LA-2367 Addenda
MATHEMATICS AND COMPUTERS
TID-4500 (18th Ed.)

LOS ALAMOS SCIENTIFIC LABORATORY
OF THE UNIVERSITY OF CALIFORNIA LOS ALAMOS NEW MEXICO

REPORT WRITTEN: November 1, 1962

REPORT DISTRIBUTED: January 14, 1963

**THE SOLUTION OF THE GENERAL LEAST SQUARES PROBLEM
WITH SPECIAL REFERENCE TO HIGH-SPEED COMPUTERS***

by

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*This report extends and revises LA-2367.

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Contract W-7405-ENG. 36 with the U. S. Atomic Energy Commission

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1. INTRODUCTION

During the past few years, several important changes have been incorporated in the Los Alamos non-linear least squares program. The purpose of this exposition is twofold: (1) to outline these changes, (2) to present a condensed guide for the data card arrangement.

It should be noted that the general "package" is now labeled PAKAG, the present form of the code is written in FORTRAN language for the IBM-7090, and the Stromberg Carlson 4020 plotter is used for the plot output option. Attachment 1 is the tape arrangement of the monitor system which the Laboratory uses.

2. GENERAL OBJECTIVE OF "PAKAG" CODE

The system to be described "fits" (in the sense of least squares) a given function to a given data set. The function to be fitted can be any "well-behaved" mathematical function for which the derivatives exist and for which the data set does not give rise to points of singularity. By supplying the correct function and its respective derivatives (in the form of a subroutine), the user will find the function parameters which best fit the data.

3. THE DECK AND OPERATING PROCEDURE

3.1 General

The "package" concept is used. There is now one basic package with

the following capacities: 5 or fewer independent variables, 1000 or fewer data points, 40 or fewer parameters.

3.2 Binary Deck

The package contains all necessary subroutines except for the particular subroutine (called YP subroutine) which defines the function and its parameters. Thus one must add this routine in order to run.

3.3 Procurement of YP Subroutine

Many of the more common functions are permanently filed in the statistical section (in binary form). Any new function must be compiled to generate a binary deck for this subroutine. Report LA-2367 (pp. 49-54) tells how to accomplish this. On the LASL's IBM-7090, one merely uses the load-and-go feature.

3.4 Control and Data Cards

Attachment 2 is a detailed example of how a set of control and data cards would be made up.

3.4.1 Control Cards

3.4.1.1 ID Card

- a. Col. #1: must contain a 1.
- b. Col. #2-72: contains any Hollerith statement desired.

3.4.1.2 Point Control and Parameter Card. (All input values fixed point integers, I3 format.)

- a. Col. #1-3: No. of data points to be loaded.
- b. Col. #4-6: No. of parameters to be used.
- c. Col. #7-9: Weighting options as follows:

0 = unity weights.

1 = weights included as additional data.

2 = weight = reciprocal of the dependent variable ($w_i = 1/y_i$).

3 = causes code to solve different problem, namely, minimizes percentage error rather than usual procedure; that is,

$$\phi = \sum_{i=1}^n \left[\frac{y_i - y_i'}{y_i} \right]^2$$

is minimized, where

y_i = dependent variable

y_i' = corresponding value on fitted curve.

It should be strongly emphasized that this procedure is not recommended since the rest of the code computes parameter errors, etc., based on the conventional least squares model. Thus using this option is a user's risk situation.

- d. Col. #10-12: denotes number of independent variables. If only 1 independent variable, may be left blank.
- e. Col. #13-15: If = 0, denotes block loading of data. If = 1, denotes point-wise loading of data.
- f. Col. #16-18: If = 0, the test convergent value (see LA-2367, p. 44) will be 10^{-6} . If $\neq 0$, the user will supply the desired convergent value on a later card (see 3.4.5).
- g. Col. #19-21: A control number that determines if values for the variable DUM are not required (=0), or if they are to be loaded from cards ($\neq 0$).
- h. Col. #22-24: If Col. #19-21 $\neq 0$, Col. #22-24 indicates how many values of DUM are to be loaded.
- i. Col. #25-27: If = 0, the program iterations and final matrices are not printed on tape 9. If $\neq 0$, iterations and matrices are printed.

- j. Col. #28-30: Control of algebraic sign of the parameter set. The following options prevail:
 - 0 = does not allow the sign of any parameter to change for 5 iterations; then sign changes are permissible for remaining iterations.
 - 1 = signs always free to change.
 - 2 = signs never free to change.
- k. Col. #31-33: The 4020 plotter is available to put out a graph of the input data and the fitted function. The following options govern this:
 - 0 = no plot output.
 - 1 = plot output with the program determining plot limits. A few comments in regard to limits: The only guarantee for the internal mechanical method is that the resulting graph will use at least 50 per cent of the area, usually more. This saves the user the trouble of generating potential limits of both points and fitted function.
 - 2 = plot output with user determining limits.
 - 3 = plot output, semi-log or log-log. If plot options 1 to 3 are used, there is a set of plot control cards incorporated in the data deck (see 3.4.3).
- l. Col. #34-36: If either the x or y values are identical in the first 3 digits, the graph needs to be scaled to give a meaningful plot. Thus,
 - 0 = no scale factors used.
 - 1 = scale factors to be used. If so, a scale card is also incorporated (see 3.4.4).

3.4.1.3 Parameters Fixed Card. Of the parameters to be used, a subset may be held fixed. This card particularizes the subset. If no parameters are to be held fixed, place a blank card here. (All input values are fixed point integers.)

- a. Col. #1-3: number of parameters held fixed.

- b. Col. #4-6: index number of 1st parameter held fixed.
- c. Col. #7-9: index number of 2nd parameter held fixed.
- d. Col. #10-12: etc.

3.4.1.4 Parameter Initial Estimate Cards. These are the initial estimates of the parameters to be fitted. There are 6 entries per card, format E12.7. There is quite naturally a 1-to-1 correspondence between the order of parameters and the parameter estimation.

3.4.2 Data Cards.

Punch up to 6 entries per card, format E12.7.

3.4.2.1 Block Loading of Data

- a. If Col. #13-15 of Point Control and Parameter Card (see 3.4.1.2e) = 0, data are entered in blocks as follows:
 block #1: $Y(1), Y(2), \dots$, punched consecutively on cards until $Y(N)$ is read.
 block #2: $X(1,1), X(1,2), \dots$, punched consecutively until $X(1,N)$ is read.
 block #3: $X(2,1), X(2,2), \dots$, punched consecutively until $X(2,N)$ is read.
 etc., for all independent variables.
- b. If Col. #7-9 of Point Control and Parameter Card (see 3.4.1.2c) = 1, then a block of weight values are now included.

3.4.2.2 Point-wise Loading of Data. If the Point Control and Parameter Card indicates pointwise loading (see 3.4.1.2e), the data are loaded as follows: $Y(I), X(1,I), X(2,I), \dots, X(M,I), W(I)$. (On the I th card) where M = number of independent parameters, and $I = 1, 2, \dots, N$, where N is total number of points. Again, if weights are not put in, $W(I)$ may be blank.

Then all weights will be internally set equal to 1.0.

3.4.3 Plot Control Cards.

Use only if Col. #31-33 of control card 2 $\neq$ 0.

Plot Card (1): Label card for y-axis. Uses 1st 36 columns only.

Plot Card (2): Label card for x-axis. Uses 1st 36 columns only.

Plot Card (3): Label card for data set. Uses 72 columns; writes this message below x-axis.

Use Plot Card 4 only if plot option = 2 or 3.

Plot Card (4): Limit card, format 4E12.7, 2I12, with

- a. Col. #1-12: X minimum
- b. Col. #13-24: X maximum
- c. Col. #25-36: Y minimum
- d. Col. #37-48: Y maximum

Use e and d only if plot option is for semi-log or log-log, i.e., = 3.

- e. Col. #59-60:
 - (1) 10 or fewer insures linear coordinate on x-axis
 - (2) 11 or greater insures log coordinate on x-axis
- f. Col. #71-72:
 - (1) 10 or fewer insures linear coordinate on y-axis
 - (2) 11 or greater insures log coordinate on y-axis

See attachment 3 for exact coordinate assignment.

3.4.4 Scale Factor Card

Use only if Col. #34-36 of control card 2 $\neq$ 0. Format is 4E12.7 with the following entries

- Col. #1-12: X factor
- Col. #13-24: X constant

Col. #25-36: Y factor

Col. #37-48: Y constant

where $x_{\text{plotted}} = x_{\text{input}} \cdot \text{XFACTOR} + \text{XCONSTANT}$

$y_{\text{plotted}} = y_{\text{input}} \cdot \text{YFACTOR} + \text{YCONSTANT}.$

3.4.5 Synopsis of Card Ordering.

In order to simplify the forementioned, the following card ordering constitutes a useable data set:

1. ID Card	ref. 3.4.1.1
2. Point Control and Parameter Card	ref. 3.4.1.2
3. Parameters Fixed Card	ref. 3.4.1.3
4. Parameter Initial Estimate Cards	ref. 3.4.1.4
5. Data Cards	ref. 3.4.2
**6. DUM Cards	ref. 3.4.1.2g, 3.4.1.2h
**7. Test Card	ref. 3.4.1.2f
**8. Plot Control Cards	ref. 3.4.3
**9. Scale Factor Card	ref. 3.4.4

**these cards are optional, governed by control card 2.

3.5 Output.

An example of the off-line output may be found in LA-2367, pp. 88-89. The fitted parameters, input and fitted values for the data points, deviations between y input and y calculated, plus other pertinent facts are listed. Attachment 4 is an example of the 4020 output.

Attachment 1

7090 TAPE ARRANGEMENT

For On-Line Operation

<u>Unit No.</u>	<u>Logical No.</u>	<u>Function</u>	<u>Remarks</u>
A1	1	System Tape	X
A2	10	Input Tape	X
A3	9	Output Tape	X
A4	4	Compiling Tape	Y
A5	2	Always available	-
A6	7	Always available	-
B1	5	Temporary System Tape	X
B2	6	Compiling and dump	Y
B3	3	Compiling	Y
B4	11	Binary Output	X
B5	12	4020 Output	X
B6	8	Always available	-

X = Never available to the problem programmer.

Y = Available when not using specified function.

Attachment 2

Suppose the given data set is as follows:

<u>x</u>	<u>y</u>
0	100.0
1	64.0
2	45.5
3	33.5
4	27.0
5	22.2
6	18.7
.	.
.	.
.	.
60	.035

The desired function is $y = P_1 e^{P_2 x} + P_3 e^{P_4 x}$.

The following attachments show the exact preparation of the data sheet, an explanatory output listing, and finally a plot of the results.

ATTACHMENT 2A

704 LA S 080																								PAGE		OF			
PROGRAMMER												PROBLEM												DATE					
1	6	7	12	13	18	19	24	25	30	31	36	37	42	43	48	49	54	55	60	61	66	67	72	73	80				
1																								CONTROL					
EXAMPLE- SUM OF 3 EXPONENTIALS FOR BIOLOGICAL RETENTION DATA																								CARD #1					
28 6 1 1 1																								CONTROL					
0																								CARD #2					
216 +01-105 -01 46 +01-289 -01 324 +01-13 +00																								CONTROL					
1 +02 0 +00																								CARD #3					
64 +01 1 +00																								CONTROL					
455 +01 2 +00																								CARD #4					
335 +01 3 +00																								1ST DATA PT					
27 +01 4 +00																								2ND "					
222 +01 5 +00																								3RD "					
187 +01 6 +00																								4TH "					
:																								5TH "					
:																								6TH "					
:																								7TH "					
35 -02 6 +01																								28TH "					
PERCENT RETENTION																								1ST PLOT CARD					
DAYS AFTER ADMINISTRATION																								2ND "					
ATTACHMENT 4 CS 184 MICE IP 10 A 56 BIOL RET WBODY 2207 LASAC																								3RD "					
THE ABOVE ILLUSTRATES THE POINT-LOADING OPTION-BY ELIMINATION THE PUNCH																													
IN COL 15 OF CONTROL CARD 2, THE DATA MAY NOW BE BLOCK LOADED, I. E.,																													
1 +02 64 +01 455 +01 335 +01 27 +01 222 +01																								BLOCK OF					
187 +01 ETC.																								Y'S					
0 +00 1 +00 2 +00 3 +00 4 +00 5 +00																								BLOCK OF					
6 +00 ETC.																								X'S					

EXAMPLE SUM OF 3 EXPONENTIALS FOR BIOLOGICAL RETENTION DATA

Attachment 2B

TEST = 1.0000000E-06

WEIGHTED SUM OF
SQUARES OF DEVIATIONS = $\sum_1 v_i (y_{input_i} - y_{calculated_i})^2$

Where y_{cal} = y value in equation
using (i-1)st parameters

* 1	1.0000000E 00**	1.9267972E 01	1.4669009E 01	-6.9309910E 00
1	2.1600000E 01	2.1600000E 01	-9.4030261E-02	1.0969737E-02
2	-1.0500000E-01	-1.0500000E-01	4.6640286E 01	6.4028738E-01
3	4.6000000E 01	4.6000000E 01	-2.5992333E-01	2.9076666E-02
4	-2.8900000E-01	-2.8900000E-01	3.8673824E 01	6.2738249E 00
5	3.2399999E 01	3.2399999E 01	-7.5193275E-01	6.3306723E-01
6	-1.3850000E 00	-1.3850000E 00		
* 2	1.0000000E 00**	3.3722128E 01	1.1408817E 01	-3.2601915E 00
1	2.1600000E 01	1.4669009E 01	-8.4896424E-02	9.1338369E-03
2	-1.0500000E-01	-9.4030261E-02	4.3346282E 01	-3.2940035E 00
3	4.6000000E 01	4.6640286E 01	-2.2564235E-01	3.4280972E-02
4	-2.8900000E-01	-2.5992333E-01	4.5249330E 01	6.5755062E 00
5	3.2399999E 01	3.8673824E 01	-8.8566275E-01	-1.3373000E-01
6	-1.3850000E 00	-7.5193275E-01		
* 3	1.0000000E 00	1.5585438E 00	1.1655778E 01	2.4696047E-01
1	2.1600000E 01	1.1408817E 01	-8.5527943E-02	-6.3151886E-04
2	-1.0500000E-01	-8.4896424E-02	4.2594665E 01	-7.5161759E-01
3	4.6000000E 01	4.3346282E 01	-2.2599820E-01	-3.5584615E-04
4	-2.8900000E-01	-2.2564235E-01	4.5752466E 01	5.0313691E-01
5	3.2399999E 01	4.5249330E 01	-8.5860084E-01	2.7061901E-02
6	-1.3850000E 00	-8.8566275E-01		
* 4	1.0000000E 00	1.4027479E 00	1.1708589E 01	5.2811567E-02
1	2.1600000E 01	1.1655778E 01	-8.5645957E-02	-1.1801506E-04
2	-1.0500000E-01	-8.5527943E-02	4.2576291E 01	-1.8373293E-02
3	4.6000000E 01	4.2594665E 01	-2.2636159E-01	-3.6338760E-04
4	-2.8900000E-01	-2.2599820E-01	4.5719708E 01	-3.2757931E-02
5	3.2399999E 01	4.5752466E 01	-8.5984286E-01	-1.2420208E-03
6	-1.3850000E 00	-8.5860084E-01		
* 5	1.0000000E 00	1.4019550E 00	1.1679834E 01	-2.8755139E-02
1	2.1600000E 01	1.1708589E 01	-8.5568656E-02	7.7300985E-05
2	-1.0500000E-01	-8.5645957E-02	4.2586395E 01	1.0103317E-02
3	4.6000000E 01	4.2576291E 01	-2.2619366E-01	1.6792280E-04
4	-2.8900000E-01	-2.2636159E-01	4.5738229E 01	1.8521631E-02
5	3.2399999E 01	4.5719708E 01	-8.5961703E-01	2.2582574E-04
6	-1.3850000E 00	-8.5984286E-01		
* 6	1.0000000E 00	1.4019547E 00	1.1692722E 01	1.2887760E-02
1	2.1600000E 01	1.1679834E 01	-8.5603749E-02	-3.5093512E-05
2	-1.0500000E-01	-8.5568656E-02	4.2580993E 01	-5.4010514E-03
3	4.6000000E 01	4.2586395E 01	-2.2626584E-01	-7.2180488E-05
4	-2.8900000E-01	-2.2619366E-01	4.5730783E 01	-7.4462360E-03
5	3.2399999E 01	4.5738229E 01	-8.5970438E-01	-8.7347192E-05
6	-1.3850000E 00	-8.5961703E-01		
* 7	1.0000000E 00	1.4019544E 00	1.1687107E 01	-5.6147220E-03
1	2.1600000E 01	1.1692722E 01	-8.5588399E-02	1.5349114E-05
2	-1.0500000E-01	-8.5603749E-02	4.2583388E 01	2.3951284E-03
3	4.6000000E 01	4.2580993E 01	-2.2623459E-01	3.1254367E-05
4	-2.8900000E-01	-2.2626584E-01	4.5733986E 01	3.2032581E-03
5	3.2399999E 01	4.5730783E 01	-8.5966700E-01	3.7369696E-05
6	-1.3850000E 00	-8.5970438E-01		
* 8	1.0000000E 00	1.4019543E 00	1.1689558E 01	2.4511581E-03
1	2.1600000E 01	1.1687107E 01	-8.5595094E-02	-6.6948187E-06
2	-1.0500000E-01	-8.5588399E-02	4.2582341E 01	-1.0458696E-03
3	4.6000000E 01	4.2583388E 01	-2.2624823E-01	-1.3647393E-05
4	-2.8900000E-01	-2.2623459E-01	4.5732588E 01	-1.3972096E-03
5	3.2399999E 01	4.5733986E 01	-8.5968330E-01	-1.6301254E-05
6	-1.3850000E 00	-8.5966700E-01		
* 9	1.0000000E 00	1.4019544E 00	1.1688493E 01	-1.0650109E-03
1	2.1600000E 01	1.1689558E 01		

Δ PARAMETER FOR THIS ITERATION CORRECTION FACTOR.
ΔP = FINAL CORRECTION TO BE APPLIED, THIS ITERATION.

** = MULTIPLICATION CORRECTION FACTOR: IF=1.0,
FULL CORRECTION APPLIED; IF < 1, ONE OR MORE
PARAMETERS ARE TRYING TO CHANGE SIGN.

* = ITERATION NO. e.g., 1st, 2nd, etc.

2	-1.0500000E-01	-8.5595094E-02	-8.5592182E-02	2.9117303E-06
3	4.6000000E 01	4.2582341E 01	4.2582799E 01	4.5756370E-04
4	-2.8900000E-01	-2.2624823E-01	-2.2624232E-01	5.9166047E-06
5	3.2399999E 01	4.5732588E 01	4.5733193E 01	6.0467774E-04
6	-1.3850000E 00	-8.5968330E-01	-8.5967628E-01	7.0232318E-06
10	1.0000000E 00	1.4019543E 00		
1	2.1600000E 01	1.1688493E 01	1.1688950E 01	4.5735790E-04
2	-1.0500000E-01	-8.5592182E-02	-8.5593435E-02	-1.2530362E-06
3	4.6000000E 01	4.2582799E 01	4.2582599E 01	-2.0007550E-04
4	-2.8900000E-01	-2.2624232E-01	-2.2624484E-01	-2.5271201E-06
5	3.2399999E 01	4.5733193E 01	4.5732938E 01	-2.5477884E-04
6	-1.3850000E 00	-8.5967628E-01	-8.5967926E-01	-2.9864800E-06
11	1.0000000E 00	1.4019553E 00		
1	2.1600000E 01	1.1688950E 01	1.1688756E 01	-1.9419888E-04
2	-1.0500000E-01	-8.5593435E-02	-8.5592903E-02	5.3175982E-07
3	4.6000000E 01	4.2582599E 01	4.2582684E 01	8.4951038E-05
4	-2.8900000E-01	-2.2624484E-01	-2.2624377E-01	1.0720776E-06
5	3.2399999E 01	4.5732938E 01	4.5733047E 01	1.0920876E-04
6	-1.3850000E 00	-8.5967926E-01	-8.5967797E-01	1.2792522E-06
12	1.0000000E 00	1.4019542E 00		
1	2.1600000E 01	1.1688756E 01	1.1688832E 01	7.5844216E-05
2	-1.0500000E-01	-8.5592903E-02	-8.5593108E-02	-2.0495293E-07
3	4.6000000E 01	4.2582684E 01	4.2582656E 01	-2.7484237E-05
4	-2.8900000E-01	-2.2624377E-01	-2.2624421E-01	-4.3938205E-07
5	3.2399999E 01	4.5733047E 01	4.5732998E 01	-4.8182405E-05
6	-1.3850000E 00	-8.5967797E-01	-8.5967855E-01	-5.8179563E-07
13	1.0000000E 00	1.4019548E 00		
1	2.1600000E 01	1.1688832E 01	1.1688802E 01	-2.9247438E-05
2	-1.0500000E-01	-8.5593108E-02	-8.5593030E-02	7.7121812E-08
3	4.6000000E 01	4.2582656E 01	4.2582662E 01	6.6157877E-06
4	-2.8900000E-01	-2.2624421E-01	-2.2624402E-01	1.8274569E-07
5	3.2399999E 01	4.5732998E 01	4.5733021E 01	2.2723447E-05
6	-1.3850000E 00	-8.5967855E-01	-8.5967823E-01	3.1325922E-07
14	1.0000000E 00	1.4019541E 00		
1	2.1600000E 01	1.1688802E 01	1.1688814E 01	1.2070688E-05
2	-1.0500000E-01	-8.5593030E-02	-8.5593061E-02	-3.1605141E-08
3	4.6000000E 01	4.2582662E 01	4.2582660E 01	-1.9394236E-06
4	-2.8900000E-01	-2.2624402E-01	-2.2624410E-01	-7.8104361E-08
5	3.2399999E 01	4.5733021E 01	4.5733012E 01	-9.0232048E-06
6	-1.3850000E 00	-8.5967823E-01	-8.5967838E-01	-1.4489456E-07
15	1.0000000E 00	1.4019546E 00		
1	2.1600000E 01	1.1688814E 01	1.1688822E 01	7.3802211E-06
2	-1.0500000E-01	-8.5593061E-02	-8.5593083E-02	-2.1635727E-08
3	4.6000000E 01	4.2582660E 01	4.2582657E 01	-2.7649789E-06
4	-2.8900000E-01	-2.2624410E-01	-2.2624414E-01	-4.0085776E-08
5	3.2399999E 01	4.5733012E 01	4.5733008E 01	-3.5226707E-06
6	-1.3850000E 00	-8.5967838E-01	-8.5967845E-01	-7.7703936E-08

PARAMETER
NUMBER

↑
INITIAL
PARAMETER
GUESSES

↑
1-1st PARAMETER
ESTIMATE

↑
1th PARAMETER
ESTIMATE

EXAMPLE SUM OF 3 EXPONENTIALS FOR BIOLOGICAL RETENTION DATA

I	A(K,L)					B(K)
1	5.4047754E 00 4.7425824E 01	2.4651628E 02	3.5664228E 00	3.5227402E 02	1.6352694E 00	-2.7874193E-08
2	2.4651628E 02 1.2495252E 03	2.6770021E 04	9.6698246E 01	2.1037022E 04	1.2121486E 01	-2.4555251E-05
3	3.5664228E 00 3.5157112E 01	9.6698246E 01	2.7128213E 00	1.8855717E 02	1.5095727E 00	1.8044323E-07
4	3.5227402E 02 3.0139761E 03	2.1037022E 04	1.8855717E 02	3.1569075E 04	3.2735289E 01	-3.0012476E-05
5	1.6352694E 00 1.2162565E 01	1.2121486E 01	1.5095727E 00	3.2735289E 01	1.2182956E 00	2.0047459E-07
6	4.7425824E 01 7.9904760E 02	1.2495252E 03	3.5157112E 01	3.0139761E 03	1.2162565E 01	4.9278967E-06

VALUE OF DETERMINANT = 2.7182680E 06

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I	INVERSE OF A(K,L)				
1	6.6136371E 02 -3.5554734E 00	-1.8313298E 00	-3.3600064E 02	-3.4771342E 00	-3.2424255E 02
2	-1.8313274E 00 8.9799315E-03	5.1977267E-03	9.9626257E-01	9.3008167E-03	8.3238804E-01
3	-3.3599700E 02 1.8695817E-01	9.9625369E-01	2.7751877E 02	1.3487339E 00	5.9106897E 01
4	-3.4771487E 00 2.4720493E-02	9.3008690E-03	1.3487605E 00	2.0021646E-02	2.1187004E 00
5	-3.2424623E 02 3.3265961E 00	8.3239939E-01	5.9110566E 01	2.1187126E 00	2.6437894E 02
6	-3.5555281E 00 4.6130894E-02	8.9800953E-03	1.8700545E-01	2.4720704E-02	3.3266034E 00

16 ITERATIONS

EXAMPLE SUM OF 3 EXPONENTIALS FOR BIOLOGICAL RETENTION DATA

$P(1) \cdot \text{EXP}(P(2)Z) + \dots + P(K-1) \cdot \text{EXP}(P(K)Z)$

THIS PROBLEM CONTAINS 28 DATA POINTS, 1 INDEPENDENT VARIABLE, AND 6 PARAMETER(S) (0 OF THEM HELD CONSTANT).

THE WEIGHTED VARIANCE IS 6.372521E-02 AND THE UNWEIGHTED SUM OF SQUARES OF THE DEVIATIONS IS 1.4019547E 00.

K	GUESSTIMATE OF K-TH PARAMETER	FINAL VALUE OF K-TH PARAMETER	S.D. OF K-TH PARAMETER	EXACT LEAST SQUARES EQUATIONS FITTED FUNCTION	EQUATIONS INPUT DATA
1	2.160000E 01	1.1688809E 01	6.4919599E 00	2.8982902E 02	2.8982907E 02
2	-1.0500000E-01	-8.5593047E-02	1.8199622E-02	7.5534989E 03	7.5534992E 03
3	4.6000000E 01	4.2582664E 01	4.2053469E 00	2.2624373E 02	2.2624373E 02
4	-2.8900000E-01	-2.2624408E-01	3.5719514E-02	1.3644022E 04	1.3644022E 04
5	3.2399999E 01	4.5733013E 01	4.1045833E 00	1.3911231E 02	1.3911231E 02
6	-1.3850000E 00	-8.5967839E-01	5.4219009E-02	2.6076665E 03	2.6076665E 03

MATRIX OF CORRELATIONS BETWEEN FREE PARAMETERS

1	1.000	-0.988	-0.784	-0.956	-0.775	-0.644
2	-0.988	1.000	0.830	0.912	0.710	0.580
3	-0.784	0.830	1.000	0.572	0.218	0.052
4	-0.956	0.912	0.572	1.000	0.921	0.813
5	-0.775	0.710	0.218	0.921	1.000	0.953
6	-0.644	0.580	0.052	0.813	0.953	1.000

EXAMPLE SUM OF 3 EXPONENTIALS FOR BIOLOGICAL RETENTION DATA

I	WEIGHT	INDEPENDENT VARIABLE	DEPENDENT VARIABLE	CALCULATED FUNCTION	DEVIATION	STD. DEV. OF PREDICTED MEAN
1	1.0000000E 00	0.	1.0000000E 02	1.0000449E 02	-4.4870377E-03	2.5148434E-01
2	1.0000000E 00	1.0000000E 00	6.4000000E 01	6.4049323E 01	-4.9324036E-02	2.2247528E-01
3	1.0000000E 00	2.0000000E 00	4.5500000E 01	4.5128682E 01	3.7131739E-01	1.5328027E-01
4	1.0000000E 00	3.0000000E 00	3.3500000E 01	3.4110937E 01	-6.1093760E-01	1.5228845E-01
5	1.0000000E 00	4.0000000E 00	2.7000000E 01	2.6995216E 01	4.7833920E-03	1.3898433E-01
6	1.0000000E 00	5.0000000E 00	2.2200000E 01	2.1979533E 01	2.2046614E-01	1.1850919E-01
7	1.0000000E 00	6.0000000E 00	1.8700000E 01	1.8214286E 01	4.8571420E-01	1.1533762E-01
8	1.0000000E 00	7.0000000E 00	1.5000000E 01	1.5270269E 01	-2.7026892E-01	1.2435443E-01
9	1.0000000E 00	8.0000000E 00	1.2800000E 01	1.2910022E 01	-1.1002171E-01	1.3239057E-01
10	1.0000000E 00	1.0000000E 01	9.4000000E 00	9.4075669E 00	-7.5669289E-03	1.3489475E-01
11	1.0000000E 00	1.6000000E 01	3.7500000E 00	4.1123611E 00	-3.6236107E-01	1.2521909E-01
12	1.0000000E 00	1.8000000E 01	3.1300000E 00	3.2296403E 00	-9.9640340E-02	1.1627470E-01
13	1.0000000E 00	2.0000000E 01	2.7200000E 00	2.5716024E 00	1.4834756E-01	1.0397697E-01
14	1.0000000E 00	2.2000000E 01	2.5800000E 00	2.0716574E 00	5.0834262E-01	9.1448374E-02
15	1.0000000E 00	2.4000000E 01	1.6200000E 00	1.6850719E 00	-6.5071896E-02	8.1819240E-02
16	1.0000000E 00	2.5000000E 01	1.7200000E 00	1.5243582E 00	1.9564183E-01	7.8726491E-02
17	1.0000000E 00	2.7000000E 01	1.1400000E 00	1.2537623E 00	-1.1376236E-01	7.6101446E-02
18	1.0000000E 00	2.8000000E 01	1.1600000E 00	1.1395085E 00	2.0491540E-02	7.6242222E-02
19	1.0000000E 00	3.1000000E 01	8.3000000E-01	8.6134546E-01	-3.1345464E-02	7.9494305E-02
20	1.0000000E 00	3.2000000E 01	7.0999999E-01	7.8607343E-01	-7.6073445E-02	8.0781311E-02
21	1.0000000E 00	3.6000000E 01	4.2900000E-01	5.4884379E-01	-1.1984380E-01	8.3603226E-02
22	1.0000000E 00	3.7000000E 01	5.2999999E-01	5.0233228E-01	2.7667709E-02	8.3503193E-02
23	1.0000000E 00	4.0000000E 01	2.9000000E-01	3.8594894E-01	-9.5948942E-02	8.1269804E-02
24	1.0000000E 00	4.3000000E 01	2.6000000E-01	2.9721517E-01	-3.7215169E-02	7.6651089E-02
25	1.0000000E 00	4.8000000E 01	2.1000000E-01	1.9290004E-01	1.7099962E-02	6.5793692E-02
26	1.0000000E 00	4.9000000E 01	1.1000000E-01	1.7697745E-01	-6.6977447E-02	6.3386295E-02
27	1.0000000E 00	5.1999999E 01	8.4999999E-02	1.3672519E-01	-5.1725187E-02	5.6062090E-02
28	1.0000000E 00	5.9999999E 01	3.4999999E-02	6.8826711E-02	-3.3826711E-02	3.7946088E-02

Attachment 3

SELECT GRID

PURPOSE: To select various grids both horizontally and vertically for the
S-C 4020 tape to film device.

CALLING SEQUENCE: CALL SELGRD (I, J)

where I is the horizontal option

J is the vertical option

option	number of intervals
≤ 1	1 (Border only)
2	2
3	3
4	4
5	5
6	10
7	15
8	20
9	25
10	50
11	1 cycle logarithmic
12	2 cycle logarithmic
13	3 cycle logarithmic
14	4 cycle logarithmic
15	5 cycle logarithmic
16	6 cycle logarithmic
≥ 17	Border only

SELECT GRID

DESCRIPTION: Whenever this routine is used a border is drawn as follows:

The grids are always drawn inside this border, leaving additional room on the left and bottom edges of each frame for labeling purposes. (The dashed lines are not drawn on film.)

EXAMPLE: With $I = 2$, $J = 1$, the following would result:

$I = 1$, $J = 2$

SELECT GRID

$$I = 4, J = 2$$

STORAGE: 351_{10} words (537_8)

- NOTE:
1. On the logarithm grids the main division lines are drawn twice, making them heavier on film.
 2. All combinations of options may be used.

Attachment 4