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FRANTIC Program for Analysis of Exponential Growth and Decay Curves

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FRANTIC PROGRAM FOR ANALYSIS OF

EXPONENTIAL GROWTH AND DECAY CURVES

1. GENERAL DESCRIPTION

A computer program called FRANTIC has been written to process raw counting data and fit to these data, by the least-squares techniques, equations for multiple exponential growth and decay. This program, written in FORTRAN for IBM computers, is sufficiently general to be used for almost any sum of exponentials with positive, negative, or zero exponents and positive or negative coefficients. FRANTIC is designed so that each independent group of operations such as data processing, matrix inversion, and input-output routines may be removed and modified or replaced without disturbing the rest of the program.

The least-squares best fit of a calculated curve to actual data is defined as that fit in which the sum of the weighted squares of the residuals (differences between the calculated values and the observed values) is a minimum. This sum, divided by the number of degrees of freedom, is known as the "variance of fit". In order for a least-squares analysis to be applicable, there must exist a set of simultaneous equations which are linear in the parameters whose values are to be determined. The number of equations in the set must be at least as large as the number of parameters. When these conditions are met, a unique solution exists and the values of the parameters can be determined by a <u>Unique</u> <u>Least-Squares</u> <u>Analysis</u>.[1]

If the equations to be used are non-linear in the parameters to be determined, the least-squares method is not directly applicable as there may exist a series of minima in the variance of fit. In order

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1. D.S. Harmer, Brookhaven National Laboratory Report BNL-544 (T-141), March 1959.

to use the least-squares method the equations must be made linear. One means of accomplishing linearization is credited to Gauss and Sidel or, alternatively, to Newton. It consists of expanding each expression in a first-order Taylor series about the point defined by the previous estimates of the parameters. By neglecting all terms of the series beyond first order, there results a set of simultaneous equations which are linear in the first power of the Δ terms (differences between the estimates of the parameters and the actual values) but not necessarily linear in the original parameters themselves. With this new set of simultaneous linear equations the conditions for least-squares analysis may be met and, if so, a unique solution for the Δ terms exists.

In order to determine the values of the parameters of the non-linear equations, it is necessary only to evaluate the Δ terms and correct the previous estimates for these differences. Since all higher-order terms of the expansion are neglected some error is introduced and it is necessary to repeat the process with the corrected estimates. Each repetition is known as an iteration. Several iterations are often required to meet the given convergence criterion. This process is known as an Iterative Least-Squares Analysis.[2]

The parameters in FRANTIC are the A_o coefficients (activities at time T = 0) and λ values (decay constants) of the exact equations describing a sum of first-order reactions (see subroutine LESFIT description below). If only the A_o coefficients are to be determined (i.e. decay constants all known) then these equations are linear and a unique analysis is sufficient. If, however, one or more of the decay constants are to be determined, the equations are non-linear and an iterative analysis must be made.

2. R.H. Moore and R.K. Zeigler, Los Alamos Scientific Laboratory Report LA-2367, March 4, 1960.

2. FRANTIC OPERATION

The FRANTIC program is presently designed to accommodate up to 400 data points and to analyze for a maximum of 10 components. It is also arranged so that several runs (analyses) may be made on a given set of data and several sets of data, each with several runs, may be analyzed consecutively. A run is defined as a single analysis or series of analyses resulting from one group of controlling input information. A set is the group of runs (analyses) on one given set of data. For each set the data need to be read into the computer only once, at the beginning of the first run. For subsequent runs only the controlling information need by entered.

In the processing of a set of data each raw count is corrected for the scale factor used and remainder (if any), dead time, background, and finally the whole set of data may be normalized. In order for this processing to be carried out correctly all input constants and data must be inserted in the <u>same</u> units of time.

In the main scheme of operation the FRANTIC program, for the first iteration, holds the values of all the λ parameters and their signs fixed. This makes the equations linear in the unknown A_o coefficients (those not held fixed). These coefficients, which correspond to the initial combination of decay constants, are evaluated by a <u>Unique Least-Squares Analysis</u>. These evaluated A_o coefficients, the A_o coefficients that were held fixed, and the initial λ values are the "Original Estimates" seen in the printed results.

If one or more of the decay constants are to be determined the unique analysis is not sufficient and, in subsequent iterations, the values of the unknown A_o and λ parameters are determined by an <u>Iterative Least-Squares Analysis</u>. In each iteration the Δ terms corresponding to the unknown parameters are evaluated and correction to the previous estimates made. For the second through fifth iterations a maximum of 70% of each Δ term is added to the previous estimate of its parameter in order to minimize large swings. In subsequent iterations a maximum of 98% of the Δ term is used. This value was chosen to prevent occurrence of a nonconverging cyclic process.

In the iterative mode it is possible to predetermine the sign of each parameter while allowing its value to be determined. This is done by initially assigning to the value of each original estimate the sign of its input estimate. During each iteration the sign of each parameter is prevented from changing by progressively dividing its corrected Δ term by two until the new Δ term does not change the sign of the previous estimate of that parameter. If the signs are allowed to vary, the original estimates and corrected Δ terms are used directly.

In order for convergence to occur the value of each parameter and the variance of fit must not deviate from their values in the preceeding iteration by more than one part in 10^6. When convergence occurs, the results are printed out before the next analysis is begun. If convergence has not occured by 25 iterations the results at that time are printed out.

The main scheme of FRANTIC operation (i.e. a unique analysis followed by an iterative analysis) may be modified depending upon which parameters are held fixed. If all of the λ values are held fixed the unique analysis is sufficient to determine the best values of the unknown A_o parameters. If any λ values are to be determined an iterative analysis must be made. When all A_o and λ parameters are fixed FRANTIC merely calculates the value of the curve at each point and compares these values with the data. In one special case (see Case 3) the unique analysis is omitted and an iterative analysis is made regardless of which parameters are held fixed (except where all are fixed).

2.1 Operating Cases

Case 1. No A_o or λ estimates are entered. One analysis is made for each value of the number of components (JCALC) consecutively from one through the maximum number of components (JMAX). At the beginning of each analysis one new positive λ value is estimated. This new estimate and the absolute values of the decay constants from the previous analysis are used as the next original estimates. The signs and values of all parameters are allowed to vary (see GUESS discussion below).

Case 2. All λ original estimates are inserted as well as the A_o values to be held fixed. None, any, or all of the A_o and λ parameters may be held fixed. One analysis is made for JCALC = JMAX. If no λ parameters are allowed to vary the unique analysis is sufficient; otherwise, the unknown A_o and λ values are determined by an iterative analysis.

Case 3. All A_o and λ original estimates are inserted. None, any, or all may be held fixed. One analysis is made for JCALC = JMAX. The unique analysis is omitted and an iterative analysis is made regardless of which parameters are held fixed (except when all are fixed).

2.2 Input Options

a. IC - Case control factor

i. One may choose any one of the three operating cases described above (IC = 1, 2, or 3).

ii. Many runs of one (Cases 2 or 3) or more (Case 1) analyses may be made consecutively on a given set of input data. Each set of data need be entered only once by making IC positive (IC = +1, +2, or +3 – read in new data) in the first run of that set and IC negative (IC = -1, -2, or -3 – use previously read data) in all subsequent runs of the set. Several sets of data (each with several runs) may be stacked to be analyzed consecutively.

b. ID - Data control factor

i. One of three types of weight factors may be chosen for each run: all data points weighted equally (ID = 1); statistical weight factors (calculated internally) which depend on uncertainty in count rate, background, dead time, and counting interval (ID = 2); or special weight factors calculated externally (ID = 3).

ii. The input data may be either simple input data points (ID = +1, +2, or +3) or accumulative data points (ID = -1, -2, or -3) where the scaler was not set back to zero between counts.

c. IS(1) - Decay constant estimate control

When using Case 1 (IC = +1 or -1) one may choose the relative magnitude of each new λ original estimate. The new estimate may be either 10 times the largest absolute λ value from the previous analysis (IS(1) = 0) or 3 times this value (IS(1) $\neq$ 0).

d. IS(2) - Parameter sign control

In a Case 2 or Case 3 iterative analysis, one may predetermine the sign of each parameter while allowing its value to vary. By setting IS(2) = 0 each original estimate is given the sign of its input estimate and this sign is prevented from changing in subsequent iterations. If IS(2) $\neq$ 0, the original estimates are used directly and the signs may change at will.

In Case 2, the original estimates include the unknown A_o values determined in the unique analysis. In the input estimates for these parameters, blank or zero values are considered positive. Therefore a dummy negative value must be inserted for each negative A_o, otherwise these estimates may be left blank.

e. IS(3) - Iterative printout control

The current values of the parameters and their corrected Δ terms are printed out at the end of each iteration if IS(3) $\neq$ 0. This step is omitted if IS(3) = 0.

f. <u>IS(4) - Matrix printout control</u>

The final least-squares matrix and transformation vector as well as the inverse of the matrix and resultant transformed vector (solutions to the least-squares equations) are printed out if $IS(4) \neq 0$. This step is omitted if $IS(4) = 0$.

g. <u>IX(I) - Parameter fixing controls</u>

The input estimate of any parameter may be held constant by setting the corresponding $IX(I) \neq 0$. The parameter will be allowed to vary if $IX(I) = 0$. Each consecutive pair of IX values IX(1) and IX(2), IX(3) and IX(4), etc., corresponds respectively to the A_o and λ values of one component. The components are in the order dictated by the estimate cards. Thus:

Term	Corresponds to	
IX(1)	$A_o(1)$	Estimate card 1.
IX(2)	$\lambda(1)$	
IX(3)	$A_o(2)$	Estimate card 2.
IX(4)	$\lambda(2)$	
etc.	etc.	etc.

In addition to the above options, all of which appear on the <u>control card</u>, certain other options are available in the form of a choice of values for the data processing parameters appearing on the <u>data control card</u>. These parameters are:

(a) TAU - any arbitrary time before (+) or after (-) T = 0 used to calculate N(ORIGINAL) (see OUTPUT),

(b) TAUD - dead-time factor (τ_d) in time units,

(c) DTAU - standard deviation of dead-time factor $[\sigma(\tau_d)]$ in time units,

(d) B - background in counts per unit time,

(e) EB - uncertainty in each counting interval DT in time units,

(f) S - data scale factor (multiplier) usually 1, 64, 128, etc. (must not be zero),

(g) XNORM - data normalization factor (multiplier) usually 1 (must not be zero),

(h) TIME - time scale factor (divisor) for changing units of T and DT (INPUT-C only, see INPUT subroutine).

Further information on the input format is given in Section 5 and sample input data are given in Section 6.

2.3 Description of the Results

In order to render the following description more understandable a sample set of output results is given (Section 6). These results were obtained from the sample input data immediately preceding them.

The general output results begin a new page with the date and time the analysis was made, a one-line title consisting of the information punched on the input header card, and 12 lines of information divided into two columns. Quantities in the first column requiring further explanation are:

Line 1. ten column identification from the control card,

Line 5. number of degrees of freedom (data points minus parameters allowed to vary),

Line 7. type of weight factors used and the absolute value of the data control factor,

Line 9. the determinant of the final least-squares matrix (should never be negative, if so special notice is given), Line 10. the absolute difference between the variance of fit in the final iteration and its value in the preceding iteration in parts per 10^6 of its final value,

Line 12. the χ^2 (chi square) value for use in "goodness-of-fit" tests.

Next, the following values and their standard deviations are given for each component of the calculated decay curve. These are:

Col. 1. A(ZERO) - activity at time T = 0 in counts per unit time,

Col. 3 LAMBDA - decay constant in reciprocal time units,

Col. 5 N(ORIGINAL) - number of active atoms at time TAU from T = 0 and its σ (including uncertainty in both A_o and λ),

Col. 7 HALF LIFE - half life in time units.

It should be noted that:

(a) the σ value for each parameter held fixed is set to 0.0,

(b) when a λ value is 0.0 the corresponding N(ORIGINAL), HALF LIFE, and their σ values are set to 0.0,

(c) N(ORIGINAL), its σ, and the σ for the half life are set to -1.0 when the σ of one of the A_o or λ values is e^{37} times the corresponding A_o or λ value or if the product of $\lambda \times$ TAU is greater than 80.0 (see OUTPUT).

For each iterative analysis the original A_o and λ estimates are given. These "Original Estimates" are composed of the following:

(a) A_o and λ values held fixed (Cases 2 or 3),

(b) unknown λ values - input estimates (Cases 2 or 3) or estimated values (Case 1),

(c) unknown A_o values - input estimates (Case 3) or values from the unique analysis (Cases 1 or 2).

Next, a histogram of the distribution of deviations of the final calculated points from the data points is given. The number above each value of σ is the number of data points whose weighted residuals lie between that value and the next larger absolute value.

Several quantities are given for each data point used in the analysis. The columns requiring further comment are:

Col. 4. raw counts corrected for scale factor, remainder, and change of accumulative data to simple data,

Col. 5 column 4 corrected for counting interval, dead time, background, and normalization factor; in counts per unit time,

Col. 6 value of the calculated curve used in the analysis, AC,

Col. 7 value of the curve calculated at the midpoint of the counting interval, AINST,

Col. 9. residual (corrected data minus calculated curve) in counts per unit time, each residual greater than 2 σ units denoted by an asterisk.

If requested (IS(4) $\neq$ 0) the least-squares matrix, transformation vector, inverted matrix, and transformed vector are printed out in normal row and column form.

The intermediate results, if requested (IS(3) $\neq$ 0), are printed out at the end of each iteration (before the general results). The first line printed for each iteration is composed of:

Col. 1. identification (as above),

Col. 2. number of the iteration,

Col. 3. number of components,

Col. 4. sum of weighted squares of residuals,

Col. 5 delta variance of fit $\times 10^6$ (as above).

In subsequent lines of each group are given the A_o and its corrected Δ term and the λ and its corrected Δ term for each component (in that order - two components per line).

3. EVALUATION OF RESULTS

When using a computer for mathematical analyses it is well to remember that computers are by no means magic. They should be expected to do nothing that you could not do better with a desk calculation or, for that matter, by longhand. The main reasons for using computers are the speed with which they carry out mathematical operations and their exceedingly small probability of making an error.

In the final analysis, each set of calculated results must be scrutinized in the light of human judgment. One must attempt to answer the following three questions: How good is the fit? How does the calculated curve compare with the data? What significance have the parameters? Certain guidelines can be given for answering these questions.

How good is the fit?

This question is answered mainly by the calculated values of the weighted variance of fit (VAR) and χ^2 (CHISQ). The variance of fit is the sum of the weighted squares of the residuals divided by the degrees of freedom (DF), where each weighted residual is expressed in units of its individual σ. The σ values include uncertainty in the observed count rate, background, dead-time, and counting interval.

The value of VAR is also the square of the standard deviation of the distribution of residuals about zero. The value of VAR for a fit to data having only statistical deviations (i.e., the expectation value of VAR) is unity and the value corresponding to the 2 σ level of confidence (i.e. value where an identical measurement has 97.73% chance of having a smaller VAR) is approximately $(1+ 3/\sqrt{DF})$.

Chi square (χ^2) is similar to VAR except that in computing the former quantity the sum of the weighted squares of the residuals is not divided by DF and the weighting factors include only uncertainty in the calculated count rates (not observed count rates). Thus, when the dead-time and counting interval errors and background are negligibly small or zero $(VAR \times DF) \simeq \chi^2$; otherwise $(VAR \times DF) < \chi^2$. In the usual χ^2 vs DF tables VAR × DF will give a more realistic measure than χ^2 of the probability of performing a better experiment or finding a better fit with different parameters.

How does the calculated curve compare with the data?

To answer this question one must look at the "Analysis of the Deviations" and the actual residuals themselves. The printed histogram of residuals should be Gaussian with standard deviation equal to (VAR). In the histogram, 31.7% of the residuals would be expected to be outside σ, 4.55% outside 2σ, and 0.272% outside 3σ.

The column containing the actual residuals, if placed in order of time of observation, should show statistical variations in the signs of the residuals (i.e. alternate positive and negative values with no long series of residuals having the same sign). Such non-statistical variations may indicate a missing component or change in the counting equipment.

No significance can be attached to VAR and the residuals histogram in an analysis with unit weight factors or to χ^2 in an analysis with special weight factors. In the latter case VAR and the residuals histogram are significant only if the special weight factors used correspond, in the proper units, to the reciprocal squares of some assumed standard deviations.

Large values for VAR and χ^2/DF and wide dispersion of the residuals histogram may indicate the presence of components not considered in the analysis or experimental counting errors larger than the assumed statistical deviations.

What significance have the parameters?

Decay Constants. For any radioactive decay these should be positive, indicating a decreasing exponential curve. The decay constants may have any combination of values with the single restriction that the partial derivatives of the functions with respect to the A_o parameters over the time covered in the experiment must vary appreciably from one component to another (i.e. no two components may have nearly identical half lives). In actual practice it is difficult to determine the decay constants for components which:

(a) have half lives very long or very short compared with the time covered in the experiment,

(b) are very similar in half life to other components (considerable difficulty occurs when one is < 1.5 times another),

(c) contribute only a very small portion to the total decay curve.

If a decay curve is analyzed for more components than are actually present, the extra components may be thrown out of the analysis entirely. This is indicated by a λ value which becomes very large or very small (with a large σ) or approaches the λ of one of the actual components.

A_o Coefficients. The A_o values determined in a decay-curve analysis should always be positive unless real parent-daughter relationships exist. If so, the parent (1) and daughter (2) should be entered as only two components where the A_o values determined in the analysis are related to the actual initial activities, A_o', by

$$A_o(1) = A_o'(1)\left[1 + \frac{C(2)}{C(1)}\ \frac{\lambda(2)}{\lambda(2) - \lambda(1)}\right] ,$$

$$A_o(2) = A_o'(2) - \frac{C(2)}{C(1)}\ \frac{\lambda(2)}{\lambda(2) - \lambda(1)}\ A_o'(1),$$

$$A_o(1) + A_o(2) = A_o'(1) + A_o'(2) ,$$

where the C(i) values are the counting efficiencies. For an assumed component not actually present, whose λ is held fixed, the resulting A_o will be a small value with a large σ. A better result for the other components may be obtained by omitting the absent component. An A_o value that becomes negative or, when its sign is held fixed, approaches zero may indicate improper dead-time correction or instrumental gain shift.

It should be pointed out that the σ for a parameter from any one analysis is often smaller than the actual standard deviation computed on the basis of a series of identical analyses (i.e. the value of the parameter is not as reproducible as would be expected on the basis of the quoted σ).

Notes on Possible Applications

a. An unknown amount of background and/or a long-lived component that does not decay appreciably during the time of the counting measurements may be included as a component with $\lambda = 0$ (fixed).

b. Individually measured background values (e.g. those measured from day to day over a long-term experiment) may be included as a negative remainder ($-R_n$) with S = 1. The value of each background must correspond to the same DT_n as the count (C_n). However, when used in this manner the statistical weight factors are computed improperly.

c. In any run but the first of a set the value of N may be smaller than the initial number of data points inserted (i.e. the last data points may be dropped in subsequent runs without reading in the lesser number of data points as a new set).

d. In addition to analyzing decay-curves, FRANTIC may be used to determine the weighted best value of a series of measurements of the same quantity. The measured values are inserted as counts with T = 0 and DT = 1, weight factors are inserted as special weights, and the analysis is made for JMAX = 1 with λ = 0 (fixed). If unit weight factors are used the simple average is computed.

4. DESCRIPTION OF THE FRANTIC PROGRAM

4.1 General Discussion

The FRANTIC program consists of 8 semi-independent subprograms written in FORTRAN.[3] Each subprogram performs one specific set of operations and may be replaced or modified without recompiling the remaining subprograms. There are no program stops in FRANTIC although normal FORTRAN stops may occur. For FRANTIC in its present form (up to 10 components and 400 data points) values used in the analysis require 8,143 storage locations and the 8 subprograms require approximately 3,687 locations.

This FRANTIC program, except for the FR-II master subprogram, may be used directly in its compiled (column binary) form at most IBM 709 or 7090 computer installations. For other types of computers it may be necessary to recompile the entire program from the FORTRAN deck.

4.2 FR-II (MAIN) Subprogram

This master subprogram is designed to direct the continuity of each analysis by calling upon the subroutines in the appropriate order. It must be specifically designed for use at each installation. In particular, there are included three FORTRAN statements which must be made compatible with the given installation,

```
ITAPE = 4
JTAPE = 2
CALL CLOCK (JTAPE).
```

3. Reference Manual 709/7090 FORTRAN Programming System, International Business Machines Corp. (1961).

ITAPE and JTAPE must be given the input- and output-tape-unit numbers respectively. CLOCK causes printout of the date and time, and may be left out entirely if not available at the installation.

4.3 Subroutines

INPUT

This subroutine is the first one called by FR-II. In it the controls and data for each run are read and stored in the computer memory. At present, three different INPUT subroutines have been written, called INPUT - A, INPUT - B, and INPUT - C. Each one has been designed for a certain type of available input data. The requirements for the header card, control card, and estimate cards are the same in each one.

INPUT - A. This is a general input subroutine requiring one card per observation.

INPUT - B. This subroutine is designed for data in groups of equally-spaced, consecutive values with no intervals between observations (as from a multiscaler). Twelve data points per card are entered and no remainders or special weight factors are allowed.

INPUT - C. This subroutine is designed especially for use with the data cards (one observation per card) from the automatic counting arrangement of the Los Alamos Scientific Laboratory P-12 group. No special weight factors are allowed.

Only <u>one</u> of these subroutines may be included with the FRANTIC binary deck at a time.

DATA

In this subroutine the corrected counts per unit time are calculated from the raw data points. Each raw count (C_n) is corrected for the scale factor (S) and remainder (R_n):

$$C_n' = C_n S + R_n.$$

Accumulative data are changed to simple data:

$$C_n' = (C_n S + R_n) - (C_{n-1} S + R_{n-1}).$$

The raw count rate is calculated (and stored in R_n):

$$R_n = C_n' / DT_n.$$

This rate is corrected for the dead-time factor (TAUD) and background (B) and each point is normalized (XNORM) to yield the corrected data:

$$A_n = \left[\frac{R_n}{1 - R_n \, TAUD} - B \right] XNORM.$$

The unit (ID = 1) or statistical (ID = 2) weight factors are calculated in this subroutine if they are to be used:

$$W_n = \frac{1}{\sigma(T)_n^2} = 1.0 \qquad \text{(unit weight factors)},$$

or

$$W_n = \frac{1}{\sigma(T)_n^2 \ XNORM^2} \qquad \text{(statistical weight factors),}$$

where

$$\sigma(T)_n^2 = \sigma(C)_n^2 + \sigma(B)_n^2 + \sigma(\tau_d)_n^2 + \sigma(DT)_n^2$$

and

$$\sigma(C)_n^2 = \left(\frac{\sqrt{C_n}}{DT_n}\right)^2 = \frac{R_n}{DT_n} \qquad \text{(uncertainty in count rate),}$$

$$\sigma(B)_n^2 = \frac{B}{DT_n} \qquad \text{(uncertainty in background),}$$

$$\sigma(\tau_d)_n^2 = \Delta A_n^2 \qquad \text{[from uncertainty in dead-time factor } \sigma(\tau_d)\text{],}$$

$$\sigma(DT)_n^2 = \Delta A_n^2 \qquad \text{(from uncertainty in counting interval EB).}$$

The value of $\sigma(\tau_d)_n^2$ is evaluated in the following manner:

$$A_n = \frac{R_n}{1 - R_n\tau_d} \quad ,$$

$$A_n + \Delta A_n = \frac{R_n}{(1 - R_n\tau_d) - R_n \ \sigma(\tau_d)} \ ,$$

$$A_n - \Delta A_n = \frac{R_n}{(1 - R_n\tau_d) + R_n \ \sigma(\tau_d)} \ ,$$

$$\sigma(\tau_d)_n^2 = \Delta A_n^2 = \left\{ \frac{R_n\left[R_n \ \sigma(\tau_d)\right]}{(1 - R_n\tau_d)^2 - \left[R_n \ \sigma(\tau_d)\right]^2} \right\}^2 \ .$$

similarly

$$\sigma(DT)_n^2 = \Delta A_n^2 = \left[\frac{R_n(EB/DT_n)}{1 - (EB/DT_n)^2}\right]^2$$

The square of the total standard deviation for each point is given by

$$\sigma(T)_n^2 = \frac{R_n}{DT_n} + \frac{B}{DT_n} + \left\{ \frac{R_n\left[R_n \sigma(\tau_d)\right]}{(1-R_n\tau_d)^2 - \left[R_n \sigma(\tau_d)\right]^2} \right\}^2 + \left[\frac{R_n(EB/DT_n)}{1-(EB/DT_n)^2} \right]^2$$

GUESS

In this subroutine, used in Case 1 only, the necessary λ original estimates for each analysis of the run are calculated. When using Case 1 and this subroutine, the analysis is limited to decaying exponentials (positive λ values). The first and last data points inserted must correspond to the first and last observations made. The first λ estimate made (one component, JCALC = 1) is

$$\lambda_1 = \left| \frac{\ln(A_1/A_N)}{T_N - T_1} \right| .$$

Following each analysis, the previous decay constants are made positive and a new λ value estimated:

$$\lambda_{n+1} = 10 \times (\text{maximum previous } |\lambda|) \qquad (IS(1) = 0),$$

or

$$\lambda_{n+1} = 3 \times (\text{maximum previous } |\lambda|) \qquad (IS(1) \neq 0).$$

This new λ estimate and the previous values (which were made positive) are placed in order of decreasing value (increasing half life) and then used as original estimates for the next analysis.

In this subroutine the IX(I) values are all set to zero and IS(2) is set to unity allowing the signs and values of all parameters to vary during each analysis.

LESFIT

In this subroutine, with the aid of MATRIX and MATINV, the least-squares analysis is performed on the N corrected data points and A_o and λ parameters for I components. In subroutine MATRIX the least-squares matrix and transformation vector are calculated and, in MATINV, this matrix is inverted and the transformed vector is obtained. In subroutine LESFIT the required A_o and λ parameters as determined, the curve is calculated, and the residuals and the sum of the weighted squares of these residuals (called VAR) are computed. Then, three tests are made for criteria for exit to the OUTPUT subroutine.

In the following discussion $\{A\}$ denotes a matrix, $\{\tilde{A}\}$ the transform of $\{A\}$, and $\vec{B}$ a column vector.

The usual equation describing a sum of first-order reactions (e.g. multiple radioactive decay) is

$$AC_n = \sum_{i=1}^{I} A_{o_i} \, e^{-\lambda_i T_n} \quad .$$

This expression is valid only for the case of an instantaneous observation interval ($DT_n \rightarrow 0$). For use with finite intervals it is necessary to integrate this expression over the observation interval:

$$\int_{T_n}^{T_n + DT_n} AC_n \, dT_n = \int_{T_n}^{T_n + DT_n} \sum_{i=1}^{I} A_{o_i} \, e^{-\lambda_i T_n} \, dT_n$$

or, as used in LESFIT,

$$AC_n = \sum_{i=1}^{I} A_{o_i} \, e^{-\lambda_i T_n} \left(\frac{1 - e^{-\lambda_i DT_n}}{\lambda_i DT_n} \right).$$

This expression, although mathematically rigorous, is not adequate for small values of $\lambda_i DT_n$. When evaluated by a computer, the portion in parentheses tends toward zero instead of the proper value of unity for $\lambda_i DT_n$ values approaching zero. This situation may introduce substantial error into the final result. However, the equation can also be expressed:

$$AC_n = \sum_{i=1}^{I} A_{o_i} \, e^{-\lambda_i (T_n + DT_n/2)} \left[\frac{\text{Sinh } (\lambda_i DT_n/2)}{\lambda_i DT_n/2} \right] ,$$

or expanding,

$$AC_n = \sum_{i=1}^{I} A_{o_i} \, e^{-\lambda_i (T_n + DT_n/2)} \left[1 + \frac{X^2}{3!} + \frac{X^4}{5!} + \frac{X^6}{7!} + \ldots \right] ,$$

where

$$X = \lambda_i DT_n/2.$$

This series expansion, truncated after the fourth term, is adequate in the region where the original expression is inapplicable, but becomes inaccurate for large values of $\lambda_i DT_n$. Therefore, in LESFIT the series approximation is used for $\lambda_i DT_n$ up to 1.0 and the original expression above that.

In the Unique Least-Squares Analysis all λ_i values are held fixed and the above expressions are linear in the A_{o_i} coefficients. Thus, the set of simultaneous linear equations describing the values of the corrected data $(\vec{A})$ are given by,

$$\vec{A} = \{AE\} \, \vec{PC}$$

where $\vec{PC}$ contains the I values of A_{o_i}, and $\{AE\}$ the $(N \times I)$ partial derivatives of the N expressions with respect to the I values of A_{o_i}.

Thus the elements of the $\{AE\}$ matrix are

$$AE_{ni} = \frac{\partial AC_n}{\partial A_{o_i}} = e^{-\lambda_i T_n} \left(\frac{1 - e^{-\lambda_i DT_n}}{\lambda_i DT_n} \right) \quad \text{for } (\lambda_i DT_n > 1.0)$$

and

$$AE_{ni} = e^{-\lambda_i (T_n + DT_n/2)} \left[1 + \frac{(\lambda_i DT_n/2)^2}{3!} + \frac{(\lambda_i DT_n/2)^4}{5!} + \frac{(\lambda_i DT_n/2)^6}{7!} \right]$$

for

$$(\lambda_i DT_n \leq 1.0).$$

In order to solve for $\vec{PC}$ it is necessary to make the following transformations:

$$\{\widetilde{AE}\}\{W\}\vec{A} = \{\widetilde{AE}\}\{W\}\{AE\}\vec{PC}$$

and redefining

$$\vec{BM} = \{AM\}\vec{PC} \; ,$$

where,

$$\{\widetilde{AE}\}\{W\}\vec{A} \equiv \vec{BM} \qquad \text{(transformation vector)}$$

$$\{\widetilde{AE}\}\{W\}\{AE\} \equiv \{AM\} \qquad \text{(least-squares matrix)}$$

and

$$\vec{PC} = \{AM\}^{-1}\vec{BM} \qquad \text{(transformed vector)} \; .$$

In the actual analysis the I index is replaced by K, the number of unknown A_{o_i} values. Thus, $\{AM\}$ is the $(K \times K)$ least-squares matrix, $\vec{BM}$ the transformation vector of length K, and $\{W\}$ the $(N \times N)$ diagonal matrix of the weight factors.

The residuals are given by

$$\vec{DA} = \vec{A} - \vec{AC}$$

and

$$VAR = \tilde{\vec{DA}} \{W\} \vec{DA}.$$

In the <u>Iterative Least-Squares Analysis</u> the exact expression given above is expanded in a first-order Taylor series about the point defined by the previous estimates of the A_o and λ parameters:

$$A_n = AC_n + \sum_{i=1}^{IMA} \frac{\partial AC_n}{\partial A_{o_i}} \Delta A_{o_i} + \sum_{i=1}^{IML} \frac{\partial AC_n}{\partial \lambda_i} \Delta \lambda_i,$$

where

$$\vec{A} - \vec{AC} = \vec{DA} = \{PART\} \vec{DP} .$$

DP contains the K unknown ΔA_{o_i} and $\Delta\lambda_i$ values, where $K = IMA + IML$ (the number of unknown A_o and unknown λ values, respectively) and $\{PART\}$ contains the $(N \times K)$ corresponding partial derivatives. The partial derivatives with respect to A_{o_i} are the same AE_{ni} values as in the unique analysis. Those with respect to λ_i are defined in the MATRIX discussion.

The evaluation of $\vec{DP}$ is the same as the evaluation of $\vec{PC}$ in the unique analysis:

$$\vec{DA} = \{PART\}\ \vec{DP} \quad ,$$

$$\{\widetilde{PART}\}\{W\}\ \vec{DA} = \{\widetilde{PART}\}\{W\}\{PART\}\ \vec{DP}.$$

Redefining, as above,

$$\vec{BM} = \{AM\}\ \vec{DP}$$

and

$$\vec{DP} = \{AM\}^{-1}\ \vec{BM} \quad .$$

The corrected Δ term is added to each previous A_{o_i} and λ_i estimate; the columns of $\{AE\}$ are recalculated for any new λ values; and the calculated curve, residuals, and VAR are evaluated as before.

Before beginning the unique analysis IMA, IML, $\{AE\}$, and K (= JCALC - IMA) are evaluated. If a unique analysis is necessary ($K \neq 0$ and $IC \neq 3$) MATRIX and MATINV are called, yielding the unknown A_o values. If all λ values are held fixed (IML = JCALC) or if $K = 0$, senselight 1 is turned on. The curve, residuals, and VAR are calculated and the tests for the exit criteria are made. Any one of these tests, if positive, will stop the further operation of the LESFIT subroutine and send control back to the (MAIN) subprogram. These exit tests are:

1. senselight 1 turned on ($K = 0$ or all λ values fixed - after the unique analysis),

2. number of iterations, IT = 25,

3. convergence occurred (i.e. all parameters as well as VAR differ from their values in the preceding iteration by less than one part in 10^6).

If none of these exit tests is positive after the first iteration (only the first is applicable) a test of IS(2) is made to see if the signs of the parameters are to be held as initially specified during the subsequent iterative analysis. If so, the original estimates of the A_o values are given the signs of their input estimates before becoming the initial estimates for the second iteration.

For each subsequent iteration MATRIX and MATINV return the values of the Δ terms. These Δ terms are multiplied by the scale correction factor (0.70 for IT $\leq$ 5 and 0.98 for IT > 5) and added to the previous estimates. If the signs are to be held fixed the new estimate of each parameter is tested for a change of sign. If the sign has changed the corrected Δ term is progressively divided by 2 until this no longer occurs. The columns of $\{AE\}$ are re-evaluated for any new λ estimates and the curve, residuals, and VAR calculated. Finally, the tests for exit criteria are made (only 2 and 3 are applicable) before another iteration is begun.

MATRIX

In this subroutine the least-squares matrix $\{AM\}$ and transformed vector $\vec{BM}$ are calculated. For the unique analysis only previously calculated quantities are necessary ($\{AE\}$, $\{W\}$, and $\vec{A}$). However, for the iterative analysis, where $\vec{DA}$ replaces $\vec{A}$, the partial derivatives of the functions with respect to the unknown λ_i parameters must be calculated. These are given by

$$\frac{\partial AC_n}{\partial \lambda_i} = A_{o_i} \frac{e^{-\lambda_i T_n}}{\lambda_i DT_n} \left[\left(\frac{1}{\lambda_i} + T_n + DT_n \right) e^{-\lambda_i DT_n} - \left(\frac{1}{\lambda_i} + T_n \right) \right] .$$

As in the case of LESFIT, this expression is inapplicable for small values of $\lambda_i DT_n$. In the region where it is inapplicable this equation may be expanded:

$$\frac{\partial AC_n}{\partial \lambda_i} = A_{o_i} e^{-\lambda_i T_n} \left\{ -T_n - DT_n/2 + \lambda_i (DT_n/2)(T_n + DT_n) \right.$$

$$\left. - \left(\frac{1}{\lambda_i} + T_n + DT_n \right) \left[\frac{(\lambda_i DT_n)^2}{3!} - \frac{(\lambda_i DT_n)^3}{4!} + \frac{(\lambda_i DT_n)^4}{5!} - \frac{(\lambda_i DT_n)^5}{6!} \right] \right\}$$

In MATRIX the series approximation is used for $\lambda_i DT_n$ up to 0.2 and the original expression above that.

MATINV

This subroutine is a modified version of share subroutine number 664 ANF402. The least-squares matrix is inverted and the least-squares solutions (transformed vector) are evaluated. This inversion and concurrent solution is accomplished by a transformation of rows and columns. The inverted matrix and solution vector are stored in the original $\{AM\}$ and $\vec{BM}$, respectively.

OUTPUT

In this subroutine, the results from the LESFIT analysis are used to calculate the quantities appearing in the printed output which were not a direct result of the basic analysis. Following these calculations the general output results are recorded on magnetic tape for future printout off line.

The standard deviation of each parameter evaluated in the least-squares analysis is given by

$$\sigma_i = \left(VAR \times AM_{ii}^{-1} \right)^{\frac{1}{2}}$$

and, for each parameter held fixed, σ_i is set equal to zero. VAR is the actual variance of fit (the VAR value calculated in LESFIT divided by the number of degrees of freedom, DF = N-K). In addition, for each component, the following quantities are calculated:

$$N(\text{ORIGINAL}) = \frac{A_o}{\lambda} \; e^{\lambda \times \text{TAU}} \;,$$

$$\sigma N(\text{ORIGINAL}) = \left| N(\text{ORIGINAL}) \left[\left(\frac{\sigma A_o}{A_o} \right)^2 + \left(\frac{\sigma_\lambda}{\lambda} \right)^2 \right]^{\frac{1}{2}} \right| \;,$$

$$\text{HALF LIFE} = \frac{0.693147}{\lambda} \;,$$

and

$$\sigma(\text{HALF LIFE}) = \left| \text{HALF LIFE} \left(\frac{\sigma_\lambda}{\lambda} \right) \right| \;.$$

In the following two situations special values are given these four quantities:

1. when $\lambda = 0.0$, all are set to 0.0,
2. when σA_o or σ_λ is e^{37} times the corresponding A_o or λ value or when $\lambda \times \text{TAU}$ is > 80.0 all except half life are set to -1.0.

Next, χ^2 (CHISQ) and the instantaneous rate at each point (AINST_n) are evaluated and an analysis is made of the number versus value of the weighted residuals. These quantities are:

$$\chi^2 = \frac{1}{\text{XNORM}} \sum_{n=1}^{N} DA_n^2 \left(\frac{DT_n}{AC_n} \right) \;,$$

$$\text{AINST}_n = \sum_{i=1}^{N} A_{o_i} \; e^{-\lambda_i (T_n + DT_n/2)} \;,$$

and each residual in $\sigma(T)_n$ units is given by

$$\frac{DA_n}{\sigma(T)_n} = DA_n \left[W_n\right]^{\frac{1}{2}} .$$

This program was written in cooperation with the M.I.T. Computation Center.

5. NOTES ON THE INPUT FORMATS AND QUANTITIES APPEARING IN FRANTIC

INPUT QUANTITIES

CONTROL CARD

```
XID     IDENTIFICATION  (ANY 10 CHARACTERS)
N       NUMBER OF OBSERVATIONS
JMAX    MAXIMUM NUMBER OF COMPONENTS
IC      CASE CONTROL FACTOR       = CASE NUMBER (1,2, OR 3)
                                  = +  READ IN NEW DATA
                                  = -  USE PREVIOUS DATA
ID      DATA CONTROL FACTOR       = 1  UNIT WEIGHT FACTORS
                                  = 2  STATISTICAL WEIGHT FACTORS
                                  = 3  SPECIAL WEIGHT FACTORS
                                  = +  SIMPLE DATA POINTS
                                  = -  ACCUMULATIVE DATA POINTS
IS(1)       = 0  NEW LAMBDA ESTIMATE 10X LARGEST PREVIOUS VALUE (CASE 1)
        NOT = 0  NEW LAMBDA ESTIMATE  3X LARGEST PREVIOUS VALUE
IS(2)       = 0  DO NOT PERMIT PARAMETERS TO CHANGE SIGN
        NOT = 0  PERMIT PARAMETERS TO CHANGE SIGN
IS(3)       = 0  DO NOT PRINT OUT RESULTS EACH ITERATION
        NOT = 0  PRINT OUT RESULTS EACH ITERATION
IS(4)       = 0  DO NOT PRINT OUT LEAST-SQUARES MATRICES
        NOT = 0  PRINT OUT LEAST-SQUARES MATRICES
IS(5)       NOT USED
IS(6)       NOT USED
IX(I)       = 0  DO NOT HOLD CORRESPONDING PARAMETER FIXED
        NOT = 0  HOLD CORRESPONDING PARAMETER FIXED
```

ESTIMATE CARDS

```
PG      ESTIMATES OF THE LAMBDA AND A(0) PARAMETERS FOR EACH COMPONENT
```

DATA CONTROL CARD

```
TAU     TIME BEFORE OR AFTER TIME T = 0
TAUD    DEAD-TIME FACTOR
DTAU    STANDARD DEVIATION OF THE DEAD-TIME FACTOR
B       BACKGROUND COUNTS PER UNIT TIME
EB      UNCERTAINTY IN COUNTING INTERVAL IN TIME UNITS
S       DATA SCALE FACTOR  (MUST NOT BE 0)
XNORM   DATA NORMALIZATION FACTOR (MUST NOT BE 0)
TIME    TIME SCALE FACTOR   (INPUT-C ONLY)
```

DATA CARDS

```
T       TIME AT THE BEGINNING OF AN OBSERVATION
DT      LENGTH OF AN OBSERVATION
C       RAW COUNTS OBSERVED
R       REMAINDER   (MAY BE LEFT BLANK)
W       WEIGHT FACTORS  (MAY BE BLANK UNLESS SPECIAL WEIGHTS ARE USED)
```

QUANTITIES APPEARING ELSEWHERE IN FRANTIC

ITAPE	INPUT TAPE-UNIT NUMBER
JTAPE	OUTPUT TAPE-UNIT NUMBER
JMAX2	TWICE JMAX
JCALC	NUMBER OF COMPONENTS FOR WHICH THE ANALYSIS IS MADE
JCALC2	TWICE JCALC
IMA	NUMBER OF A(0) VALUES HELD FIXED
IML	NUMBER OF LAMBDA VALUES HELD FIXED
K	NUMBER OF VARIABLES NOT HELD FIXED
KP	K + 1
IT	NUMBER OF ITERATIONS
H	LEAST-SQUARES SCALE CORRECTION FACTOR
A	CORRECTED DATA
AC	CALCULATED CURVE
AE	VALUES OF THE PARTIAL DERIVATIVES WITH RESPECT TO A(0)
DA	RESIDUALS
P	VALUES OF THE PARAMETERS AT THE BEGINNING OF AN ITERATION
PC	CORRECTED PARAMETERS AT THE END OF THE ITERATION
DP	CORRECTED DELTA TERMS FOR ITERATIVE ANALYSIS
PART	PARTIAL DERIVATIVES
PIVOT	VALUES USED IN MATRIX INVERSION
IPIVOT	PIVOT TERM USED IN MATRIX INVERSION
INDEX	INDEXING TERMS USED IN MATRIX INVERSION
AM	LEAST-SQUARES MATRIX AND LATER THE INVERSE
BM	TRANSFORMATION VECTOR AND LATER THE TRANSFORMED VECTOR
AMO	LEAST-SQUARES MATRIX
BMO	TRANSFORMATION VECTOR
VAR2	SUM OF THE WEIGHTED SQUARES OF RESIDUALS, LATER VARIANCE OF FIT
DVAR	DELTA VARIANCE OF FIT BETWEEN CONSECUTIVE ITERATIONS
IDF	DEGREES OF FREEDOM
DET	LEAST-SQUARES DETERMINANT
SP	STANDARD DEVIATION OF EACH PARAMETER
XNORIG	N(ORIGINAL) VALUE AT TIME TAU FROM TIME T = 0
ENORIG	STANDARD DEVIATION OF N(ORIGINAL)
HL	HALF LIFE OF A COMPONENT
EHL	STANDARD DEVIATION OF THE HALF LIFE
AINST	INSTANTANEOUS RATE
IDEV	SIGMA ANALYSIS OF THE RESIDUALS
CHISQ	CHI SQUARE VALUE
NP2S	NUMBER OF POINTS DEVIATING MORE THAN 2 SIGMA UNITS

FORMATS FOR INPUT OF DATA INTO FRANTIC

NOTE - ALL QUANTITIES INVOLVING TIME MUST BE ENTERED IN THE SAME TIME UNITS.

A. HEADER CARD - ONE CARD OF ANY DESIRED INFORMATION.

B. CONTROL CARD - CONTROL VALUES PUNCHED IN INTEGER FORM.

	COL.		COL.	FOR
XID	1-10	IX(1)	33-34	A(1)
N	11-14	IX(2)	35-36	LAMBDA(1)
JMAX	15-16	IX(3)	37-38	A(2)
IC	17-18	IX(4)	39-40	LAMBDA(2)
ID	19-20	IX(5)	41-42	A(3)
IS(1)	21-22	IX(6)	43-44	LAMBDA(3)
IS(2)	23-24	IX(7)	45-46	A(4)
IS(3)	25-26	IX(8)	47-48	LAMBDA(4)
IS(4)	27-28	IX(9)	49-50	A(5)
IS(5)	29-30	IX(10)	51-52	LAMBDA(5)
IS(6)	31-32	ETC.	ETC.	ETC.

C. ESTIMATE CARDS - ESTIMATES OF LAMBDA AND A(0) FOR EACH COMPONENT PUNCHED PAIRWISE IN EXPONENTIAL FORM ONE COMPONENT PER CARD. (JMAX CARDS FOR CASE 2 OR CASE 3 AND NONE FOR CASE 1)

FORMAT (1PE12.7)

	COL.		
CARD 1			
PG(2)	1-12	LAMBDA(1)	
PG(1)	13-24	A(1)	(MAY BE BLANK FOR CASE 2)
CARD 2			
PG(4)	1-12	LAMBDA(2)	
PG(3)	13-24	A(2)	(MAY BE BLANK FOR CASE 2)
ETC.			

DATA

INCLUDE THESE CARDS IN THE FIRST RUN OF A SET (IC = +) AND OMIT THEM FOR ALL OTHER RUNS OF THAT SET (IC = -).

D. DATA CONTROL CARD - DATA PROCESSING CONTROLS PUNCHED IN EXPONENTIAL FORM.

	INPUT-A	INPUT-B	INPUT-C
FORMAT	(1P7E10.5)	(1P7E10.5)	(1P8E9.4)
	COL.	COL.	COL.
TAU	1-10	1-10	1 -9
TAUD	11-20	11-20	10-18
DTAU	21-30	21-30	19-27
B	31-40	31-40	28-36
EB	41-50	41-50	37-45
S	51-60	51-60	46-54
XNORM	61-70	61-70	55-63
TIME			64-72

E. DATA CARDS - THE RAW DATA.

```
INPUT-A           COL.     GENERAL CASE OF ONE CARD PER OBSERVATION PUNCHED
   FORMAT (1P5E12.7)       IN EXPONENTIAL FORM.
    T(I)           1-12
   DT(I)          13-24
    C(I)          25-36
    R(I)          37-48    (MAY BE BLANK)
    W(I)          49-60    (MAY BE BLANK)


INPUT-B           COL.     SPECIAL CASE OF ALL DT THE SAME AND T VALUES
                           CONSECUTIVE IN EACH SUBGROUP.
                           NO REMAINDERS OR SPECIAL WEIGHTS ALLOWED.
   FORMAT (I3,1P2E12.7)    FIRST CARD OF THE SUBGROUP.
      N             1-3    INTEGER NUMBER OF DATA POINTS IN SUBGROUP.
    T(1)           4-15    TIME OF FIRST OBSERVATION IN EXPONENTIAL FORM.
   DT(1)          16-27    STANDARD OBSERVATION LENGTH IN EXPONENTIAL FORM.
    FORMAT (12F6.0)        REMAINING CARDS OF THE SUBGROUP.
    C(1)            1-6    DATA CONSECUTIVE FROM 1 THROUGH N PUNCHED IN
    C(2)           7-12    DECIMAL 12 WORDS PER CARD AND 6 SPACES PER WORD.
    ETC.          ETC.
            SEVERAL SUBGROUPS MAY BE STACKED CONSECUTIVELY


INPUT-C           COL.     SPECIAL INPUT FOR LASL P-12 GROUP.
   FORMAT (2F6.0,13X,F5.0,1X,10F1.0)
    T(I)            1-6
   DT(I)           7-12
    C(I)          26-30
    X(1)             32    2(9)    (BINARY REPRESENTATION OF REMAINDER)
    X(2)             33    2(8)
    X(3)             34    2(7)
    ETC.           ETC.    ETC.
   X(10)             41    2(0)
```

THE THREE TYPES OF FORMAT SPECIFICATIONS USED IN FRANTIC ARE (IW), (FW.D), AND (1PEW.D). IN EACH OF THESE SPECIFICATIONS W IS THE FIELD WIDTH (NUMBER OF SPACES FOR THE WORD) AND D IS THE NUMBER OF DIGITS TO THE RIGHT OF THE DECIMAL.

INTEGER VALUES (IW).
THESE QUANTITIES ARE PUNCHED AT THE FAR RIGHT OF THEIR ALLOTED FIELD.

DECIMAL VALUES (FW.D).
THESE ARE PUNCHED AT THE RIGHT OF THEIR FIELD AS THOUGH THEY WERE INTEGERS. THE DECIMAL POINT IS ASSUMED TO THE RIGHT OF THE EXTREME-RIGHT FIELD POSITION.

EXPONENTIAL VALUES (1PEW.D).
THESE ARE TREATED IN THE FORM V X 10(K) WHERE V IS A DECIMAL VALUE (1.00 TO 10.00) AND K IS AN INTEGER (+37 TO -39). EACH WORD IS DIVIDED INTO

A. SIGN OF THE WORD (FIRST SPACE),
B. (D + 1) DIGITS DESCRIBING V,
C. SIGN AND VALUE OF K (LAST THREE SPACES).

THE DECIMAL POINT IN V NEED NOT BE PUNCHED AS IT IS ASSUMED TO LIE BETWEEN THE SECOND AND THIRD SPACES OF THE WORD (AFTER THE UNITS VALUE OF V).
THUS, THE VALUE +1234.5678 WOULD BE PUNCHED

```
    FORMAT          (1PE12.7)           (1PE10.5)
                  +12345678+03         +123457+03      .
```

FRANTIC INPUT CARD ARRANGEMENT

FORMAT FOR INPUT CARDS FOR SEVERAL SETS OF DATA EACH WITH SEVERAL RUNS.

FRANTIC BINARY DECK

- SET - 1
  - RUN - 1
    - HEADER CARD
    - CONTROL CARD (IC = +)
    - ESTIMATE CARDS (IF IC = 2 OR 3)
    - DATA CONTROL CARD
    - DATA CARDS
  - RUN - 2
    - HEADER CARD
    - CONTROL CARD (IC = -)
    - ESTIMATE CARDS (IF IC = 2 OR 3)
  - RUN - 3
    - HEADER CARD
    - CONTROL CARD (IC = -)
    - ESTIMATE CARDS (IF IC = 2 OR 3)
  - ETC.
- ETC.

6. SAMPLE DATA AND RESULTS

THESE DATA ARE FOR ANALYSIS OF THE HALF LIVES OF F-18 (110.3 ± 0.5 MIN.) AND NA-24 (900 ± 4 MIN.) PUNCHED FOR USE WITH INPUT-A.

```
    SAMPLE ANALYSIS OF F(18) AND NA(24) HALF LIVES IN MINUTES
F-18 NA-24   24 2 2 2
+62445900-03
+77068000-04
+100000+02+400000-08+200000-08+128000+02+300000-03+100000+00+100000+00
+00000000+00+10000000+00+60842000+04
+30000000+00+10000000+00+60575000+04
+47000000+01+10000000+00+55209000+04
+12250000+02+10000000+00+48443000+04
+17700000+02+10000000+00+43840000+04
+21350000+02+10000000+00+41606000+04
+21650000+02+10000000+00+41549000+04
+26650000+02+10000000+00+39366000+04
+43500000+02+10000000+00+33192000+04
+54750000+02+91666667-01+27342000+04
+56200000+02+10000000+00+29492000+04
+12260000+03+10000000+00+17556000+04
+13600000+03+10000000+00+15656000+04
+15360000+03+10000000+00+13715000+04
+16570000+03+10000000+00+12727000+04
+16600000+03+10000000+00+12503000+04
+26910000+03+20000000+00+11207000+04
+26955000+03+20000000+00+11190000+04
+27505000+03+20000000+00+10870000+04
+28965000+03+20000000+00+96900000+03
+30145000+03+20000000+00+90940000+03
+40980000+03+50000000+00+99910000+03
+43720000+03+70000000+00+11559000+04
+45660000+03+50000000+00+73500000+03
```

THE DATE IS JUNE 28, 1962.
THE TIME IS 1044.1

SAMPLE ANALYSIS OF F(18) AND NA(24) HALF LIVES IN MINUTES

F-18 NA-24 = FRANTIC IDENTIFICATION
2 = NUMBER OF COMPONENTS
0 = NUMBER OF PARAMETERS HELD FIXED
24 = NUMBER OF DATA POINTS
20 = DEGREES OF FREEDOM
8 = ITERATIONS
2 = STATISTICAL WEIGHTS
0 = NUMBER OF POINTS (*) DEVIATING MORE THAN 2 SIGMA
07967181.00000 = LEAST SQUARES DETERMINANT
0.10781 = DELTA VARIANCE OF FIT X 10(6)
1.32690 = WEIGHTED VARIANCE OF FIT
32.68209 = CHI SQUARE

100.00000 = TAU (TIME TO COUNTING)
0.04000 = TAUD (DEAD TIME FACTOR IN MICRO TIME UNITS)
0.02000 = ERROR IN DEAD TIME FACTOR (MICRO TIME UNITS)
128.00000 = BACKGROUND
0.00300 = UNCERTAINTY IN TIMING INTERVAL IN TIME UNITS
1.00000 = DATA SCALE FACTOR
1.00000 = NORMALIZATION FACTOR

A(ZERO)	SIGMA	LAMBDA	SIGMA	N(ORIGINAL)	SIGMA	HALF LIFE	SIGMA
16341.443	332.882	0.006638639	0.000261754	4781055.	212184.	104.4110	4.1168
44749.806	267.309	0.000773363	0.000002451	62516273.	422810.	896.2732	2.8426

ORIGINAL ESTIMATES

16510.036	0.006244585
44410.143	0.000770673

ANALYSIS OF THE DEVIATIONS

	0	0	0	0	0	0	0	2	1	4	6	4	2	1	4	0	0	0	0	0	0	0
SIGMA	-XS	-4.5	-4.0	-3.5	-3.0	-2.5	-2.0	-1.5	-1.0	-0.5	-0.0	0.0	0.5	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	XS

	BEGINNING TIME	INTERVAL TIME	ORIGINAL COUNTS	CORRECTED DATA	CALCULATED RATE	INSTANTANEOUS RATE	WEIGHTS X 10(3)	DELTA RATE
1	0.	1.000	60842.0	60862.431	61019.826	61019.795	0.01002	-157.395
2	3.000	1.000	60575.0	60594.130	60594.994	60594.964	0.01008	-0.864
3	47.000	1.000	55209.0	55203.191	55057.582	55057.559	0.01156	145.610
4	122.500	1.000	48443.0	48409.051	47911.374	47911.360	0.01391	497.678
5	177.000	1.000	43840.0	43789.013	44039.507	44039.497	0.01594	-250.494
6	213.500	1.000	41606.0	41547.358	41871.424	41871.417	0.01709	-324.066
7	216.500	1.000	41549.0	41490.167	41705.702	41705.694	0.01712	-215.534
8	266.500	1.000	39366.0	39300.085	39177.577	39177.571	0.01838	122.508
9	435.000	1.000	33192.0	33108.127	32860.822	32860.820	0.02287	247.305
10	547.500	0.917	27342.0	29735.266	29722.005	29722.004	0.02351	13.261
11	562.000	1.000	29492.0	29398.832	29354.863	29354.862	0.02649	43.969
12	1226.000	1.000	17556.0	17440.337	17336.747	17336.747	0.04879	103.590
13	1360.000	1.000	15656.0	15537.811	15627.749	15627.748	0.05551	-89.938
14	1536.000	1.000	13715.0	13594.528	13637.935	13637.934	0.06431	-43.407
15	1657.000	1.000	12727.0	12605.482	12419.345	12419.345	0.06982	186.137
16	1660.000	1.000	12503.0	12381.256	12390.560	12390.559	0.07119	-9.304
17	2691.000	2.000	11207.0	5476.756	5579.989	5579.988	0.34051	-103.233
18	2695.500	2.000	11190.0	5468.252	5560.603	5560.603	0.34103	-92.351
19	2750.500	2.000	10870.0	5308.182	5329.042	5329.041	0.35109	-20.860
20	2896.500	2.000	9690.0	4717.939	4760.059	4760.059	0.39377	-42.120
21	3014.500	2.000	9094.0	4419.827	4344.901	4344.900	0.41943	74.926
22	4098.000	5.000	9991.0	1870.360	1877.426	1877.425	2.34366	-7.066
23	4372.000	7.000	11559.0	1523.395	1517.746	1517.745	3.92638	5.648
24	4566.000	5.000	7350.0	1342.086	1307.303	1307.303	3.12130	34.783

7. FRANTIC FORTRAN LISTING

```
*     LIST
*     LABEL
CFR-II
C     FRANTIC II   PROGRAM FOR DECAY CURVE ANALYSIS  P.C.ROGERS  3/6/62
C            FRANTIC II  MASTER PROGRAM
      DIMENSION T(400), DT(400), C(400), R(400), W(400), A(400), AC(400)
     1, AE(10,400), DA(400), IX(20), IS(6), PC(20), PG(20), BM(20),
     2BMO(20), AM(20,20), AMO(20,20), FMT(14), XID(2)
      COMMON K,DET,AM,BM,AMO,BMO,FMT,ITAPE,JTAPE,XID,N,JMAX,IC,ID,IS,IX,
     1JCALC,JCALC2,IT,TAU,TAUD,B,EB,S,XNORM,VAR2,DVAR,SUM,DTAU,T,DT,C,R,
     2W,A,AC,DA,AE,PG,PC
    1 FORMAT (1H1)
      ITAPE = 4
      JTAPE = 2
   10 SENSELIGHT 0
      CALL INPUT
      JCALC = JMAX
      JCALC2 = JMAX + JMAX
      CALL DATA
      IF (IC - 1) 10,11,13
   11 JCALC = 0
   12 CALL GUESS
   13 WRITE OUTPUT TAPE JTAPE, 1
      CALL LESFIT
      WRITE OUTPUT TAPE JTAPE, 1
      CALL CLOCK (JTAPE)
      CALL OUTPUT
      IF (JCALC - JMAX) 12,10,10
      END
```

```
*     LIST
*     LABEL
CINPUTA
      SUBROUTINE INPUT
      DIMENSION T(400), DT(400), C(400), R(400), W(400), A(400), AC(400)
     1, AE(10,400), DA(400), IX(20), IS(6), PC(20), PG(20), BM(20),
     2BMO(20), AM(20,20), AMO(20,20), FMT(14), XID(2)
      COMMON K,DET,AM,BM,AMO,BMO,FMT,ITAPE,JTAPE,XID,N,JMAX,IC,ID,IS,IX,
     1JCALC,JCALC2,IT,TAU,TAUD,B,EB,S,XNORM,VAR2,DVAR,SUM,DTAU,T,DT,C,R,
     2W,A,AC,DA,AE,PG,PC
   10 FORMAT (13A6,A2)
   11 FORMAT (A6,A4,I4,29I2)
   12 FORMAT (1P6E12.7)
   13 FORMAT (1P7E10.5)
      READ INPUT TAPE ITAPE, 10, (FMT(I), I = 1,14)
      READ INPUT TAPE ITAPE ,11, XID(1), XID(2), N, JMAX, IC, ID,
     1(IS(I), I = 1,6), (IX(I), I = 1,20)
      IF (XABSF(IC)-2) 103,101,101
  101 DO 102 I = 1, JMAX
  102 READ INPUT TAPE ITAPE, 12, PG(2*I), PG(2*I-1)
  103 IF (IC) 110,110,104
  104 READ INPUT TAPE ITAPE, 13, TAU,TAUD,DTAU,B,EB,S,XNORM
      DO 105 I = 1,N
  105 READ INPUT TAPE ITAPE, 12, T(I), DT(I), C(I), R(I), W(I)
  110 RETURN
      END
```

```
*      LIST
*      LABEL
CINPUTB
      SUBROUTINE INPUT
      DIMENSION T(400), DT(400), C(400), R(400), W(400), A(400), AC(400)
     1, AE(10,400), DA(400), IX(20), IS(6), PC(20), PG(20), BM(20),
     2BMO(20), AM(20,20), AMO(20,20), FMT(14), XID(2)
      COMMON K,DET,AM,BM,AMO,BMO,FMT,ITAPE,JTAPE,XID,N,JMAX,IC,ID,IS,IX,
     1JCALC,JCALC2,IT,TAU,TAUD,B,EB,S,XNORM,VAR2,DVAR,SUM,DTAU,T,DT,C,R,
     2W,A,AC,DA,AE,PG,PC
   10 FORMAT (13A6,A2)
   11 FORMAT (A6,A4,I4,29I2)
   12 FORMAT (1P6E12.7)
   13 FORMAT (I3,1P2E12.7)
   14 FORMAT (12F6.0)
   15 FORMAT (1P7E10.5)
      READ INPUT TAPE ITAPE, 10, (FMT(I), I = 1,14)
      READ INPUT TAPE ITAPE ,11, XID(1), XID(2), N, JMAX, IC, ID,
     1(IS(I), I = 1,6), (IX(I), I = 1,20)
      IF (XABSF(IC)-2) 103,101,101
  101 DO 102 I = 1, JMAX
  102 READ INPUT TAPE ITAPE, 12, PG(2*I), PG(2*I-1)
  103 IF (IC) 110,110,104
  104 READ INPUT TAPE ITAPE, 15, TAU,TAUD,DTAU,B,EB,S,XNORM
      IT = 0
  105 K = IT + 1
      READ INPUT TAPE ITAPE, 13, J, T(K), DT(K)
      IT = IT + J
      READ INPUT TAPE ITAPE, 14, (C(I), I = K,IT)
      R(K) = 0.0
      K = K + 1
      DO 106 I = K,IT
      R(I) = 0.0
      T(I) = T(I-1) + DT(I-1)
  106 DT(I) = DT(I-1)
      IF (N-IT)  110,110,105
  110 RETURN
      END
```

```
*      LIST
*      LABEL
CINPUTC
       SUBROUTINE INPUT
       DIMENSION T(400), DT(400), C(400), R(400), W(400), A(400), AC(400)
      1, AE(10,400), DA(400), IX(20), IS(6), PC(20), PG(20), BM(20),
      2BMO(20), AM(20,20), AMO(20,20), FMT(14), XID(2)
       COMMON K,DET,AM,BM,AMO,BMO,FMT,ITAPE,JTAPE,XID,N,JMAX,IC,ID,IS,IX,
      1JCALC,JCALC2,IT,TAU,TAUD,B,EB,S,XNORM,VAR2,DVAR,SUM,DTAU,T,DT,C,R,
      2W,A,AC,DA,AE,PG,PC
    10 FORMAT (13A6,A2)
    11 FORMAT (A6,A4,I4,29I2)
    12 FORMAT (1P6E12.7)
    13 FORMAT (1P8E9.4)
    14 FORMAT (2F6.0,13X,F5.0,1X,10F1.0)
       READ INPUT TAPE ITAPE, 10, (FMT(I), I = 1,14)
       READ INPUT TAPE ITAPE ,11, XID(1), XID(2), N, JMAX, IC, ID,
      1(IS(I), I = 1,6), (IX(I), I = 1,20)
       IF (XABSF(IC)-2) 103,101,101
   101 DO 102 I = 1, JMAX
   102 READ INPUT TAPE ITAPE, 12, PG(2*I), PG(2*I-1)
   103 IF (IC) 110,110,104
   104 READ INPUT TAPE ITAPE, 13, TAU,TAUD,DTAU,B,EB,S,XNORM,TIME
       DO 105 I = 1,N
       READ INPUT TAPE ITAPE, 14, T(I),DT(I),C(I),(X(J), J = 1,10)
       T(I) = T(I)/TIME
       DT(I) = DT(I)/TIME
       R(I) = 0.0
       DO 105 J = 1,10
   105 R(I) = R(I) + X(J)*2.0**(10-J)
   110 RETURN
       END
```

```
*       LIST
*       LABEL
C DATA
        SUBROUTINE DATA
        DIMENSION T(400), DT(400), C(400), R(400), W(400), A(400), AC(400)
       1, AE(10,400), DA(400), IX(20), IS(6), PC(20), PG(20), BM(20),
       2BMO(20), AM(20,20), AMO(20,20), FMT(14), XID(2)
        COMMON K,DET,AM,BM,AMO,BMO,FMT,ITAPE,JTAPE,XID,N,JMAX,IC,ID,IS,IX,
       1JCALC,JCALC2,IT,TAU,TAUD,B,EB,S,XNORM,VAR2,DVAR,SUM,DTAU,T,DT,C,R,
       2W,A,AC,DA,AE,PG,PC
        IF (IC) 210,210,201
  201 DO 203 I = 1,N
  203 C(I) = C(I)*S + R(I)
        IF (ID) 204,204,206
  204 ID = -ID
      SUM = 0.0
      DO 205 I = 1,N
      C(I) = C(I) - SUM
  205 SUM = SUM + C(I)
  206 DO 207 I = 1,N
      R(I) = C(I)/DT(I)
  207 A(I) = (R(I)/(1.0 - R(I)*TAUD) - B) * XNORM
  210 IC = XABSF(IC)
      IF (ID-2) 211,213,215
  211 DO 212 I = 1,N
  212 W(I) = 1.0
      RETURN
  213 DO 214 I = 1,N
      R(I) = C(I)/DT(I)
      X = (R(I)*DTAU) / ((1.0-R(I)*TAUD)**2 - (R(I)*DTAU)**2)
      Y = (EB/DT(I)) / (1.0 - (EB/DT(I))**2)
  214 W(I) = 1.0 / (((R(I)+B)/DT(I) + R(I)**2 * (X**2+Y**2)) * XNORM**2)
  215 RETURN
      END
```

```
*     LIST
*     LABEL
C GUESS
      SUBROUTINE GUESS
      DIMENSION T(400), DT(400), C(400), R(400), W(400), A(400), AC(400)
     1, AE(10,400), DA(400), IX(20), IS(6), PC(20), PG(20), BM(20),
     2BMO(20), AM(20,20), AMO(20,20), FMT(14), XID(2)
      COMMON K,DET,AM,BM,AMO,BMO,FMT,ITAPE,JTAPE,XID,N,JMAX,IC,ID,IS,IX,
     1JCALC,JCALC2,IT,TAU,TAUD,B,EB,S,XNORM,VAR2,DVAR,SUM,DTAU,T,DT,C,R,
     2W,A,AC,DA,AE,PG,PC
      IF (JCALC) 400,400,402
  400 DO 401 I = 1,20
      IX(I) = 0
  401 PG(I) = 0.0
      PG(2) = ABSF(LOGF(A(1)/A(N))/(T(N) - T(1)))
      IS(2) = 1
      JCALC = 1
      JCALC2 = 2
      RETURN
  402  DO 403 I = 1,JCALC2,2
      PG(I) = 0.0
  403 PC(I+1) = ABSF(PC(I+1))
      X=MAX1F(PC(2),PC(4),PC(6),PC(8),PC(10),PC(12),PC(14),PC(16),PC(18)
     1)
      IF (IS(1)) 405,404,405
  404 PC(JCALC2 + 2) = X*10.0
      GO TO 406
  405 PC(JCALC2 + 2) = X*3.0
  406 J = 0
      DO 409 I = 2, JCALC 2, 2
      IF(PC(I) - PC(I + 2)) 407,407,408
  407 X = PC(I)
      PC(I) = PC(I + 2)
      PC(I + 2) = X
      GO TO 409
  408 J = J + 1
  409 CONTINUE
      IF (J-JCALC) 406,410,410
  410 JCALC = JCALC + 1
      JCALC2 = JCALC2 + 2
      DO 411 I = 2, JCALC2, 2
  411 PG(I) = PC(I)
      RETURN
      END
```

```
*       LIST
*       LABEL
CLESFIT
        SUBROUTINE LESFIT
        DIMENSION T(400), DT(400), C(400), R(400), W(400), A(400), AC(400)
       1, AE(10,400), DA(400), IX(20), IS(6), PC(20), PG(20), BM(20),
       2BMO(20), AM(20,20), AMO(20,20), FMT(14), XID(2)
        COMMON K,DET,AM,BM,AMO,BMO,FMT,ITAPE,JTAPE,XID,N,JMAX,IC,ID,IS,IX,
       1JCALC,JCALC2,IT,TAU,TAUD,B,EB,S,XNORM,VAR2,DVAR,SUM,DTAU,T,DT,C,R,
       2W,A,AC,DA,AE,PG,PC
        DIMENSION DP(20), P(20)
  501   FORMAT (//1X,A6,A4,F18.4,6PF18.2/(1P8E15.7))
        EXPPF(X) = 1.0 + X/6.0 + X**2/120.0 + X**3/5040.0
        IT = 0
        IMA = 0
        IML = 0
        VAR1 = 0.0
        DO 514 I = 1, JCALC2, 2
        IF (IX(I)) 510,511,510
  510   IMA = IMA + 1
  511   IF (IX(I + 1)) 512,513,512
  512   IML = IML + 1
  513   IX(I + 1) = IX(I + 1) + 100
        DP(I) = 0.0
        DP(I+1) = 0.0
        PC(I) = PG(I)
  514   PC(I + 1) = PG(I + 1)
        DO 520 L = 1,N
        DO 520 I = 1, JCALC
        J = 2*I
        X = PC(J)*DT(L)
        Y = PC(J)*T(L)
        IF (X-1.0) 519,519,518
  518   AE(I,L) = EXPF(-Y)*(1.0 - EXPF(-X))/X
        GO TO 520
  519   AE(I,L) = EXPF(-Y-X/2.0)*EXPPF((X/2.0)**2)
  520   CONTINUE
        K = JCALC - IMA
        IF (K) 526,526,521
  521   IT = 1
        IF (IC-2) 523,523,550
  523   CALL MATRIX
        CALL MATINV
        J = 1
        DO 525 I = 1, JCALC2, 2
        IF (IX(I)) 525,524,525
  524   PC(I) = BM(J)
        J = J + 1
  525   CONTINUE
  526   IF (JCALC - IML) 527,527,550
  527   SENSELIGHT 1
        GO TO 550
C
C       ITERATIVE SECTION
C
  535   IT = IT + 1
        CALL MATRIX
        CALL MATINV
        J = 1
```

```
      IF (IT - 5) 536,536,537
  536 H = 0.7
      GO TO 538
  537 H = 0.98
  538 DO 545 I = 1,JCALC2
      IF (IX(I)) 545,540,545
  540 DP(I) = H*BM(J)
  541 PC(I) = P(I) + DP(I)
      IF (IS(2)) 544,542,544
  542 IF (PC(I)*P(I)) 543,543,544
  543 DP(I) = DP(I)/2.0
      GO TO 541
  544 J = J + 1
  545 CONTINUE
C
C     CALCULATION OF FIT
C
  550 VAR2 = 0.0
      DO 563 L = 1,N
      AC(L) = 0.0
      DO 562 I = 1,JCALC
      J = 2*I
      IF (IX(J)) 562,559,562
  559 X = PC(J)*DT(L)
      Y = PC(J)*T(L)
      IF (X - 1.0) 561,561,560
  560 AE(I,L) = EXPF(-Y)*(1.0 - EXPF(-X))/X
      GO TO 562
  561 AE(I,L) = EXPF(-Y-X/2.0)*EXPPF((X/2.0)**2)
  562 AC(L) = AC(L) + PC(J - 1)*AE(I,L)
      DA(L) = A(L) - AC(L)
  563 VAR2 = VAR2 + DA(L)**2*W(L)
C
C     TEST FIT
C
      DVAR = ABSF((VAR2 - VAR1)/VAR2)
      IF (IS(3)) 564,565,564
  564 WRITE OUTPUT TAPE JTAPE, 501, XID(1), XID(2), IT, JCALC, VAR2,
     1DVAR, (PC(I),DP(I), I = 1,JCALC2)
  565 IF (SENSELIGHT 1) 575,566
  566 IF (IT - 25) 567,575,575
  567 DO 569 I = 1,JCALC2
      IF (IX(I)) 569,568,569
  568 IF (ABSF(DP(I)/PC(I)) - 0.000001) 569,569,570
  569 CONTINUE
      IF (DVAR - 0.000001) 575,575,570
  570 DO 571 I = 1,JCALC2
  571 P(I) = PC(I)
      VAR1 = VAR2
      IF (IT - 1) 572,572,535
  572 DO 574 I = 1,JCALC2,2
      IX(I + 1) = IX(I + 1) - 100
      IF (IS(2)) 574,573,574
  573 P(I) = ABSF(P(I))
      IF (PG(I)) 576,574,574
  576 P(I) = -P(I)
  574 PG(I) = PC(I)
      K = JCALC2 - IMA - IML
      GO TO 535
  575 RETURN
      END
```

```
*     LIST
*     LABEL
CMATRIX
      SUBROUTINE MATRIX
      DIMENSION T(400), DT(400), C(400), R(400), W(400), A(400), AC(400)
     1, AE(10,400), DA(400), IX(20), IS(6), PC(20), PG(20), BM(20),
     2BMO(20), AM(20,20), AMO(20,20), FMT(14), XID(2)
      COMMON K,DET,AM,BM,AMO,BMO,FMT,ITAPE,JTAPE,XID,N,JMAX,IC,ID,IS,IX,
     1JCALC,JCALC2,IT,TAU,TAUD,B,EB,S,XNORM,VAR2,DVAR,SUM,DTAU,T,DT,C,R,
     2W,A,AC,DA,AE,PG,PC
      DIMENSION PART(20)
      DO 606 I = 1,K
      DO 605 J = 1,K
  605 AM(I,J) = 0.0
  606 BM(I) = 0.0
      DO 625 L = 1,N
      J = 1
      DO 613 I = 1,JCALC
      JA = 2*I
      IF (IX(JA-1)) 608,607,608
  607 PART(J) = AE(I,L)
      J = J + 1
  608 IF (IX(JA)) 613,609,613
  609 X = PC(JA)*DT(L)
      IF (X-0.2) 611,611,610
  610 PART(J) =((1.0/PC(JA)+T(L)+DT(L))*EXPF(-X)-1.0/PC(JA)-T(L))/X
      GO TO 612
  611 PART(J) = -T(L)-DT(L)/2.0+X/2.0*(T(L)+DT(L))-(1.0/PC(JA)+T(L)+
     1DT(L))*((X**2)/6.0-(X**3)/24.0+(X**2)**2/120.0-(X**2)*(X**3)/720.)
  612 PART(J) = PART(J)*PC(JA-1)*EXPF(-PC(JA)*T(L))
      J = J + 1
  613 CONTINUE
      DO 620 I = 1,K
      DO 620 J = 1,K
  620 AM(I,J) = AM(I,J) + PART(I)*PART(J)*W(L)
      IF (IT-1) 621,621,623
  621 DO 622 I = 1,K
  622 BM(I) = BM(I) + PART(I)*W(L)*A(L)
      GO TO 625
  623 DO 624 I = 1,K
  624 BM(I) = BM(I) + PART(I)*W(L)*DA(L)
  625 CONTINUE
      DO 627 I = 1,K
      DO 626 J = 1,K
  626 AMO(I,J) = AM(I,J)
  627 BMO(I) = BM(I)
      RETURN
      END
```

```
*     LIST
*     LABEL
CMATINV
      SUBROUTINE MATINV
      COMMON K,DET,AM,BM
      DIMENSION AM(20,20), BM(20), PIVOT(20), IPIVOT(20), INDEX(20,2)
      EQUIVALENCE (IROW,JROW), (ICOLUM,JCOLUM), (AMAX, TA, SWAP)
  701 DET = 1.0
  702 DO 703 J = 1,K
  703 IPIVOT (J) = 0
  704 DO 741 I = 1,K
  705 AMAX = 0.0
  706 DO 715 J = 1,K
  707 IF(IPIVOT(J)-1) 708,715,708
  708 DO 714 M = 1,K
  709 IF ( IPIVOT(M)-1) 710,714,753
  710 IF (ABSF(AMAX)-ABSF(AM(J,M))) 711,714,714
  711 IROW = J
  712 ICOLUM = M
  713 AMAX = AM(J,M)
  714 CONTINUE
  715 CONTINUE
  716 IPIVOT (ICOLUM) = IPIVOT (ICOLUM) + 1
  717 IF (IROW-ICOLUM) 718,726,718
  718 DET = -DET
  719 DO 722 L = 1,K
  720 SWAP = AM(IROW,L)
  721 AM(IROW,L) = AM(ICOLUM,L)
  722 AM(ICOLUM,L) = SWAP
  723 SWAP = BM(IROW)
  724 BM(IROW) = BM(ICOLUM)
  725 BM(ICOLUM) = SWAP
  726 INDEX(I,1) = IROW
  727 INDEX(I,2) = ICOLUM
  728 PIVOT(I) = AM(ICOLUM,ICOLUM)
  729 DET = DET*PIVOT(I)
  730 AM(ICOLUM,ICOLUM) = 1.0
  731 DO 732 L =1,K
  732 AM(ICOLUM,L) = AM(ICOLUM,L)/PIVOT(I)
  733 BM(ICOLUM) = BM(ICOLUM)/PIVOT(I)
  734 DO 741 L1 = 1,K
  735 IF(L1-ICOLUM) 736,741,736
  736 TA = AM(L1,ICOLUM)
  737 AM(L1,ICOLUM) = 0.0
  738 DO 739 L = 1,K
  739 AM(L1,L) = AM(L1,L)-AM(ICOLUM,L)*TA
  740 BM(L1) = BM(L1)-BM(ICOLUM)*TA
  741 CONTINUE
  742 DO 752 I = 1,K
  743 L = K+1-I
  744 IF(INDEX(L,1)-INDEX(L,2)) 745,752,745
  745 JROW = INDEX(L,1)
  746 JCOLUM = INDEX(L,2)
  747 DO 751 M = 1,K
  748 SWAP = AM(M,JROW)
  749 AM(M,JROW) = AM(M,JCOLUM)
  750 AM(M,JCOLUM) = SWAP
  751 CONTINUE
  752 CONTINUE
  753 RETURN
      END
```

```
*       LIST
*       LABEL
COUTPUT
      SUBROUTINE OUTPUT
      DIMENSION T(400), DT(400), C(400), R(400), W(400), A(400), AC(400)
     1, AE(10,400), DA(400), IX(20), IS(6), PC(20), PG(20), BM(20),
     2BMO(20), AM(20,20), AMO(20,20), FMT(14), XID(2)
      COMMON K,DET,AM,BM,AMO,BMO,FMT,ITAPE,JTAPE,XID,N,JMAX,IC,ID,IS,IX,
     1JCALC,JCALC2,IT,TAU,TAUD,B,EB,S,XNORM,VAR2,DVAR,SUM,DTAU,T,DT,C,R,
     2W,A,AC,DA,AE,PG,PC
      DIMENSION SP(20), XNORIG(10), ENORIG(10), HL(10), EHL(10),
     1AINST(400), NP(400), Y(3), IDEV(23)
  801 FORMAT(//5X,A6,A4,25H = FRANTIC IDENTIFICATION,19X,F10.5,25H = TAU
     1 (TIME TO COUNTING))
  802 FORMAT (I15,23H = NUMBER OF COMPONENTS,21X,6PF10.5,46H = TAUD (DEA
     1D TIME FACTOR IN MICRO TIME UNITS))
  800 FORMAT (I15,34H = NUMBER OF PARAMETERS HELD FIXED,10X,6PF10.5,47H
     1= ERROR IN DEAD TIME FACTOR (MICRO TIME UNITS))
  803 FORMAT (I15,24H = NUMBER OF DATA POINTS,20X,F10.5,13H = BACKGROUND
     1)
  804 FORMAT (I15,21H = DEGREES OF FREEDOM,23X,F10.5,47H = UNCERTAINTY I
     1N TIMING INTERVAL IN TIME UNITS)
  805 FORMAT (I15,13H = ITERATIONS,31X,F10.5,20H = DATA SCALE FACTOR)
  806 FORMAT (I15,15H = UNIT WEIGHTS)
  807 FORMAT (I15,22H = STATISTICAL WEIGHTS)
  808 FORMAT (I15,18H = SPECIAL WEIGHTS)
  809 FORMAT (1X,F14.5,28H = LEAST SQUARES DETERMINANT)
  810 FORMAT (1H+,50X,12H(LOUSY LUCK))
  811 FORMAT (1X,F14.5,27H = WEIGHTED VARIANCE OF FIT)
  812 FORMAT (1X,F14.5,13H = CHI SQUARE)
  813 FORMAT (1H+,35X,26H(BEASTLY FIT - CHECK DATA))
  814 FORMAT (1H+,58X,F10.5,23H = NORMALIZATION FACTOR)
  815 FORMAT (///118H        A(ZERO)          SIGMA          LAMBDA
     1  SIGMA        N(ORIGINAL)          SIGMA        HALF LIFE       SIGMA
     2 //)
  816 FORMAT (1X,F14.3,F15.3,2F15.9,2F15.0,2F15.4)
  817 FORMAT (27H0         ORIGINAL ESTIMATES//)
  818 FORMAT (1X,F14.3,F30.9)
  819 FORMAT (///6X,111HBEGINNING    INTERVAL       ORIGINAL        CORRE
     1CTED        CALCULATED    INSTANTANEOUS    WEIGHTS           DELTA/
     29X,4HTIME,8X,4HTIME,10X,6HCOUNTS,11X,4HDATA,12X,4HRATE,12X,4HRATE,
     38X,7HX 10(3),10X,4HRATE//)
  820 FORMAT (I4,F11.3,F12.3,F15.1,3F16.3,3PF15.5,0PF14.3)
  821 FORMAT (///4H   I,39X,6HA(I,J),61X,4HB(I)//)
  822 FORMAT (I4,1P5E17.7/(1PE21.7,1P4E17.7))
  823 FORMAT (1H+,1PE119.7//)
  824 FORMAT (4H   I,35X,17HINVERSE OF A(I,J)//)
  825 FORMAT (6PF15.5,32H = DELTA VARIANCE OF FIT X 10(6))
  826 FORMAT (I15,51H = NUMBER OF POINTS (*) DEVIATING MORE THAN 2 SIGMA
     1)
  827 FORMAT (1H+,118X,1H*)
  828 FORMAT (20X,13A6,A2)
  829 FORMAT (///40X,26HANALYSIS OF THE DEVIATIONS//)
  830 FORMAT (5X,22I5/1X,114HSIGMA -XS  -4.5 -4.0 -3.5 -3.0 -2.5 -2.0 -1
     1.5 -1.0 -0.5 -0.0  0.0  0.5  1.0  1.5  2.0  2.5  3.0  3.5  4.0  4.
     25  XS)
      IDF = N-K
      K = JCALC2 - K
      IF(IDF) 832,832,831
```

```
831 VAR2 = VAR2/FLOATF(IDF)
832 J = 1
    DO 835 I = 1,JCALC2
    IF  (IX(I)) 834,833,834
833 SP(I) = SQRTF(ABSF(AM(J,J)*VAR2))
    J = J + 1
    GO TO 835
834 SP(I) = 0.0
835 CONTINUE
    DO 841 I = 1,JCALC
    J = 2*I
    IF (PC(J)) 837,836,837
836 XNORIG(I) = 0.0
    ENORIG(I) = 0.0
    HL(I) = 0.0
    EHL(I) = 0.0
    GO TO 841
837 HL(I) = 0.693147 / PC(J)
    DO 839 JP = 1,2
    JPP = J - 2 + JP
    Y(JP) = ABSF(SP(JPP)/PC(JPP))
    IF (Y(JP))  839,839,838
838 IF (LOGF(Y(JP)) - 37.0)  839,840,840
839 CONTINUE
    X = PC(J)*TAU
    IF (X - 80.0)  842,840,840
842 XNORIG(I) = PC(J-1)/PC(J)*EXPF(X)
    ENORIG(I) = ABSF(XNORIG(I)*SQRTF(Y(1)**2 + Y(2)**2))
    EHL(I) = ABSF(HL(I)*Y(2))
    GO TO 841
840 XNORIG(I) = -1.0
    ENORIG(I) = -1.0
    EHL(I) = -1.0
841 CONTINUE
    NP2S = 0
    CHISQ = 0.0
    DO 844 I = 1,23
844 IDEV(I) = 0
    DO 847 L = 1,N
    NP(L) = 0
    AINST(L) = 0.0
    DO 845 I = 1,JCALC2,2
845  AINST(L) = AINST(L) + PC(I)*EXPF(-PC(I+1)*(T(L)+DT(L)/2.0))
    X = DA(L)**2
    CHISQ = CHISQ + DT(L)/AC(L)*X
    X = SQRTF(X*W(L))
    I = 12.0 + SIGNF(2.0*X,DA(L))
    IF (I)  850,850,851
850 I = 1
    GO TO 853
851 IF (I - 22)  853,853,852
852 I = 22
853 IDEV(I) = IDEV(I) + 1
    IF (X - 2.0)  847,846,846
846 NP2S = NP2S + 1
    NP(L) = 1
847 CONTINUE
    CHISQ = CHISQ/XNORM
    WRITE OUTPUT TAPE JTAPE, 828, (FMT(I), I = 1,14)
```

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      WRITE OUTPUT TAPE JTAPE, 801, XID(1), XID(2), TAU
      WRITE OUTPUT TAPE JTAPE, 802, JCALC, TAUD
      WRITE OUTPUT TAPE JTAPE, 800, K, DTAU
      WRITE OUTPUT TAPE JTAPE, 803, N, B
      WRITE OUTPUT TAPE JTAPE, 804, IDF, EB
      WRITE OUTPUT TAPE JTAPE, 805, IT, S
      IF (ID-2) 859,861,863
  859 WRITE OUTPUT TAPE JTAPE, 806, ID
      GO TO 864
  861 WRITE OUTPUT TAPE JTAPE, 807, ID
      GO TO 864
  863 WRITE OUTPUT TAPE JTAPE, 808, ID
  864 WRITE OUTPUT TAPE JTAPE, 814, XNORM
      WRITE OUTPUT TAPE JTAPE, 826, NP2S
      WRITE OUTPUT TAPE JTAPE, 809, DET
      IF (DET) 866,867,867
  866 WRITE OUTPUT TAPE JTAPE, 810
  867 WRITE OUTPUT TAPE JTAPE, 825, DVAR
      WRITE OUTPUT TAPE JTAPE, 811, VAR2
      WRITE OUTPUT TAPE JTAPE, 812, CHISQ
      IF (CHISQ/FLOATF(IDF) - 16.0) 876,875,875
  875 WRITE OUTPUT TAPE JTAPE, 813
  876 WRITE OUTPUT TAPE JTAPE, 815
      WRITE OUTPUT TAPE JTAPE, 816, (PC(2*I-1),SP(2*I-1),PC(2*I),SP(2*I)
     1,XNORIG(I), ENORIG(I), HL(I), EHL(I), I = 1,JCALC)
      IF (IT-1)  880,880,881
  881 WRITE OUTPUT TAPE JTAPE, 817
      WRITE OUTPUT TAPE JTAPE, 818, (PG(I), I = 1,JCALC2)
  880 IF (ID-1)  883,883,882
  882 WRITE OUTPUT TAPE JTAPE, 829
      WRITE OUTPUT TAPE JTAPE, 830, (IDEV(I), I = 1,22)
  883 WRITE OUTPUT TAPE JTAPE, 819
      DO 885 L = 1,N
      WRITE OUTPUT TAPE JTAPE, 820, L,T(L),DT(L),C(L),A(L),AC(L),
     1AINST(L),W(L),DA(L)
      IF (NP(L)) 885,885,884
  884 WRITE OUTPUT TAPE JTAPE, 827
  885 CONTINUE
      IF (IS(4)) 887,895,887
  887 WRITE OUTPUT TAPE JTAPE, 821
      DO 890 I = 1,K
      WRITE OUTPUT TAPE JTAPE, 822, I, (AMO(I,J), J = 1,K)
  890 WRITE OUTPUT TAPE JTAPE, 823, BMO(I)
      WRITE OUTPUT TAPE JTAPE, 824
      DO 894 I = 1,K
      WRITE OUTPUT TAPE JTAPE, 822, I, (AM(I,J), J = 1,K)
  894 WRITE OUTPUT TAPE JTAPE, 823, BM(I)
  895 RETURN
      END
```