as its graduate students, participate in the consultation program to varying degrees. Some recent activities of the program are now described.

Consultation/Cooperative Research at the University of Chicago

1. Statistical Analysis of Moon Rocks. Dr. John Morgan (Department of Chemistry) brought the following problem to Rod Little for statistical advice. The proportion of various metals in rock samples collected by Apollo missions should provide information about meteoritic activity on the surface of the moon. On the basis of 74 samples, Dr. Morgan and colleagues thought that the rocks could be grouped into 6 groups or clusters, and they wanted more objective evidence that the groupings existed. Factor analysis had been tried with little success. Little rejected factor analysis and cluster analysis as unsuitable for the small sample size. With the help of graduate student Stella Machado, a principal component analysis was carried out on a selection of 38 substantial rock samples, and the rock samples plotted out in the coordinates of the first two principal components, which captured most of the variability in the measurements. The results provided a useful picture of the data, but provided very little evidence of grouping.

2. Statistical Estimation of Particle Counts from an Orbiting Spacecraft.

Mr. John Jump (Laboratory for Astrophysics and Space Research) consulted on an indirect method for counting atomic particles arriving at an orbiting space-

craft, as a substitute for a malfunctioning direct recording device. An estimated rate for the particle in question was obtained by assuming a Poisson distribution for arrivals, and Mr. Jump had been given a formula for the standard error of the estimate which he mistrusted. His doubts proved well founded, for Little's analysis, using propagation of error and the theory of conditional probability, indicated a missing term in the formula. Mr. Jump was also advised about how to analyze the data for fluctuations in the particle rates over time.

Consultation/Cooperative Research at Argonne National Laboratories

1. Visit of the Department of Statistics to Argonne: 13 January 1976. Six faculty members and seven graduate students from the Department of Statistics visited Argonne on 13 January 1976 at the invitation of Dr. James Pool, Associate Director of the Applied Mathematics Division of Argonne National Laboratories. Statistical problems arising in research projects at Argonne were presented in talks by Dr. Tom Baldwin (Energy and Environmental Systems Division), Dr. George Sacher (Biological and Medical Research Division), Dr. Stephen Spigarelli (Radiological and Environmental Research Division). These discussions were general in nature, and emphasized the need for statistical expertise in the analysis of a wide range of data. Dr. David Rasky (Material Sciences Division) presented a particular problem in some detail, and received statistical advice. A brief account of this discussion follows.

Dr. Rasky described data collected from a fatigue analysis, where a metal is subjected to repeated flexing under various physical conditions, and the number of cycles to breakage (N) recorded. The aim is to find a prediction equation for N as a function of four independent variables: T, the temperature of metal, S, the log strain range, R, the log strain rate, and H, the hold

time. From a sample of 430 observations, Dr. Rasky had fitted linear regressions of various functions of N on polynomial functions of T , S , R , and H , and had arrived at a prediction equation, expressing $\frac{1}{\log_{10} N}$ as a linear function of 18 polynomials in T , S , R , and H . The equation explained 96% of the variance of the dependent variable, and produced residuals which appeared to be normally distributed with constant variance. An evaluation of his procedure was requested.

Professor David L. Wallace criticized the choice $\frac{1}{\log_{10} N}$ for the dependent variable for its lack of physical meaning, and advocated a transformation such as the rate $1/N$, which is more easily interpretable. He was also worried by the complexity of the final equation, and suggested the following principles for fitting equations: (a) the use of orthogonal polynomials, (b) the inclusion of all lower order terms of a variable for which a high order term is included, (c) the retention only of terms which improve the fit significantly. In this example 93% of the variation was explained by an equation with just three terms, which was considered adequate. In addition, the reasons for transformations were discussed, and Professors Haberman and Izenman commented further on when interactions can be estimated satisfactorily, and on checking whether the fit was in accord with metallurgical principles. Dr. Rasky discussed these points in more detail over lunch, and was interested in further collaboration in the future.

2. Visit of Drs. James Pool, James Lyness, and party to Department of Statistics, University of Chicago: 18 February 1976. A party of four from the Argonne Applied Mathematics Division visited the Statistics Department of the University of Chicago on 18 February 1976. In the morning, Dr. James Lyness gave a consulting seminar entitled "Evaluating Quadrature Routines." The

performance profile of various automatic quadrature routines were compared over a family $f(\lambda)$ of integrands, for a suitable range of the parameter λ . The family $f(\lambda)$ was chosen so that the integrals could be evaluated analytically, and the attained accuracy $\epsilon_{\text{act}}(\lambda, \epsilon_{\text{req}})$ measured as the deviation of the calculated value from the true value of the integral. The parameter ϵ_{req} is a required accuracy, a parameter read into the routine. Also measured was $v(\lambda, \epsilon_{\text{req}})$, the number of function evaluations, a measure of the cost of the integration.

The performance profile of a given routine is $\epsilon_{\text{act}}(\lambda, \epsilon_{\text{req}})$ as a function of λ for fixed ϵ_{req} . Since for automatic routines this often has a profile "like the Chicago skyline," comparisons of routines are highly dependent on the value of λ chosen. Thus large numbers of λ in the given range are generated by a random number generator, and the random variables $\epsilon_{\text{act}}(u, \epsilon_{\text{req}})$ and $v(u, \epsilon_{\text{req}})$ studied, where u is a uniform variable over the range of λ .

Dr. Lyness had found that 5-10% of the time an automatic routine can fail, in the sense that ϵ_{act} was much larger than the required accuracy ϵ_{req} . He presented ways of calibrating ϵ_{req} to be 90% sure that ϵ_{act} is less than a given accuracy, ϵ_0 . He also estimated the mean number of function evaluations, $\bar{v}_{.90}(\epsilon_0)$, required at the calibrated value of ϵ_{req} . This was used to compare the performance of different quadrature routines on the given problem.

Dr. Lyness' talk stimulated a lively discussion over a period of two hours, straddled by lunch at the Quadrangle Club. Active participation for the Department of Statistics included Professors Wallace, Little, Haberman, Izenman, Wichura, Zabell, and Perlman. Among the points discussed were the following:

(a) An economical presentation of the data, in view of the apparently Gaussian nature of the distribution of $\epsilon_{\text{act}}(u, \epsilon_{\text{req}})$; (b) further study of ϵ_{act} and v as joint random variables, for example, by plots of ϵ_{act} against v to

explore dependence, possibly leading to other measures such as $\epsilon_{\text{act}}/\nu$, the attained accuracy per function evaluation. (c) The use of the statistical theory of estimating a distribution function to suggest the number of λ -values needed to estimate the distribution of ϵ_{act} to a given accuracy.

The discussion was stimulating to both sides. Dr. Lyness appreciated the interest shown in the problem, and the statisticians learned about some of the problems of numerical integration when function evaluation is very expensive. In particular, Professor Michael Wichura presented Dr. Lyness with a spiky curve and received advice about how best to find the area beneath it. Thus the consultation cut both ways, and future meetings are anticipated.

* * * * *

As the above discussion indicates, scientific interaction between the Department of Statistics and scientists at Argonne National Laboratories can be extremely fruitful for both groups. We consider this interaction to comprise a major activity under ERDA Contract No. E(11-1)-2751 and desire to continue and expand this activity in subsequent years. A letter from Dr. James Pool of Argonne, which reflects the mutuality of this desire, follows immediately.

ARGONNE NATIONAL LABORATORY

January 19, 1976

Professor Michael Perlman
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Dear Professor Perlman:

The visit to Argonne on Tuesday, January 13 of faculty members and students from the Department of Statistics of the University of Chicago represents, I believe, a significant milestone in our investigation of the potential role of an "Applied Statistics Program" in the Applied Mathematics Division. The review of activities in the various Argonne divisions, indeed, identified several new areas where expertise in statistics can contribute. More importantly, a spectrum of applicable statistical techniques is beginning to emerge.

While I anticipate that several topics could lead to mutually beneficial collaboration, I feel we should initially concentrate on a limited spectrum of problems. With this approach, we can demonstrate more definitively the impact of an enhanced level of statistical expertise at Argonne. Based upon our discussions, I anticipate that, for example, the two priority areas should be discussions of the examination of the fatigue testing problem of Argonne's Materials Science Division and the statistical analysis of numerical software performance, an activity of the Research Program in AMD. I understand that two members of the Materials Science Division will be contacting Rod Little. I would like to reschedule our tentative date for discussing the performance of numerical software from February 11 to February 18, since two of the primary Argonne participants will not be available on February 11.

I would particularly like to pursue further the feasibility of a joint appointment between the Department of Statistics at the University and the Applied Mathematics Division at the Laboratory. While there are, of course, the problems we discussed, I feel that this venture would yield significant benefits to both organizations. I will examine examples of existing joint appointments and would like to discuss this possibility further with you February 18.

Professor Michael Perlman

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January 19, 1976

We will continue our examination of the basis, both financially and technically, for establishing an "Applied Statistics Group" in AMD during the next month. Consequently, any additional comments will be welcomed.

Please call me if February 18 is an inconvenient date for us to visit the University.

Sincerely,

James C. T. Pool
Associate Director
Applied Mathematics Division

JCTP:dmp

cc: R. G. Sachs, OTD/ANL
R. J. Royston, AMD/ANL

D. TECHNICAL REPORTS PREPARED OR IN PREPARATION UNDER FULL OR
PARTIAL ERDA SUPPORT: 15 June 1975 - 14 June 1976

CURRENT FACULTY

R. R. Bahadur

"Some aspects of estimation." In preparation.

"Large deviation probabilities concerning Markov chains." In preparation.

"Asymptotic efficiency of estimates of the parameters of a Markov chain." In preparation.

"Large deviation probabilities of randomly stopped means." In preparation.

"A simple proof of Sanov's theorem." (With Sandy Zabell). In preparation.

"The asymptotic variance of functions of the transition counts for a Markov chain." In preparation.

"Small-sample efficiencies of the Pearson chi-square and likelihood ratio tests for multinomial goodness-of-fit." (With James A. Koziol and David L. Wallace). In preparation.

Michael D. Perlman

"Combining independent chi-square tests." (With James A. Koziol). Technical Report No. 19.

"Combining independent non-central F-tests." (With James A. Koziol and U. Rasmussen). In preparation.

"A simple procedure for testing equality of correlation matrices." (With Kinley Larntz). In preparation.

"Estimation of a covariance matrix with a general quadratic loss function." In preparation.

"Invariant tests for means in the presence of covariates." (With John Marden). In preparation.

"A note on the matrix-variate F distribution." Technical Report No. 20.

David L. Wallace

"Pearson curves as asymptotic approximations." In preparation.

"Analytic approximations to distributions of largest eigenvalues." In preparation.

"Small-sample efficiencies of the Pearson chi-square and likelihood ratio tests for multinomial goodness-of-fit." (With R. R. Bahadur and James A. Koziol). In preparation.

Michael J. Wichura

"Functional laws of the iterated logarithm for the large values of the partial sums of iid random variables in the domain of attraction of a stable law." In preparation.

"Boundary-crossing probabilities for extremal processes." In preparation.

"Boundary-crossing probabilities associated with Chung's law of the iterated logarithm." In preparation.

"Asymptotic boundary-crossing probabilities for Bessel diffusions." In preparation.

"Another general form of the so-called law of the iterated logarithm." In preparation.

Sandy Zabell

"A limit theorem for conditional expectations." In preparation.

"A simple proof of Sanov's theorem." (With R. R. Bahadur). In preparation.

DOCTORAL DISSERTATIONS

S. P. Lin (Research Advisor: Michael D. Perlman)

"Improved procedures for the estimation of correlation matrices." (Completion expected September, 1976).

S. G. Machado (Research Advisor: David L. Wallace)

"On transformations of multivariate data." (Completion expected April, 1976).

A. G. de Wet (Research Advisor: David L. Wallace)

"Linear functional and structural relationships."
(Completion expected November, 1976).