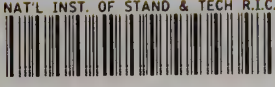


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# A New Method of Assigning Uncertainty in Volume Calibration

James A. Lechner, Charles P. Reeve, Clifford H. Spiegelman

Issued December 1980



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**U.S. DEPARTMENT OF COMMERCE, Philip M. Klutznick, *Secretary***  
**Jordan J. Baruch, *Assistant Secretary for Productivity, Technology, and Innovation***  
**NATIONAL BUREAU OF STANDARDS, Ernest Ambler, *Director***



\*A NEW METHOD OF ASSIGNING UNCERTAINTY IN VOLUME CALIBRATION

by

James A. Lechner  
Charles P. Reeve  
Clifford H. Spiegelman

with programming assistance from  
Martin Ross Cordes and Janice M. Knapp

---

\*Work supported (in part) by the U. S. Nuclear Regulatory Commission.



## ABSTRACT

This paper presents a practical statistical overview of the pressure-volume calibration curve for large nuclear materials processing tanks. It explains the appropriateness of applying splines (piecewise polynomials) to this curve, and it presents an overview of the associated statistical uncertainties. In order to implement these procedures a practical and portable FORTRAN IV program is provided along with its users' manual. Finally, the recommended procedure is demonstrated on actual tank data collected by NBS.

Key Words: Volume calibration; differential pressure; splines; accountability; statistics.

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## 1. Introduction.

The direct measurement of liquid volume in large processing tanks, especially with internal structure, is impractical at best. Measuring (differential) pressure is simple and quick. However, in order to estimate the volume indirectly by observing pressure, it is necessary to use the relationship between volume and pressure. This relationship is known as a calibration curve; its estimation is the process known as calibration.

Fitting a calibration curve is much like regression, in that for "known" values  $v_i$  of volume, one obtains one or more observations  $p_{ij}$  of the differential pressure  $p_i = p(v_i)$ , and "fits" a response function  $p(v)$  by statistical methods - usually by least squares. At this point, the correspondence stops. Whereas regression is used to predict values of the dependent variable ( $p$ ) for given values of the independent variable ( $v$ ), or to test a proposed relationship between the variables, a calibration curve is used to estimate values of the independent variable  $v$  corresponding to new measured values of the dependent variable  $p$ . Furthermore, the confidence interval (or uncertainty measure) which is desired is not for  $p$ , but rather for  $v$ . And finally, systematic error is introduced by lack of fit of the calibration curve, and in a materials accounting situation this may be crucial.

This paper presents a method for producing valid uncertainty limits for the pressure-volume tank calibration curve by using calibration functions which are smooth, piecewise polynomial functions called "splines." Taking advantage of an approach to calibration originated by Scheffé [1] and further elucidated by Scheffé, Rosenblatt and

Spiegelman [2], it provides statistically sound uncertainty limits, not just for a single estimated value of volume, but for all volumes estimated by use of the fitted curve. This approach overcomes a major theoretical problem with earlier methods: it makes proper allowance for the contribution to the overall uncertainty of errors in fitting the curve.

The procedure presented herein has been implemented, based upon a spline-fitting program due to deBoor [3]. The resulting FORTRAN program has been tested on various sets of data, including actual tank data.

The remainder of this paper is organized as follows. Section 2 contains a discussion of the pressure-volume model, and the statistics of calibration. Section 3 contains a discussion of an example, and of the printout produced by the program. Section 4 is essentially a users' manual for the program. In Section 5 will be found a discussion of open questions, work in progress, cautions, and possible extensions of this technique. Finally, Appendix 1 contains a discussion of Scheffe's constant  $c$ , used as an input to the program, and Appendix 2 contains a listing of the program.

## 2. The Scientific Basis for, and Interpretation of, a Calibration Curve.

In order to provide statistically valid uncertainty limits for the volume estimates obtained through the use of a calibration curve, it is necessary to have a prior model for the pressure-volume relationship. That is, while the constants in the model for the relationship may be determined from the data, the form of the model must not depend on the data to be used in fitting the relationship. In addition, the less accurately the hypothesized model describes this relationship, the less

valid will be the resulting uncertainty statements. That is, inaccuracies in the hypothesized model will lead to systematic differences between true and fitted curves. In order to obtain valid uncertainty statements, bounds for such differences must be determined, and added to the statistical uncertainty as systematic error limits.

The interiors of large processing tanks do not generally conform to idealized geometrical shapes, such as cylinders. Often, however, the tank can be considered to be composed only of segments for which an idealized model is a good representation. In this paper it is assumed that the tank is composed of a finite number,  $k+1$ , of distinct and known regions where the idealized relationship between the two variables pressure,  $p$ , and volume,  $v$ , is given by

$$\begin{aligned}
 p &= f(v) \\
 &= g_1(v) && \xi_0 < v < \xi_1 \\
 &= g_2(v) && \xi_1 < v < \xi_2 \\
 &\vdots \\
 &= g_{k+1}(v) && \xi_k < v < \xi_{k+1} .
 \end{aligned}$$

In addition, continuity of the relationship at the interior "knots"  $\xi_i$ ,  $i=1, \dots, k$  is required.

In all that follows, volume and height refer to the portion of the tank above the bottom of the diptube used to measure pressure. The portion of the tank below that point is known as the heel, and is not treated in this paper. The pressure measured is the difference in

pressure between the bottom of the diptube and a reference point at the top of the tank.

The pressure-volume relationship can be ascertained from the following two equations. At height  $h$  the volume in the container is

$$v = \int_0^h A(x) dx$$

where  $A(x)$  is the cross-sectional area at height  $x$ . Also, when the liquid height is  $h$ ,  $p = h\rho g$ , where  $\rho$  is the density of the homogeneous liquid and  $g$  is the acceleration due to gravity. Using these two equations one easily obtains

$$v = \int_0^{p/\rho g} A(x) dx .$$

Thus  $\frac{\partial v}{\partial p} = \frac{1}{\rho g} A(p/\rho g)$  and hence in areas of the tank where  $A(x)$  is

constant the volume-pressure relationship is a straight line.

If  $A(x)$  is constant\* in region  $i$ , as it obviously is for at least some regions of the tank shown in Figure 1, then

$$(1) \quad p = g_i(v) = \gamma_i + \beta_i v \text{ for } \xi_{i-1} < v < \xi_i, \quad i=1, \dots, k+1.$$

We assume that each pressure measurement has a random error associated with it, and that these errors are independent and

---

\* If  $A(x)$  is not constant on an interval, then  $p$  is not a linear function of  $v$  on that interval. The program under discussion uses the B-spline basis when higher-order polynomial splines are required, because as pointed out in reference [4], the use of simpler representations of polynomial splines may lead to numerical instability.

normally-distributed, with mean zero and constant variance  $\sigma^2$ . (Recall that volume is assumed to be measured with no significant error.) Because of these errors, only estimates of the coefficients  $\gamma_i$  and  $\beta_i$  are obtained during the calibration process (experiment). These coefficient estimates are then used during plant operation to obtain estimates of the volume in the tank, utilizing the inverse of the relationship (1).

Determination of uncertainty limits on these estimates is not trivial. There are two sources of random error: estimation of the coefficients  $\gamma$  and  $\beta$  in the calibration experiment, and measurement of  $p$  during operational use of the tank. The familiar linear regression model has properties, such as the nonexistence of means and variances of reciprocals, which make the analysis difficult. Special justification involving asymptotic (large sample-size) behavior is thus required in order to use a propagation-of-error approach to obtain appropriate approximate uncertainty limits on the estimated volumes. Furthermore, unless the  $p$ - $v$  relationship is linear, normally distributed errors in the  $p$ -measurements during operation produce non-normal errors in the resulting estimates of  $v$ . The usual propagation-of-error technique does not take into account the differing characteristics of these errors. The new technique presented in this paper, in contrast to the propagation-of-error approach just mentioned, does allow a correct accounting for both.

The calibration chart (i.e., the table of uncertainty limits) is produced after choosing two probabilities,  $\alpha$  and  $\delta$ . An exact statement giving the interpretation of these probabilities may be found in Scheffé

[1] and in Scheffé, Rosenblatt, and Spiegelman [2]. However, an expanded, more heuristic explanation is given here. First, we require bounds for the calibration curve which will contain the entire curve with a prechosen probability  $1-\delta$ . (Thus,  $\delta$  can be thought of as describing the uncertainty level to be associated with the outcome of the initial calibration experiment.) These bounds guarantee, with probability  $1-\delta$ , that for any and every future volume  $v$  within the range of calibration of the tank, the  $v$ -interval (see Figure 2) that would be obtained by projection of the value  $f(v)$  through the curves to  $\underline{v}$  and  $\bar{v}$  would contain  $v$ . The second probability level to be chosen is  $\alpha$ . (Here  $\alpha$  can be thought of as describing the uncertainty level to be attributed to errors in future individual pressure measurements.) If  $\sigma$  were known, we could state that the true pressure  $f(v)$  at the unknown volume  $v$  lies within the  $1-\alpha$  confidence interval  $(p-z_{1-\alpha/2}\sigma, p+z_{1-\alpha/2}\sigma)$  with probability  $1-\alpha$ , where  $p$  is the observed pressure and  $z_{1-\alpha/2}$  is the two-sided  $1-\alpha$  value for a normal distribution. The Scheffé procedure expands this interval appropriately, to account for the facts that  $\sigma$  is estimated and that this estimate is used for the  $1-\delta$  bound on the curve and for bounds on many different  $f(v)$ . It then combines the  $1-\alpha$  confidence interval for  $f(v)$  with the  $1-\delta$  bounds on the calibration curve to produce calibration intervals  $I(p)$  for  $v$ . Construction of the calibration intervals is shown schematically in Figure 3. A set of intervals  $I(p_i)$  for  $p_i$  in the range of values obtained during the calibration experiment is called a calibration chart (see Figure 4).

In the discussion of the example presented in the next section, more detail on the nature of the steps that make up a calibration run will be found.

### 3. An Example.

This example relates to a processing tank, roughly circular in cross section, but with internal structure consisting of cooling coils, stirrers, braces, etc. [5]. This tank is pictured in Figure 1. The data from calibration runs on this tank have graciously been made available by the author of reference [5].

There were five calibration runs for which the data were useful for this analysis. One run was done in the canyon where the tank is to be used. The other four, done in a mock-up area, used smaller tubing in the pressure-measuring system. This smaller tubing was known to cause systematic differences in the pressure measurement, which were expected to be linearly related to pressure for each run. Since the tubing in the canyon was sufficiently large to render the pressure drop insignificant, the systematic error was estimated for each of the other four runs, and a correction made by applying a linear transformation to the measured pressure. It should be noted that these corrections, made to four of the five runs, effectively decrease the degrees of freedom for the error sum of squares by eight (two correction parameters times four runs corrected).

The calibration program was applied to these data, as were various other techniques available on the large central computer at NBS. The results will now be presented and their use described.

In the version of the program described here, the knot locations are input by the analyst. It is presumed that the knot locations can be adequately prescribed from the blueprints and other knowledge about the tank. (A refinement which allows the automatic determination of the

number and location of knots is being investigated.) The program displays the given knot locations and other input data, as shown in Figure 5. Next come the results of the fitting operation, as shown in part in Figure 6. Note that the fit here is a fit of observed pressure (y) as a function of the accurately-dispensed volume (x); it is pressure which is subject to errors of observation, and volume which is essentially known. The residual standard deviation, an estimate of the standard deviation of the pressure measurements, is derived from the residuals or deviations of the measured pressures from the fitted curve. In this case, its value is 1.49 pascals. This value, the corresponding degrees of freedom, and the coefficients (which are in general not immediately interpretable, since they refer to the so-called B-splines, a representation chosen for computational stability), are part of these results. The calibration intervals for estimation of volume from measured pressure are printed next (see Figure 4). An ordinary polynomial representation and a residual plot are also printed as shown in Figures 7 and 8.

It will be instructive to examine the printout and discuss the approach in more detail, and this will now be done.

As can be seen from Figure 5, the program duplicates the end knots. This is just a simple way to define the B-spline basis functions which are used to perform the fit, and need not concern the analyst. The input values for knot locations, degree of fit, and other miscellaneous parameters are printed out for verification.



At this point, the program does a linear least squares fit of the specified model to the (v,p) data, and prints out a reasonably standard summary (Figure 6). The column labels are self-explanatory. At the bottom of this summary are found the residual standard deviation and its associated degrees of freedom, and the estimated coefficients with the corresponding estimated standard deviations.

The program next computes some intermediate results which generally are of no interest to the analyst, and therefore are only printed out if requested. These are confidence intervals for p, at 300 evenly-spaced points covering the range of v between the extreme knots. Input values of  $\alpha$ ,  $\delta$ , and c are used in this procedure, so these values are printed.

The calibration chart comes next, giving the predicted value of v and the corresponding lower and upper limits for each of the specified set of p-values (see Figure 4). It is obtained by inverse interpolation from the confidence intervals for p discussed in the preceding paragraph. Usually, the extreme values of p will be at least partially outside the range of at least one of the curves. When this happens, the intervals should extend either to zero volume or to full volume. This is indicated by "<" and ">" respectively on the printout.

Since the coefficients actually fitted are the B-spline coefficients, the program converts the B-spline representation to a simple polynomial representation. The printout shows the endpoints and the coefficients of the fitted polynomial for each of the specified intervals (see Fig. 7).

Finally, the residuals from the fitted model are plotted in order of increasing volume to allow a visual check of the adequacy of the chosen model [6] (see Fig. 8).

At NBS, with the aid of the central computer and the OMNITAB system [7], a number of other things were tried which strengthen the conviction that this program does indeed work well. These will now be discussed.

Various subsets of the data were fitted to the same model. No inconsistencies were found.

The sensitivity to position and presence of the different knots was checked. The results were rather sensitive to the knot locations, which implies that good estimates of the locations are required for good fits. It should also be noted that where a knot bounds a short segment, the removal of that knot might make very little difference in any global measure of fit quality, unless there are many data points in that short stretch. Nevertheless, the systematic error introduced by deleting that knot can be a consistent source of inventory losses or gains, apparent or real. Thus it is important to include all real segments in the model to be fitted.

A separate program was written to perform linear spline fitting, while the main package was being put together. The answers did not differ between the two programs, providing a partial check that no programming errors were committed.

Smooth higher-order spline fits were tried (quadratic and cubic). There was no improvement in fit. The linear spline appears to provide an adequate representation of the pressure/volume relationship.

Probability plots were done in various ways, looking for possible troubles with the data or the method. Nothing suspicious was found.

#### 4. User's Manual.

This fixed-knot spline package for calibration consists of a "main" subroutine SPLEEN and 29 additional subroutines. The manner in which they interact is diagrammed in Figure 9. All programs are written in FORTRAN and have been checked for portability by the Bell Laboratories PFORT verifier [8]. It was decided that SPLEEN should be a subroutine rather than a main program so that the user could enter the parameter values in the way most convenient for him. The user then must write a main program which sets up the required dimensioned variables and assigns values to the necessary parameters (those with asterisks in the list which follows). These parameters are passed to subroutine SPLEEN via the statement

```
CALL SPLEEN(H,X,Y,W,R1,R2,RES,N,NX,NKX,T,BCOEF,XXI,Q,DIAG,K,  
           KX,YY,NY,NYX,MD,SCRATCH,JX,AL,DL,C,IP)
```

where

- \* H(80) = Up to 80 characters in 80A1 format identifying the data
- \* X(NX) = Vector (length N) of X-values where observations were made (independent variable)
- \* Y(NX) = Vector (length N) of observations
- \* W(NX) = Vector (length N) of weights for observations
- R1(NKX) = Vector (length N+K) for scratch area
- R2(NKX) = Vector (length N+K) for scratch area
- RES(NKX) = Vector (length N+K) of residuals from spline fit
- \* N = Number of observations
- \* NX = Dimension (>N) of vectors X,Y,W
- \* NKX = Dimension (>N+K) of vectors R1,R2,RES
- \* T(KX) = Vector (length K+2\*MD) of knot locations

BCOEF(KX) = Vector (length  $K+MD-1$ ) of B-spline coefficients

XXI(KX,KX) = Variance-covariance matrix (size  $[K+MD-1] \times [K+MD-1]$ ) of B-spline coefficients

Q(JX,KX) = Matrix (size  $[MD+1] \times [K+MD-1]$ ) for scratch area

DIAG(KX) = Vector (length  $K+MD-1$ ) for scratch area

- \* K = Number of knots specified by user (later increased to  $K+2*MD$  by program)
- \* KX = Dimension ( $>K+2*MD$ ) of vectors T,BCOEF,DIAG and matrices XXI and Q (column only for Q)
- \* YY(NYX) = Vector (length NY) of Y-values for which predicted X-values (with confidence intervals) are to be computed
- \* NY = Number of Y-values for which predicted X-values are to be computed
- \* NYX = Dimension ( $>NY$ ) of vector YY
- \* MD = Degree of spline ( $\leq 19$ ); for example, 1=linear, 2=quadratic, 3=cubic)

SCRATCH(JX,JX) = Matrix (size  $[MD+1] \times [MD+1]$ ) for scratch area

- \* JX = Dimension of square matrix SCRATCH and row dimension of matrix Q = 20
- \* AL = Alpha level of significance
- \* DL = Delta level of significance
- \* C = Constant in the interval (0.85,1.25) associated with Scheffé's calibration technique (see Appendix 1 for a discussion of this constant)

0 For abbreviated printout

- \* IP = 1 For full printout (residuals, PP representation)
- 2 For full printout plus Y-confidence intervals for 300 evenly spaced X-values over knot span

Variables which appear with an asterisk (\*) require input values from the main program. The subscripts on vectors and matrices indicate the dimensions which must be assigned in the main program.

Variable names which begin with the letters I,J,K,L,M, or N are of the INTEGER type. The remaining variable names are of the REAL single precision type.

The print parameter IP gives the user a certain amount of control over the amount of information to be printed out. Normally the most suitable value is IP=1. A value of IP=0 suppresses the printout of the weights, independent variable, observations, predicted values, and residuals. This option may save quite a bit of paper in case there are several hundred observations, but it deprives the user of the chance to visually examine the residuals. A value of IP=2 causes a listing of certain intermediate vectors which are somewhat lengthy and would not normally be of use to the user.

In the interest of minimizing the number of variables needed in the CALL statement, not all of the printed information can be recovered through the passed parameters. Furthermore, three of the variables (X, K, and T) return values different from their input values.

The data points  $(X_i, Y_i, W_i)$  may be input in arbitrary order, as may the knot locations  $T_i$  and the vector of  $YY_i$  specifying the y-values on the calibration chart.

There are two subroutines which check for consistency among the input parameters. Each inconsistency causes a diagnostic message to be printed. If one or more inconsistencies is detected then the program execution is terminated. Observations outside the knot span are flagged and weighted zero. The number of observations is then reduced by one for each flagged point and a diagnostic is printed. This is not a fatal error unless it reduces the number of degrees of freedom to zero or less.

Although this package can handle splines of any degree up to 19 it was primarily intended for splines of lower degree, i.e., linear, quadratic, or cubic. Test runs on sets of both real and artificial data have given valid results up to about degree 9. Beyond that the limitation of single precision arithmetic on the 36-bit NBS central computer begins to cause roundoff errors that invalidate the results. The user should exercise caution when fitting the higher degree splines.

If the user wants to change some of the continuity conditions at a given knot he may do so by duplicating that knot in the knot vector which is passed to subroutine SPLEEN. If a knot appears  $M$  times in the fitting of a spline of degree  $N$  then the functional value and the first  $N-M$  derivatives of the function will be continuous at that knot. If  $M = N+1$ , neither the function nor its derivatives are required to be continuous.

The package may be applied to both monotone increasing and decreasing calibration curves.

## 5. Summary and Discussion.

An approach to calibration curves and their uncertainty bands has been presented, complete with a FORTRAN program to perform the required calculations. An example involving a large process tank has been used to illustrate the approach and the program. The results include not only the curve for estimating volume from measured pressure, but also valid uncertainty limits for repeated applications of the calibration curve obtained.

The interval estimates of volume comprise two parts: a long-term component which changes only at recalibration, and a random component.

The contribution due to the long-term component may be estimated in large scale calibration experiments by the volume interval estimate obtained when  $\alpha=1$ . Similarly, the contribution due to the random component may be estimated by the volume interval estimate obtained when  $\delta=1$ . When the calibration experiment is of a more modest size involving less than 100 data points the above component estimates may not be realistic. However a more comprehensive treatment for combining interval estimates (and hence their components) obtained from a calibration curve is under development by C. Spiegelman and K. Eberhardt [9].

The results of a calibration will be used repeatedly, usually without any further opportunity to verify their correctness, until the next calibration. Therefore it is important that the measurement system be under control. In the work reported here, the run-to-run differences observed in the mock-up area were due to a known source (the small diameter of the tubing), and could be corrected. If any anomalous behavior is observed which cannot be satisfactorily explained, then of course the entire statistical analysis must be approached with caution.

Little has been written about the design of calibration experiments - i.e., the selection of volumes at which pressure is to be measured, the number of measurements to be taken at each volume, and the arrangement of these measurement points into a sequence of runs. One solution to this question has been achieved by Spiegelman and Studden, and will be published in the NBS Journal of Research [10]. In general, later runs will concentrate on certain sections of a tank, but it is good practice to ensure that at least two runs cover each section, and that several runs cover the whole tank. If this precaution is not taken, there might

be very little cross-validation between runs.

Certain caveats ought to be mentioned here. The program under discussion assumes that the knot locations are known, and that the model is correct. Consequences of failure of these assumptions could be severe. With respect to the knot locations, careful inspection of the residual plots will sometimes indicate discrepancies. These may be small; however, it is important to realize that such regions represent systematic deviations, and could be used (at least in theory) to cover the diversion of material. An approach to the problem involving unknown knot locations is being pursued at this writing.

Unlike a simple linear regression, where the inclusion of a superfluous higher-order term generally causes no major trouble (the fitted coefficient turns out insignificantly small, and the residual mean square increases minimally), choosing a higher-order model when fitting smooth splines can result in a very much worse fit. This is because of the smoothing restrictions, which greatly limit the freedom of the fitting procedure. (Imagine that the true model consists of two straight lines meeting at a point. If one chooses to fit a quadratic spline, then one is insisting on having two quadratic curves which meet at the proper x-value, and which have the same slope at that point. Thus the slope at that point is probably going to be some value between the two straight-line slopes, and the fit cannot be accurate.) One way around this difficulty is to fit piecewise polynomials (i.e., do not require smoothness), and investigate the appropriate degree from these fits. However, it is much better to know the situation well enough to choose the correct model from physical considerations.



A technique that the authors have found useful is to run the program described here with the degree of the fit set equal to zero. The result is to fit a step function to the data, and to produce a plot of the residuals from that fit; for the Example of this paper, that plot is reproduced as Figure 10. It can be seen that the residuals look as linear as a printer plot can look. Therefore, a first-degree (linear) spline fit is the proper choice. If in some segment the relationship were not linear, this plot should show it. The plot also gives some idea of the spread of points across the intervals, though of course near-duplicate points will plot as one because it is a discrete printer plot.

Note that the continuity restrictions can be relaxed when using the program under consideration, by simply duplicating the knots. See Section 4 for details.

## Appendix 1.

As stated in Section 4, a constant  $c$  must be input by the user. In order to obtain this constant from tables 1 and 2 in Scheffé (1973) for  $1 \leq k \leq 10$  the user must have calculated the standard deviation,  $SD$ , for  $\hat{p}(v)$  in the complete region of calibration. The smallest and largest values of the  $SD(\hat{p}(v))/\hat{\sigma}$  over the complete calibration region are used as input for the Scheffé tables. For  $k > 10$  Scheffé gives a mathematical algorithm for finding  $c$ , and states that for very large (asymptotic) values of  $n-k$ ,  $c=1$ . (Here  $n$  is the number of observations, and  $k$  is the number of B-spline coefficients.) If the reader does not wish to do a Scheffé table 1 or table 2 lookup, the following table gives approximate and generally larger values for this constant.

Approximate  $c$  values  
for  $1 \leq k \leq 10$

$n-k$	60-119	120-149	150 +
$c$	1.10	1.05	1.00

Appendix 2.

Program Listing.

The subroutines which make up the spline-fitting package follow, in alphabetical order.

SUBROUTINE ADKNTS ( T, K, KX, MO)

```

1  C-----
2  C ADKNTS WRITTEN BY CHARLES P. REEVE, STATISTICAL ENGINEERING
3  C DIVISION, NATIONAL BUREAU OF STANDARDS, WASHINGTON, D.C.
4  C AS PART OF THE FIXED-KNOT SPLINE PACKAGE FOR CALIBRATION
5  C FOR: DUPLICATING THE FIRST AND KTH (LAST) ENTRIES OF THE KNOT
6  C VECTOR T (MO-1) TIMES
7  C SUBPROGRAMS CALLED: -NONE-
8  C CURRENT VERSION COMPLETED OCTOBER 10, 1979
9  C-----
10 C DIMENSION T(KX)
11 C FORMAT (/1X,29(1H-)/1X,29H* SUMMARY OF KNOT LOCATIONS */1X,
12 2 29(1H-)/5X,1H1,6X,8HKNOTS(1)/)
13 C
14 20 FORMAT (2X,14,G15.6)
15 30 FORMAT (/5X,30H<<<<< EACH END KNOT DUPLICATED,13,1X,
16 2 11HTIMES >>>>>)
17 C--- SAVE END KNOT LOCATIONS
18 Q1=T(1)
19 Q2=T(K)
20 C--- INCREASE INDEX OF EACH KNOT LOCATION BY (MO-1)
21 KM=K+MO
22 DO 40 I=1,K
23 KMI=KM-I
24 KI=K-I+1
25 T(KMI)=T(KI)
26 CONTINUE
27 C--- ADD DUPLICATE END KNOT LOCATIONS AT THEIR RESPECTIVE ENDS
28 MD=MO-1
29 DO 50 I=1,MD
30 KMI=KM+I-1
31 T(I)=Q1
32 T(KMI)=Q2
33 CONTINUE
34 C--- RECOMPUTE THE LENGTH OF THE VECTOR T
35 K=K+2*MD
36 WRITE (6,30) MD
37 WRITE NEW VECTOR OF KNOT LOCATIONS
38 WRITE (6,10)
39 DO 60 I=1,K
40 WRITE (6,20) I,T(I)
41 CONTINUE
42 RETURN
43 END
ADKNTS01
ADKNTS02
ADKNTS03
ADKNTS04
ADKNTS05
ADKNTS06
ADKNTS07
ADKNTS08
ADKNTS09
ADKNTS10
ADKNTS11
ADKNTS12
ADKNTS13
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ADKNTS27
ADKNTS28
ADKNTS29
ADKNTS30
ADKNTS31
ADKNTS32
ADKNTS33
ADKNTS34
ADKNTS35
ADKNTS36
ADKNTS37
ADKNTS38
ADKNTS39
ADKNTS40
ADKNTS41
ADKNTS42
ADKNTS43

```

CPR\*NS(1).BCHFAC(2)

1 SUBROUTINE BCHFAC (W,NBNDMX,NBANDS,NROW,DIAG)  
2 FROM \* A PRACTICAL GUIDE TO SPLINES \* BY C. DE BOOR  
3 CONSTRUCTS CHOLESKY FACTORIZATION  
4 C = L \* D \* L-TRANSPOSE  
5 WITH L UNIT LOWER TRIANGULAR AND D DIAGONAL, FOR GIVEN MATRIX C OF  
6 ORDER NROW, IN CASE C IS (SYMMETRIC) POSITIVE SEMIDEFINITE  
7 AND Banded, HAVING NBANDS DIAGONALS AT AND BELOW THE  
8 MAIN DIAGONAL.  
9  
10 C\*\*\*\*\* I N P U T \*\*\*\*\*  
11 C NROW..... IS THE ORDER OF THE MATRIX C .  
12 C NBNDMX.... THE ACTUAL ROW DIMENSION OF W.  
13 C NBANDS.... INDICATES ITS BANDWIDTH, I.E.,  
14 C C(I,J) = 0 FOR ABS(I-J) .GT. NBANDS .  
15 C W..... WORKARRAY OF SIZE (NBANDS,NROW) CONTAINING THE NBANDS DIAGO-  
16 C NALS IN ITS ROWS, WITH THE MAIN DIAGONAL IN ROW 1 . PRECISELY, BCHFAC16  
17 C W(I,J) CONTAINS C(I+J-1,J), I=1,.....,NBANDS, J=1,....,NROW. BCHFAC17  
18 C FOR EXAMPLE, THE INTERESTING ENTRIES OF A SEVEN DIAGONAL SYM-  
19 C METRIC MATRIX C OF ORDER 9 WOULD BE STORED IN W AS  
20 C  
21 C 11 22 33 44 55 66 77 88 99  
22 C 21 32 43 54 65 76 87 98  
23 C 31 42 53 64 75 86 97  
24 C 41 52 63 74 85 96  
25 C  
26 C ALL OTHER ENTRIES OF W NOT IDENTIFIED IN THIS WAY WITH AN EN-  
27 C TRY OF C ARE NEVER REFERENCED .  
28 C DIAG..... IS A WORK ARRAY OF LENGTH NROW .  
29 C  
30 C\*\*\*\*\* O U T P U T \*\*\*\*\*  
31 C W.....CONTAINS THE CHOLESKY FACTORIZATION C = L\*D\*L-TRANSP, WITH  
32 C W(1,1) CONTAINING 1/D(1,1)  
33 C AND W(I,J) CONTAINING L(I-1+J,J), I=2,....,NBANDS.  
34 C  
35 C\*\*\*\*\* M E T H O D \*\*\*\*\*  
36 C GAUSS ELIMINATION, ADAPTED TO THE SYMMETRY AND BANDEDNESS OF C ,  
37 C USED .  
38 C NEAR ZERO PIVOTS ARE HANDLED IN A SPECIAL WAY. THE DIAGONAL ELE-  
39 C MENT C(N,N) = W(1,N) IS SAVED INITIALLY IN DIAG(N), ALL N. AT THE N-BCHFAC39  
40 C TH ELIMINATION STEP, THE CURRENT PIVOT ELEMENT, VIZ. W(1,N), IS COM-  
41 C PARED WITH ITS ORIGINAL VALUE, DIAG(N) . IF, AS THE RESULT OF PRIOR  
42 C ELIMINATION STEPS, THIS ELEMENT HAS BEEN REDUCED BY ABOUT A WORD  
43 C LENGTH, (I.E., IF W(1,N)+DIAG(N) .LE. DIAG(N)), THEN THE PIVOT IS DE-  
44 C CLARED TO BE ZERO, AND THE ENTIRE N-TH ROW IS DECLARED TO BE LINEARLY-  
45 C DEPENDENT ON THE PRECEDING ROWS. THIS HAS THE EFFECT OF PRODUCING  
46 C X(N) = 0 WHEN SOLVING C\*X = B FOR X, REGARDLESS OF B. JUSTIFIC-  
47 C ATION FOR THIS IS AS FOLLOWS. IN CONTEMPLATED APPLICATIONS OF THIS  
48 C PROGRAM, THE GIVEN EQUATIONS ARE THE NORMAL EQUATIONS FOR SOME LEAST-  
49 C SQUARES APPROXIMATION PROBLEM, DIAG(N) = C(N,N) GIVES THE NORM-SQUARE  
50 C OF THE N-TH BASIS FUNCTION, AND, AT THIS POINT, W(1,N) CONTAINS THE  
51 C NORM-SQUARE OF THE ERROR IN THE LEAST-SQUARES APPROXIMATION TO THE  
52 C TH BASIS FUNCTION BY LINEAR COMBINATIONS OF THE FIRST N-1 . HAVING  
53 C W(1,N)+DIAG(N) .LE. DIAG(N) SIGNIFIES THAT THE N-TH FUNCTION IS LIN-  
54 C EARLY DEPENDENT TO MACHINE ACCURACY ON THE FIRST N-1 FUNCTIONS, THERE-  
55 C FORE CAN SAFELY BE LEFT OUT FROM THE BASIS OF APPROXIMATING FUNCTIONS  
56 C THE SOLUTION OF A LINEAR SYSTEM  
57 C C\*X = B

```

58 C IS EFFECTED BY THE SUCCESSION OF THE FOLLOWING T W O CALLS: BCHFAC58
59 C CALL BCHFAC (W, NBNDMX, NBANDS, NROW, DIAG) ; TO GET FACTORIZATION BCHFAC59
60 C CALL BCHSLV (W, NBNDMX, NBANDS, NROW, DIAG) ; TO SOLVE FOR X. BCHFAC60
61 C THE VECTOR B NOW CONTAINS X. BCHFAC61
62 C BCHFAC62
63 C BCHFAC63
64 C BCHFAC64
65 C BCHFAC65
66 C BCHFAC66
67 C BCHFAC67
68 C BCHFAC68
69 C BCHFAC69
70 C BCHFAC70
71 C INTEGER NBNDMX, NBANDS, NROW, I, IMAX, J, JMAX, N BCHFAC71
72 C REAL W(NBNDMX, NROW), DIAG(NROW), RATIO BCHFAC72
73 C IF (NROW.GT.1) GO TO 10 BCHFAC73
74 C IF (W(1,1).CT.0.) W(1,1)=1./W(1,1) BCHFAC74
75 C RETURN BCHFAC75
76 C STORE DIAGONAL OF C IN DIAG. BCHFAC76
77 C BCHFAC77
78 C BCHFAC78
79 C BCHFAC79
80 C FACTORIZATION . BCHFAC80
81 C BCHFAC81
82 C BCHFAC82
83 C BCHFAC83
84 C BCHFAC84
85 C BCHFAC85
86 C BCHFAC86
87 C BCHFAC87
88 C BCHFAC88
89 C BCHFAC89
90 C BCHFAC90
91 C BCHFAC91
92 C BCHFAC92
93 C BCHFAC93
94 C BCHFAC94
95 C BCHFAC95
96 C BCHFAC96
97 C BCHFAC97
98 C BCHFAC98
99 C BCHFAC99

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IS EFFECTED BY THE SUCCESSION OF THE FOLLOWING T W O CALLS:  
 CALL BCHFAC (W, NBNDMX, NBANDS, NROW, DIAG) ; TO GET FACTORIZATION  
 CALL BCHSLV (W, NBNDMX, NBANDS, NROW, DIAG) ; TO SOLVE FOR X.  
 THE VECTOR B NOW CONTAINS X.

MODIFICATION BY.

MARTIN CORDES  
 CENTER FOR APPLIED MATHEMATICS, NBS  
 VERSION 1  
 OCT 1979

-----  
 INTEGER NBNDMX, NBANDS, NROW, I, IMAX, J, JMAX, N  
 REAL W(NBNDMX, NROW), DIAG(NROW), RATIO  
 IF (NROW.GT.1) GO TO 10  
 IF (W(1,1).CT.0.) W(1,1)=1./W(1,1)  
 RETURN

STORE DIAGONAL OF C IN DIAG.

FACTORIZATION .

DO 20 N=1, NROW  
 DIAG(N)=W(1, N)  
 DO 70 N=1, NROW  
 IF (W(1, N)+DIAG(N).CT.DIAG(N)) GO TO 40  
 DO 30 J=1, NBANDS  
 W(J, N)=0.  
 GO TO 70  
 W(1, N)=1./W(1, N)  
 IMAX=MIN0(NBANDS-1, NROW-N)  
 IF (IMAX.LT.1) GO TO 70  
 JMAX=IMAX  
 DO 60 I=1, IMAX  
 RATIO=W(I+1, N)\*W(1, N)  
 DO 50 J=1, JMAX  
 L1=N+I  
 L2=J+I  
 W(J, L1)=W(J, L1)-W(L2, N)\*RATIO  
 JMAX=JMAX-1  
 W(I+1, N)=RATIO  
 CONTINUE  
 RETURN  
 END

```

1  C  PR*NS(1) . BCHSLV(1)
2  C  SUBROUTINE BCHSLV (W,NBNDMX,NBANDS,NROW,B)
3  C  FROM * A PRACTICAL GUIDE TO SPLINES * BY C. DE BOOR
4  C  SOLVES THE LINEAR SYSTEM C*X = B OF ORDER N R O W FOR X
5  C  PROVIDED W CONTAINS THE CHOLESKY FACTORIZATION FOR THE BANDED (SYM-BCHSLV04
6  C  METRIC) POSITIVE DEFINITE MATRIX C AS CONSTRUCTED IN THE SUBROUTINEBCHSLV05
7  C  B C H F A C (QUO VIDE).
8  C
9  C ***** I N P U T *****
10 C  NROW... IS THE ORDER OF THE MATRIX C .
11 C  NBNDMX... THE ACTUAL ROW DIMENSION OF W.
12 C  NBANDS... INDICATES THE BANDWIDTH OF C .
13 C  W... CONTAINS THE CHOLESKY FACTORIZATION FOR C , AS OUTPUT FROM
14 C  SUBROUTINE BCFAC (QUO VIDE).
15 C  B... THE VECTOR OF LENGTH N R O W CONTAINING THE RIGHT SIDE.
16 C
17 C ***** O U T P U T *****
18 C  B... THE VECTOR OF LENGTH N R O W CONTAINING THE SOLUTION.
19 C
20 C ***** M E T H O D *****
21 C  WITH THE FACTORIZATION C = L*D*L-TRANSPOSE AVAILABLE, WHERE L IS
22 C  UNIT LOWER TRIANGULAR AND D IS DIAGONAL, THE TRIANGULAR SYSTEM
23 C  L*Y = B IS SOLVED FOR Y (FORWARD SUBSTITUTION), Y IS STORED IN B,
24 C  THE VECTOR D**(-1)*Y IS COMPUTED AND STORED IN B, THEN THE TRIANG-
25 C  ULAR SYSTEM L-TRANSPOSE*X = D**(-1)*Y IS SOLVED FOR X (BACKSUBSTIT-
26 C  UTION).
27 C
28 C  MODIFICATION BY.
29 C
30 C  MARTIN CORDES
31 C  CENTER FOR APPLIED MATHEMATICS, NBS
32 C  VERSION 1
33 C  OCT 1979
34 C
35 C
36 C
37 C  INTEGER NBNDMX,NBANDS,NROW,J,JMAX,N,NBNDM1
38 C  REAL W(NBNDMX,NROW),B(NROW)
39 C  IF (NROW.GT.1) GO TO 10
40 C  B(1)=B(1)*W(1,1)
41 C  RETURN
42 C
43 C  FORWARD SUBSTITUTION. SOLVE L*Y = B FOR Y, STORE IN B.
44 C  NBNDM1=NBANDS-1
45 C  DO 30 N=1,NROW
46 C  JMAX=MIN0(NBNDM1,NROW-N)
47 C  IF (JMAX.LT.1) GO TO 30
48 C  DO 20 J=1,JMAX
49 C  L=J+N
50 C  B(L)=B(L)-W(J+1,N)*B(N)
51 C  CONTINUE
52 C
53 C  BACKSUBSTITUTION. SOLVE L-TRANSP.X = D**(-1)*Y FOR X, STORE IN B.
54 C  N=NROW
55 C  B(N)=B(N)*W(1,N)
56 C  JMAX=MIN0(NBNDM1,NROW-N)
57 C  IF (JMAX.LT.1) GO TO 60
58 C  DO 50 J=1,JMAX

```

58  
59  
60  
61  
62  
63

L=J+N  
B(N)=B(N)-W(J+1,N)\*B(L)  
N=N-1  
IF (N.CT.0) GO TO 40  
RETURN  
END

50  
60

BCHSLV58  
BCHSLV59  
BCHSLV60  
BCHSLV61  
BCHSLV62  
BCHSLV63



```

CPR*NS(1).BSPLPP(1)
1 SUBROUTINE BSPLPP (T,BCOEF,N,K,SCRATCH,BREAK,COEF,L,KMX)
2 FROM * A PRACTICAL GUIDE TO SPLINES * BY C. DE BOOR
3 CALLS BSPLVB
4
5 CONVERTS THE B-REPRESENTATION T, BCOEF, N, K OF SOME SPLINE INTO ITS
6 PP-REPRESENTATION BREAK, COEF, L, K.
7
8 C***** I N P U T *****
9 C T....KNOT SEQUENCE, OF LENGTH N+K
10 C BCOEF....B-SPLINE COEFFICIENT SEQUENCE, OF LENGTH N
11 C N....LENGTH OF BCOEF AND DIMENSION OF SPLINE SPACE SPLINE(K,T)
12 C K....ORDER OF THE SPLINE
13 C KMX....ROW DIMENSION OF ARRAYS COEF AND SCRATCH
14
15 C W A R N I N G . . . THE RESTRICTION K .LE. KMAX (= 20) IS IMPO-BSPLP015
16 SED BY THE ARBITRARY DIMENSION STATEMENT FOR BIATX BELOW, BUTBSPLP016
17 IS N O W H E R E C H E C K E D F O R .
18
19 C***** W O R K A R E A *****
20 C SCRATCH....OF SIZE (KMX,K), NEEDED TO CONTAIN BCOEFFS OF A PIECE
21 OF THE SPLINE AND ITS K-1 DERIVATIVES
22
23 C***** O U T P U T *****
24 C BREAK....BREAKPOINT SEQUENCE, OF LENGTH L+1, CONTAINS (IN INCREAS-
25 ING ORDER) THE DISTINCT POINTS IN THE SEQUENCE T(K)....T(N+1)BSPLP025
26 C COEF....ARRAY OF SIZE (KMX,N), WITH COEF(I,J) = (I-1)ST DERIVATIVE
27 OF SPLINE AT BREAK(J) FROM THE RIGHT
28 C L....NUMBER OF POLYNOMIAL PIECES WHICH MAKE UP THE SPLINE IN THE IN-BSPLP028
29 Terval (T(K), T(N+1))
30
31 C***** M E T H O D *****
32 C FOR EACH BREAKPOINT INTERVAL, THE K RELEVANT B-COEFFS OF THE
33 SPLINE ARE FOUND AND THEN DIFFERENCED REPEATEDLY TO GET THE B-COEFFS
34 OF ALL THE DERIVATIVES OF THE SPLINE ON THAT INTERVAL. THE SPLINE ANDBSPLP034
35 ITS FIRST K-1 DERIVATIVES ARE THEN EVALUATED AT THE LEFT END POINT
36 OF THAT INTERVAL, USING BSPLVB REPEATEDLY TO OBTAIN THE VALUES OF
37 ALL B-SPLINES OF THE APPROPRIATE ORDER AT THAT POINT.
38
39 C PARAMETER KMAX = 20
40
41 C MODIFICATION BY.
42
43 C MARTIN CORDES
44 CENTER FOR APPLIED MATHEMATICS, NBS
45 VERSION 1
46 MAR 1980
47
48 -----
49 C INTEGER K,L,N,I,J,JP1,KMJ,LEFT,LSOFAR
50 REAL BCOEF(N),BREAK(1),COEF(KMX,1),T(1),SCRATCH(KMX,K),BIATX(20),
51 2 DIFF,FKMJ,SUM
52 *
53 C DIMENSION BREAK(L+1),COEF(K,L),T(N+K)
54 CURRENT FORTRAN STANDARD MAKES IT IMPOSSIBLE TO SPECIFY THE LENGTH OF
55 BREAK, COEF AND T PRECISELY WITHOUT THE INTRODUCTION OF OTHERWISEBSPLP056
56 SUPERFLUOUS ADDITIONAL ARGUMENTS.
57
BSPLP001
BSPLP002
BSPLP003
BSPLP004
BSPLP005
BSPLP006
BSPLP007
BSPLP008
BSPLP009
BSPLP010
BSPLP011
BSPLP012
BSPLP013
BSPLP014
BSPLP015
BSPLP016
BSPLP017
BSPLP018
BSPLP019
BSPLP020
BSPLP021
BSPLP022
BSPLP023
BSPLP024
BSPLP025
BSPLP026
BSPLP027
BSPLP028
BSPLP029
BSPLP030
BSPLP031
BSPLP032
BSPLP033
BSPLP034
BSPLP035
BSPLP036
BSPLP037
BSPLP038
BSPLP039
BSPLP040
BSPLP041
BSPLP042
BSPLP043
BSPLP044
BSPLP045
BSPLP046
BSPLP047
BSPLP048
BSPLP049
BSPLP050
BSPLP051
BSPLP052
BSPLP053
BSPLP054
BSPLP055
BSPLP056
BSPLP057

```

```

58 LSOFAR=0
59 BREAK(1)=T(K)
60 DO 60 LEFT=K,N
61 C
62 IF (T(LEFT+1).EQ.T(LEFT)) GO TO 60
63 LSOFAR=LSOFAR+1
64 BREAK(LSOFAR+1)=T(LEFT+1)
65 IF (K.GT.1) GO TO 10
66 COEF(1,LSOFAR)=BCOEF(LEFT)
67 GO TO 60
68 C
69 STORE THE K B-SPLINE COEFF.S RELEVANT TO CURRENT KNOT INTERVAL
70 IN SCRTCH(.,1) .
71 DO 20 I=1,K
72 M=LEFT-K+1
73 SCRTCH(I,1)=BCOEF(M)
74 C
75 FOR J=1,....,K-1, COMPUTE THE K-J B-SPLINE COEFF.S RELEVANT TO BSPLP074
76 CURRENT KNOT INTERVAL FOR THE J-TH DERIVATIVE BY DIFFERENCING
77 THOSE FOR THE (J-1)ST DERIVATIVE, AND STORE IN SCRTCH(.,J+1) .
78 DO 30 JPI=2,K
79 J=JPI-1
80 KMJ=K-J
81 FKMJ=FLOAT(KMJ)
82 DO 30 I=1,KMJ
83 M1=LEFT+I
84 M2=M1-KMJ
85 DIFF=T(M1)-T(M2)
86 IF (DIFF.GT.0.) SCRTCH(I,JP1)=((SCRTCH(I+1,J)-SCRTCH(I,J))/DIFF)*FBSP085
87 2KMJ
88 CONTINUE
89 C
90 FOR J = 0, ..., K-1, FIND THE VALUES AT T(LEFT) OF THE J+1
91 B-SPLINES OF ORDER J+1 WHOSE SUPPORT CONTAINS THE CURRENT
92 KNOT INTERVAL FROM THOSE OF ORDER J (IN BIATX), THEN COMB-
93 LINE WITH THE B-SPLINE COEFF.S (IN SCRTCH(.,K-J)) FOUND EARLIERBSPLP092
94 TO COMPUTE THE (K-J-1)ST DERIVATIVE AT T(LEFT) OF THE GIVEN
95 SPLINE.
96 NOTE. IF THE REPEATED CALLS TO BSPLVB ARE THOUGHT TO GENE-BSPLP095
97 RATE TOO MUCH OVERHEAD, THEN REPLACE THE FIRST CALL BY
98 BIATX(I) = 1.
99 AND THE SUBSEQUENT CALL BY THE STATEMENT
100 J = JPI - 1
101 DELTAR(J) = T(LEFT+J) - X
102 .....
103 BIATX(J+1) = SAVED
104 FROM BSPLVB . DELTAR(KMAX) AND DELTAR(KMAX) WOULD HAVE TO
105 APPEAR IN A DIMENSION STATEMENT, OF COURSE.
106 C
107 CALL BSPLVB (T,1,1,T(LEFT),LEFT,BIATX)
108 COEF(K,LSOFAR)=SCRTCH(1,K)
109 DO 50 JPI=2,K
110 CALL BSPLVB (T,JP1,2,T(LEFT),LEFT,BIATX)
111 KMJ=K+1-JPI
112 SUM=0.
113 DO 40 I=1,JP1
114 SUM=BIATX(I)*SCRTCH(I,KMJ)+SUM
115 COEF(KMJ,LSOFAR)=SUM

```

BSPLP116  
BSPLP117  
BSPLP118  
BSPLP119

CONTINUE  
L=LSOFAR  
RETURN  
END

60

116  
117  
118  
119

CPR\*NS(1),BSPLVB(1)

1 SUBROUTINE BSPLVB (T,JHIGH,INDEX,X,LEFT,BIATX)  
2 FROM \* A PRACTICAL GUIDE TO SPLINES \* BY C. DE BOOR  
3 CALCULATES THE VALUE OF ALL POSSIBLY NONZERO B-SPLINES AT X OF ORDER  
4 C  
5 C JOUT = MAX( JHIGH , (J+1)\*(INDEX-1) )  
6 C  
7 C WITH KNOT SEQUENCE T .  
8 C  
9 C\*\*\*\*\* I N P U T \*\*\*\*\*  
10 C T.....KNOT SEQUENCE, OF LENGTH LEFT + JOUT , ASSUMED TO BE NONDE-  
11 C CREATING. A S S U M P T I O N . . . . T(LEFT + 1)  
12 C  
13 C D I V I S I O N B Y Z E R O WILL RESULT IF T(LEFT) = T(LEFT+1)  
14 C JHIGH,  
15 C INDEX.....INTEGERS WHICH DETERMINE THE ORDER JOUT = MAX(JHIGH,  
16 C (J+1)\*(INDEX-1)) OF THE B-SPLINES WHOSE VALUES AT X ARE TO  
17 C BE RETURNED. INDEX IS USED TO AVOID RECALCULATIONS WHEN SEVE-  
18 C RAL COLUMNS OF THE TRIANGULAR ARRAY OF B-SPLINE VALUES ARE NEE-  
19 C DED (E.G., IN BVALUE OR IN BSPLVD) . PRECISELY,  
20 C IF INDEX = 1,  
21 C THE CALCULATION STARTS FROM SCRATCH AND THE ENTIRE TRIANGULAR  
22 C ARRAY OF B-SPLINE VALUES OF ORDERS 1,2,...,JHIGH IS GENERATED  
23 C ORDER BY ORDER , I.E., COLUMN BY COLUMN .  
24 C IF INDEX = 2,  
25 C ONLY THE B-SPLINE VALUES OF ORDER J+1, J+2, . . . , JOUT ARE GE-  
26 C NERATED, THE ASSUMPTION BEING THAT BIATX, J , DELTAL , DELTARBSPLVB26  
27 C ARE, ON ENTRY, AS THEY WERE ON EXIT AT THE PREVIOUS CALL.  
28 C IN PARTICULAR, IF JHIGH = 0, THEN JOUT = J+1, I.E., JUST  
29 C THE NEXT COLUMN OF B-SPLINE VALUES IS GENERATED.  
30 C  
31 C W A R N I N G . . . . THE RESTRICTION JOUT .LE. JMAX (= 20) IS IM-  
32 C POSED ARBITRARILY BY THE DIMENSION STATEMENT FOR DELTAL AND  
33 C DELTAR BELOW, BUT IS N O W H E R E C H E C K E D FOR .  
34 C  
35 C X.....THE POINT AT WHICH THE B-SPLINES ARE TO BE EVALUATED.  
36 C LEFT.....AN INTEGER CHOSEN (USUALLY) SO THAT  
37 C T(LEFT) .LE. X .LE. T(LEFT+1) .  
38 C  
39 C\*\*\*\*\* O U T P U T \*\*\*\*\*  
40 C BIATX.....ARRAY OF LENGTH JOUT , WITH BIATX(I) CONTAINING THE VAL-  
41 C UE AT X OF THE POLYNOMIAL OF ORDER JOUT WHICH AGREES WITH  
42 C THE B-SPLINE B(LEFT-JOUT+1,JOUT,T) ON THE INTERVAL (T(LEFT),  
43 C T(LEFT+1)) .  
44 C  
45 C\*\*\*\*\* M E T H O D \*\*\*\*\*  
46 C THE RECURRENCE RELATION  
47 C  
48 C B(I,J+1)(X) = X - T(I) T(I+J+1) - X  
49 C -----B(I,J)(X) + -----T(I+J+1)-T(I+1)(X)  
50 C T(I+J)-T(I)  
51 C  
52 C IS USED (REPEATEDLY) TO GENERATE THE (J+1)-VECTOR B(LEFT-J,J+1)(X),  
53 C ...,B(LEFT,J+1)(X) FROM THE J-VECTOR B(LEFT-J+1,J)(X),...  
54 C B(LEFT,J)(X), STORING THE NEW VALUES IN BIATX OVER THE OLD. THE  
55 C FACTS THAT  
56 C B(I,1) = 1 IF T(I) .LE. X .LT. T(I+1)  
57 C AND THAT

```

58 BSPLVB58
59 BSPLVB59
60 BSPLVB60
61 BSPLVB61
62 BSPLVB62
63 BSPLVB63
64 BSPLVB64
65 BSPLVB65
66 BSPLVB66
67 BSPLVB67
68 BSPLVB68
69 BSPLVB69
70 BSPLVB70
71 BSPLVB71
72 BSPLVB72
73 BSPLVB73
74 BSPLVB74
75 BSPLVB75
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78 BSPLVB78
79 BSPLVB79
80 BSPLVB80
81 BSPLVB81
82 BSPLVB82
83 BSPLVB83
84 BSPLVB84
85 BSPLVB85
86 BSPLVB86
87 BSPLVB87
88 BSPLVB88
89 BSPLVB89
90 BSPLVB90
91 BSPLVB91
92 BSPLVB92
93 BSPLVB93
94 BSPLVB94

C B(I,J)(XO = 0 UNLESS T(I) .LE. X .LT. T(I+J)
C ARE USED. THE PARTICULAR ORGANIZATION OF THE CALCULATIONS FOLLOWS AL-
C GORITHM (8) IN CHAPTER X OF THE TEXT.
C
C PARAMETER JMAX = 20
C INTEGER INDEX,JHIGH,LEFT,I,J,JP1
C REAL BIATX(JHIGH),T(1),X, DELTAL(JMAX),DELTAR(JMAX),SAVED,TERM
C REAL BIATX(JHIGH),T(1),X,DELTAL(20),DELTAR(20),SAVED,TERM
C DIMENSION BIATX(JOUT), T(LEFT+JOUT)
C CURRENT FORTRAN STANDARD MAKES IT IMPOSSIBLE TO SPECIFY THE LENGTH OF
C T AND OF BIATX PRECISELY WITHOUT THE INTRODUCTION OF OTHERWISE
C SUPERFLUOUS ADDITIONAL ARGUMENTS.
C DATA J /1/
C SAVE J,DELTAL,DELTAR (VALID IN FORTRAN 77)
C
C GO TO (10,20), INDEX
C J=1
C BIATX(1)=1.
C IF (J.GE.JHIGH) GO TO 40
C
C JP1=J+1
C L=LEFT+J
C DELTAR(J)=T(L)-X
C L=LEFT+1-J
C DELTAL(J)=X-T(L)
C SAVED=0.
C DO 30 I=1,J
C L=JP1-I
C TERM=BIATX(I)/(DELTAR(I)+DELTAL(L))
C BIATX(I)=SAVED+DELTAR(I)*TERM
C SAVED=DELTAL(L)*TERM
C BIATX(JP1)=SAVED
C J=JP1
C IF (J.LT.JHIGH) GO TO 20
C
C RETURN
C END

```



```

58 INTEGER JDERIV,K,N,I,ILO,IMK,J,JC,JCMIN,JCMAX,J,J,KMJ,KM1,MFLAG,NMIBVAL058
59 2,JDRVPI
60 REAL BCOEF(N),T(1),X,AJ(20),DL(20),DR(20),FKMJ
61 REAL BCOEF(N),T(1),X,AJ(KMAX),DL(KMAX),DR(KMAX),FKMJ
62 DIMENSION T(N+K)
63 CURRENT FORTRAN STANDARD MAKES IT IMPOSSIBLE TO SPECIFY THE LENGTH OF
64 C PRECISELY WITHOUT THE INTRODUCTION OF OTHERWISE SUPERFLUOUS ADDITION-
65 C AL ARGUMENTS.
66 BVALUE=0.
67 IF (JDERIV.GE.K) GO TO 170
68
69 C *** FIND I S.T. I.LE. I.LT. N+K AND T(I).LT. T(I+1) ANDBVAL069
70 T(1).LE. X.LT. T(I+1). IF NO SUCH I CAN BE FOUND, X LIES
71 C OUTSIDE THE SUPPORT OF THE SPLINE F AND BVALUE = 0.
72 C (THE ASYMETRY IN THIS CHOICE OF I MAKES F RIGHTCONTINUOUS)
73 CALL INTERV (T,N+K,X,I,MFLAG)
74 IF (MFLAG.NE.0) GO TO 170
75 C *** IF K = 1 (AND JDERIV = 0), BVALUE = BCOEF(I).
76 KM1=K-1
77 IF (KM1.GT.0) GO TO 10
78 BVALUE=BCOEF(I)
79 GO TO 170
80
81 C *** STORE THE K B-SPLINE COEFFICIENTS RELEVANT FOR THE KNOT INTERVAL
82 C (T(I),T(I+1)) IN AJ(1),...,AJ(K) AND COMPUTE DL(J) = X - T(I+1-J),
83 C DR(J) = T(I+J) - X, J=1,...,K-1. SET ANY OF THE AJ NOT OBTAINABLE
84 C FROM INPUT TO ZERO. SET ANY T.S NOT OBTAINABLE EQUAL TO T(1) OR
85 C TO T(N+K) APPROPRIATELY.
86 JCMIN=1
87 IMK=I-K
88 IF (IMK.GE.0) GO TO 40
89 JCMIN=1-IMK
90 DO 20 J=1,I
91 L=I+1-J
92 DL(J)=X-T(L)
93 DO 30 J=1,KM1
94 L=K-J
95 AJ(L)=0.
96 DL(J)=DL(I)
97 GO TO 60
98 DO 50 J=1,KM1
99 L=I+1-J
100 DL(J)=X-T(L)
101 C
102 JCMAX=K
103 NMI=N-I
104 IF (NMI.GE.0) GO TO 90
105 JCMAX=K+NMI
106 DO 70 J=1,JCMAX
107 L=I+J
108 DR(J)=T(L)-X
109 DO 80 J=JCMAX,KM1
110 AJ(J+1)=0.
111 DR(J)=DR(JCMAX)
112 GO TO 110
113 DO 100 J=1,KM1
114 L=I+J
115 DR(J)=T(L)-X

```

```

116 BVALU116
117 BVALU117
118 BVALU118
119 BVALU119
120 BVALU120
121 BVALU121
122 BVALU122
123 BVALU123
124 BVALU124
125 BVALU125
126 BVALU126
127 BVALU127
128 BVALU128
129 BVALU129
130 BVALU130
131 BVALU131
132 BVALU132
133 BVALU133
134 BVALU134
135 BVALU135
136 BVALU136
137 BVALU137
138 BVALU138
139 BVALU139
140 BVALU140
141 BVALU141
142 BVALU142
143 BVALU143
144 BVALU144

C 110 DO 120 JC=JCMIN, JCMAX
L=IMK+JC
120 AJ(JC)=BCOEF(L)
C
C *** DIFFERENCE THE COEFFICIENTS JDERIV TIMES.
IF (JDERIV.EQ.0) GO TO 140
DO 130 J=1, JDERIV
KMJ=K-J
ILO=KMJ
DO 130 JJ=1, KMJ
AJ(JJ)=((AJ(JJ+1)-AJ(JJ))/(DL(ILO)+DR(JJ)))*FKMJ
ILO=ILO-1
130
C
C *** COMPUTE VALUE AT X IN (T(I), T(I+1)) OF JDERIV-TH DERIVATIVE,
GIVEN ITS RELEVANT B-SPLINE COEFFS IN AJ(1), ..., AJ(K-JDERIV).
140 IF (JDERIV.EQ.KM1) GO TO 160
JDRVP1=JDERIV+1
DO 150 J=JDRVP1, KM1
KMJ=K-J
ILO=KMJ
DO 150 JJ=1, KMJ
AJ(JJ)=(AJ(JJ+1)*DL(ILO)+AJ(JJ)*DR(JJ))/(DL(ILO)+DR(JJ))
150 BVALUE=AJ(1)
160
C 170 RETURN
END

```



CPR\*NS(1).CHECK1(2)

1 SUBROUTINE CHECK1 (W,N,NX,K,KX,NKX,NY,NYX,JX,MO,AL,DL,C,WZ) CHECK101

2 C----- CHECK102

3 C CHECK1 WRITTEN BY CHARLES P. REEVE, STATISTICAL ENGINEERING CHECK103

4 C DIVISION, NATIONAL BUREAU OF STANDARDS, WASHINGTON, D. C. CHECK104

5 C AS PART OF THE FIXED-KNOT SPLINE PACKAGE FOR CALIBRATION CHECK105

6 C FOR: CHECKING WHETHER INPUT VALUES FALL WITHIN THEIR ALLOWABLE CHECK106

7 C LIMITS CHECK107

8 C SUBPROGRAMS CALLED: -NONE- CHECK108

9 C CURRENT VERSION COMPLETED JUNE 20, 1980 CHECK109

10 C----- CHECK110

11 C DIMENSION W(NX) CHECK111

12 C WRITE FORMATS CHECK112

13 C 10 FORMAT (/1X,21H\*\*\* VECTOR LENGTH N = ,14,2X,20HEXCEEDS DIMENSIONED CHECK113

14 2,10HVALUE NX = ,14) CHECK114

15 C 20 FORMAT (/1X,18H\*\*\* DIMENSION KX = ,14,2X,20HMUST BE AT LEAST AS , CHECK115

16 2 8HLARGE AS/5X,26HK + 2\*(DEGREE OF SPLINE) = ,14) CHECK116

17 C 30 FORMAT (/1X,22H\*\*\* VECTOR LENGTH NY = ,14,2X, CHECK117

18 2 20HEXCEEDS DIMENSIONED ,11HVALUE NYX = ,14) CHECK118

19 C 40 FORMAT (/1X,17H\*\*\* WEIGHT NUMBER,15,1X,13HIS NEGATIVE (,C10.5,1H) CHECK119

20 50 FORMAT (/1X,22H\*\*\* DEGREE OF SPLINE (,13,12H) EXCEEDS 19) CHECK120

21 C 60 FORMAT (/1X,28H\*\*\* NUMBER OF OBSERVATIONS (,14,13H) MUST EXCEED, CHECK121

22 2 15) CHECK122

23 C 70 FORMAT (/1X,33H\*\*\* ALPHA LEVEL OF SIGNIFICANCE (,F6.3, CHECK123

24 2 10H) MUST BE ,21HIN THE INTERVAL (0,1]) CHECK124

25 C 80 FORMAT (/1X,33H\*\*\* DELTA LEVEL OF SIGNIFICANCE (,F6.3, CHECK125

26 2 10H) MUST BE ,21HIN THE INTERVAL (0,1]) CHECK126

27 C 90 FORMAT (/1X,16H\*\*\* CONSTANT C (,F6.3,26H) MUST BE IN THE INTERVAL CHECK127

28 2,11H0.85,1.25]) CHECK128

29 C 100 FORMAT (/1X,14,1X,40HERROR CONDITIONS DETECTED BY SUBROUTINE , CHECK129

30 2 8H\*CHECK1\*/6X,38H\*\*\*PROGRAM EXECUTION TERMINATED\*\*\*\*//) CHECK130

31 C 110 FORMAT (/1X,47H\*\*\* MAXIMUM ORDER OF SPLINES JX MUST BE 20 (NOT,13, CHECK131

32 2 1H) ) CHECK132

33 C 120 FORMAT (/5X,42HSEE APPENDIX 1 OF THE FOLLOWING NBS PAPER://5X, CHECK133

34 2 36HA NEW APPROACH TO VOLUME CALIBRATION/5X, CHECK134

35 3 51HBY J. A. LECHNER, C. P. REEVE, AND C. H. SPIEGELMAN/) CHECK135

36 C 130 FORMAT (/1X,23H\*\*\* VECTOR LENGTH N+K = ,14,2X, CHECK136

37 2 20HEXCEEDS DIMENSIONED ,11HVALUE NKX = ,14) CHECK137

38 C--- INITIALIZE COUNT FOR ERROR CONDITIONS CHECK138

39 KOUNT=0 CHECK139

40 C--- INITIALIZE NUMBER OF ZERO WEIGHTS CHECK140

41 NZ=0 CHECK141

42 C--- CHECK FOR VECTOR LENGTHS EXCEEDING DIMENSIONED VALUES CHECK142

43 IF (N.LE.NX) GO TO 140 CHECK143

44 KOUNT=KOUNT+1 CHECK144

45 WRITE (6,10) N,NX CHECK145

46 NK=N+K CHECK146

47 IF (NK.LE.NKX) GO TO 150 CHECK147

48 KOUNT=KOUNT+1 CHECK148

49 WRITE (6,130) NK,NKX CHECK149

50 K2=K+2\*(M0-1) CHECK150

51 IF (K2.LE.KX) GO TO 160 CHECK151

52 KOUNT=KOUNT+1 CHECK152

53 WRITE (6,20) KX,K2 CHECK153

54 IF (NY.LE.NYX) GO TO 170 CHECK154

55 KOUNT=KOUNT+1 CHECK155

56 WRITE (6,30) NY,NYX CHECK156

57 C--- CHECK FOR NEGATIVE AND ZERO WEIGHTS CHECK157

```

58 170 D0 200 I=1,N
59 IF (W(I)) 180,190,200
60 C--- COUNT EACH NEGATIVE WEIGHT AS AN ERROR CONDITION
61 180 KOUNT=KOUNT+1
62 WRITE (6,40) I,W(I)
63 GO TO 200
64 C--- COUNT ZERO WEIGHTS
65 190 NZ=NZ+1
66 CONTINUE
67 200 CHECK FOR MAXIMUM ORDER OF SPLINE = 20
68 IF (JX.EQ.20) GO TO 210
69 KOUNT=KOUNT+1
70 WRITE (6,110) JX
71 C--- CHECK ORDER OF SPLINE
72 210 IF (M0.LE.20) GO TO 220
73 KOUNT=KOUNT+1
74 MD=M0-1
75 WRITE (6,50) MD
76 C--- CHECK NUMBER OF OBSERVATIONS
77 220 K2=K+M0-2+NZ
78 IF (N.GT.K2) GO TO 230
79 KOUNT=KOUNT+1
80 WRITE (6,60) N,K2
81 C--- CHECK SIGNIFICANCE LEVELS
82 230 IF (AL.GT.0.0.AND.AL.LE.1.0) GO TO 240
83 KOUNT=KOUNT+1
84 WRITE (6,70) AL
85 IF (DL.GT.0.0.AND.DL.LE.1.0) GO TO 250
86 KOUNT=KOUNT+1
87 WRITE (6,80) DL
88 C--- CHECK CONSTANT C
89 250 IF (C.LE.1.25.AND.C.CE.0.85) GO TO 260
90 KOUNT=KOUNT+1
91 WRITE (6,90) C
92 WRITE (6,120)
93 C--- CHECK WHETHER ANY ERROR CONDITIONS EXIST
94 260 IF (KOUNT.EQ.0) RETURN
95 WRITE (6,100) KOUNT
96 STOP
97 END
CHECK158
CHECK159
CHECK160
CHECK161
CHECK162
CHECK163
CHECK164
CHECK165
CHECK166
CHECK167
CHECK168
CHECK169
CHECK170
CHECK171
CHECK172
CHECK173
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CHECK197

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1  CPR*NS(1), CHECK2(1)
2  SUBROUTINE CHECK2 ( T, K, KX, X, W, N, NX, NZ, MO)
3  CHECK2
4  CHECK2 WRITTEN BY CHARLES P. REEVE, STATISTICAL ENGINEERING
5  DIVISION, NATIONAL BUREAU OF STANDARDS, WASHINGTON, D.C.
6  AS PART OF THE FIXED-KNOT SPLINE PACKAGE FOR CALIBRATION
7  FOR: CHECKING FOR OBSERVATIONS WHICH LIE OUTSIDE THE SEQUENCE OF
8  KNOTS. THE WEIGHTS OF SUCH OBSERVATIONS ARE SET TO ZERO.
9  SUBPROGRAMS CALLED: -NONE-
10 CURRENT VERSION COMPLETED MARCH 24, 1980
11 -----
12 DIMENSION T(KX), X(NX), WC(NX)
13 FORMAT (/1X, 6H** X(, 14, 3H) =, G12.6, 1X, 22HIS OUTSIDE KNOT SPAN. ,
14 2 1X, 11HSET WEIGHT(, 14, 5H) = 0.)
15 FORMAT (/1X, 48H** ADDITIONAL ZERO WEIGHTS GIVE NONPOSITIVE *** / 9XCHECK214
16 2, 32HDEGREES OF FREEDOM FOR RESIDUALS / 6X, 13H*****PROGRAM ,
17 3 25HEXECUTION TERMINATED*****//)
18 FORMAT (/1X, 15H*** VALUE OF X(, 14, 14H) CHANGED FROM, G14.8, 2X, 2HTO,
19 2 G14.8 / 5X, 45HSO THAT IT WILL BE LESS THAN THE LARGEST KNOT)
20 DO 60 I=1, N
21 IF (W(I).EQ.0.0) GO TO 60
22 IF (X(I).LT.T(1)) GO TO 50
23 IF (X(I)-T(K)) 60, 40, 50
24 XOLD=X(I)
25 X(I)=XOLD-ABS(XOLD)*0.0000001
26 WRITE (6, 30) I, XOLD, X(I)
27 GO TO 60
28 W(I)=0.0
29 NZ=NZ+1
30 WRITE (6, 10) I, X(I), I
31 CONTINUE
32 K2=K+MO-2+NZ
33 IF (N.GT.K2) RETURN
34 WRITE (6, 20)
35 STOP
36 END

```

CPR\*NS(1).CHSCDF(1)

SUBROUTINE CHSCDF (X,NU,CDF)

PURPOSE--THIS SUBROUTINE COMPUTES THE CUMULATIVE DISTRIBUTION FUNCTION VALUE FOR THE CHI-SQUARED DISTRIBUTION WITH INTEGER DEGREES OF FREEDOM PARAMETER = NU. THIS DISTRIBUTION IS DEFINED FOR ALL NON-NEGATIVE X. THE PROBABILITY DENSITY FUNCTION IS GIVEN IN THE REFERENCES BELOW.

INPUT ARGUMENTS--X = THE SINGLE PRECISION VALUE AT WHICH THE CUMULATIVE DISTRIBUTION FUNCTION IS TO BE EVALUATED.  
X SHOULD BE NON-NEGATIVE.

--NU = THE INTEGER NUMBER OF DEGREES OF FREEDOM.

OUTPUT ARGUMENTS--CDF = NU SHOULD BE POSITIVE.  
= THE SINGLE PRECISION CUMULATIVE DISTRIBUTION FUNCTION VALUE.

OUTPUT--THE SINGLE PRECISION CUMULATIVE DISTRIBUTION FUNCTION VALUE FOR THE CHI-SQUARED DISTRIBUTION WITH DEGREES OF FREEDOM PARAMETER = NU.

PRINTING--NONE UNLESS AN INPUT ARGUMENT ERROR CONDITION EXISTS. RESTRICTIONS--X SHOULD BE NON-NEGATIVE.

--NU SHOULD BE A POSITIVE INTEGER VARIABLE.

OTHER DATAPAC SUBROUTINES NEEDED--NORCDF.  
FORTRAN LIBRARY SUBROUTINES NEEDED--DSQRT, DEXP.

MODE OF INTERNAL OPERATIONS--DOUBLE PRECISION.  
LANGUAGE--ANSI FORTRAN.

REFERENCES--NATIONAL BUREAU OF STANDARDS APPLIED MATHEMATICS SERIES 55, 1964, PAGE 941, FORMULAE 26.4.4 AND 26.4.5.

--JOHNSON AND KOTZ, CONTINUOUS UNIVARIATE DISTRIBUTIONS--1, 1970, PAGE 176,  
FORMULA 28, AND PAGE 180, FORMULA 33.1.

--OWEN, HANDBOOK OF STATISTICAL TABLES, 1962, PAGES 50-55.

--PEARSON AND HARTLEY, BIOMETRIKA TABLES FOR STATISTICIANS, VOLUME 1, 1954,  
PAGES 122-131.

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UPDATED --MAY 1974.  
--SEPTEMBER 1975.  
UPDATED --NOVEMBER 1975.  
UPDATED --OCTOBER 1976.

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DOUBLE PRECISION DX,PI,CHI,SUM,TERM,AI,DCDFN

DOUBLE PRECISION DNU

DOUBLE PRECISION DSQRT,DEXP

DOUBLE PRECISION DLOG

DOUBLE PRECISION DFACT,DPOWER

DOUBLE PRECISION DW

DOUBLE PRECISION D1,D2,D3

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 CHSCD115

DOUBLE PRECISION TERM0, TERM1, TERM2, TERM3, TERM4  
 DOUBLE PRECISION B11  
 DOUBLE PRECISION B21  
 DOUBLE PRECISION B31, B32  
 DOUBLE PRECISION B41, B42, B43  
 DATA NUCUT /1000/  
 DATA PI /3.14159265358979D0/  
 DATA DPOWER /0.333333333333333D0/  
 DATA B11 /0.333333333333333D0/  
 DATA B21 /-0.0277777777777778D0/  
 DATA B31 /-0.00061728395061D0/  
 DATA B32 /-13.0D0/  
 DATA B41 /0.00018004115226D0/  
 DATA B42 /6.0D0/  
 DATA B43 /17.0D0/

C

IPR=6

CHECK THE INPUT ARGUMENTS FOR ERRORS

IF (NU.LE.0) GO TO 10  
 IF (X.LT.0.0) GO TO 20

GO TO 30

WRITE (IPR,50)

WRITE (IPR,70) NU

CDF=0.0

RETURN

WRITE (IPR,40)

WRITE (IPR,60) X

CDF=0.0

RETURN

CONTINUE

FORMAT (1H,96H\*\*\*\* NON-FATAL DIAGNOSTIC--THE FIRST INPUT ARGUMENT IS NEGATIVE \*\*\*\*\*)  
 2NT TO THE CHSCDF SUBROUTINE IS NEGATIVE \*\*\*\*\*)

FORMAT (1H,91H\*\*\*\* FATAL ERROR--THE SECOND INPUT ARGUMENT TO THE CHSCDF SUBROUTINE IS NON-POSITIVE \*\*\*\*\*)  
 2 CHSCDF SUBROUTINE IS NON-POSITIVE \*\*\*\*\*)

FORMAT (1H,35H\*\*\*\* THE VALUE OF THE ARGUMENT IS ,E15.8,6H \*\*\*\*\*)  
 FORMAT (1H,35H\*\*\*\* THE VALUE OF THE ARGUMENT IS ,I8,6H \*\*\*\*\*)

-----START POINT-----

DX=X

ANU=NU

DNU=NU

IF X IS NON-POSITIVE, SET CDF = 0.0 AND RETURN.

IF NU IS SMALLER THAN 10 AND X IS MORE THAN 200

STANDARD DEVIATIONS BELOW THE MEAN,

SET CDF = 0.0 AND RETURN.

IF NU IS 10 OR LARGER AND X IS MORE THAN 100

STANDARD DEVIATIONS BELOW THE MEAN,

SET CDF = 0.0 AND RETURN.

IF NU IS SMALLER THAN 10 AND X IS MORE THAN 200

STANDARD DEVIATIONS ABOVE THE MEAN,

SET CDF = 1.0 AND RETURN.

IF NU IS 10 OR LARGER AND X IS MORE THAN 100

STANDARD DEVIATIONS ABOVE THE MEAN,

SET CDF = 1.0 AND RETURN.

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116 C
117 IF (X.LE.0.0) GO TO 80
118 AMEAN=ANU
119 SD=SQRT(2.0*ANU)
120 Z=(X-AMEAN)/SD
121 IF (NU.LT.10.AND.Z.LT.-200.0) GO TO 80
122 IF (NU.GE.10.AND.Z.LT.-100.0) GO TO 80
123 IF (NU.LT.10.AND.Z.GT.200.0) GO TO 90
124 IF (NU.GE.10.AND.Z.GT.100.0) GO TO 90
125 GO TO 100
126 CDF=0.0
127 RETURN
128 CDF=1.0
129 RETURN
130 CONTINUE
131 C
132 DISTINGUISH BETWEEN 3 SEPARATE REGIONS
133 OF THE (X,NU) SPACE.
134 BRANCH TO THE PROPER COMPUTATIONAL METHOD
135 DEPENDING ON THE REGION.
136 NUCUT HAS THE VALUE 1000.
137 C
138 IF (NU.LT.NUCUT) GO TO 120
139 IF (NU.GE.NUCUT.AND.X.LE.ANU) GO TO 180
140 IF (NU.GE.NUCUT.AND.X.GT.ANU) GO TO 190
141 IBRAN=1
142 WRITE (IPR,110) IBRAN
143 FORMAT (1H,42H****INTERNAL ERROR IN CHSCDF SUBROUTINE--,
144 2 46HIMPOSSIBLE BRANCH CONDITION AT BRANCH POINT = ,18)
145 RETURN
146 C
147 TREAT THE SMALL AND MODERATE DEGREES OF FREEDOM CASE
148 (THAT IS, WHEN NU IS SMALLER THAN 1000).
149 METHOD UTILIZED--EXACT FINITE SUM
150 (SEE AMS 55, PAGE 941, FORMULAE 26.4.4 AND 26.4.5).
151 C
152 CONTINUE
153 CHI=DSQRT(DX)
154 IEVODD=NU-2*(NU/2)
155 IF (IEVODD.EQ.0) GO TO 130
156 C
157 SUM=0.0D0
158 TERM=1.0/CHI
159 IMIN=1
160 IMAX=NU-1
161 GO TO 140
162 C
163 SUM=1.0D0
164 TERM=1.0D0
165 IMIN=2
166 IMAX=NU-2
167 C
168 IF (IMIN.GT.IMAX) GO TO 160
169 DO 150 I=IMIN,IMAX,2
170 AI=I
171 TERM=TERM*(DX/AI)
172 SUM=SUM+TERM
173 CONTINUE

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CHSCD116
CHSCD117
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219 CHSCD219
220 CHSCD220
221 CHSCD221

CONTINUE
SUM=SUM*DEXP(-DX/2.0D0)
IF (IEVODD.EQ.0) GO TO 170
SUM=(DSQRT(2.0D0/PI))*SUM
SPCHI=CHI
CALL NORCDF (SPCHI, CDFN)
DCDFN=CDFN
SUM=SUM+2.0D0*(1.0D0-DCDFN)
CDF=1.0D0-SUM
RETURN

170
TREAT THE CASE WHEN NU IS LARGE
(THAT IS, WHEN NU IS EQUAL TO OR GREATER THAN 1000)
AND X IS LESS THAN OR EQUAL TO NU.
METHOD UTILIZED--WILSON-HILFERTY APPROXIMATION
(SEE JOHNSON AND KOTZ, VOLUME 1, PAGE 176, FORMULA 28).

CONTINUE
DFACT=4.5D0*DNU
U=((DX/DNU)**DPOWER)-1.0D0+(1.0D0/DFACT)*DSQRT(DFACT)
CALL NORCDF (U, CDFN)
RETURN

C
TREAT THE CASE WHEN NU IS LARGE
(THAT IS, WHEN NU IS EQUAL TO OR GREATER THAN 1000)
AND X IS LARGER THAN NU.
METHOD UTILIZED--HILL'S ASYMPTOTIC EXPANSION
(SEE JOHNSON AND KOTZ, VOLUME 1, PAGE 180, FORMULA 33.1).

CONTINUE
DW=DSQRT(DX-DNU-DNU*DLOG(DX/DNU))
DANU=DSQRT(2.0D0/DNU)
D1=DW
D2=DW**2
D3=DW**3
TERM0=DW
TERM1=B11*DANU
TERM2=B21*D1*(DANU**2)
TERM3=B31*(D2+B32)*(DANU**3)
TERM4=B41*(B42*D3+B43*D1)*(DANU**4)
U=TERM0+TERM1+TERM2+TERM3+TERM4
CALL NORCDF (U, CDFN)
RETURN

C
END

```

CPR\*NS(1).CHSPPF(1)

SUBROUTINE CHSPPF ( P, NU, PPF )

PURPOSE--THIS SUBROUTINE COMPUTES THE PERCENT POINT FUNCTION VALUE FOR THE CHI-SQUARED DISTRIBUTION WITH INTEGER DEGREES OF FREEDOM PARAMETER = NU. THE CHI-SQUARED DISTRIBUTION USED HEREIN IS DEFINED FOR ALL NON-NEGATIVE X, AND ITS PROBABILITY DENSITY FUNCTION IS GIVEN IN REFERENCES 2, 3, AND 4 BELOW.

NOTE THAT THE PERCENT POINT FUNCTION OF A DISTRIBUTION IS IDENTICALLY THE SAME AS THE INVERSE CUMULATIVE DISTRIBUTION FUNCTION OF THE DISTRIBUTION.

INPUT ARGUMENTS--P = THE SINGLE PRECISION VALUE ( BETWEEN 0.0 ( INCLUSIVELY ) AND 1.0 ( EXCLUSIVELY ) ) AT WHICH THE PERCENT POINT FUNCTION IS TO BE EVALUATED.

--NU = THE INTEGER NUMBER OF DEGREES OF FREEDOM.

OUTPUT ARGUMENTS--PPF = THE SINGLE PRECISION PERCENT POINT FUNCTION VALUE.

OUTPUT--THE SINGLE PRECISION PERCENT POINT FUNCTION VALUE PPF FOR THE CHI-SQUARED DISTRIBUTION WITH DEGREES OF FREEDOM PARAMETER = NU.

PRINTING--NONE UNLESS AN INPUT ARGUMENT ERROR CONDITION EXISTS. RESTRICTIONS--NU SHOULD BE A POSITIVE INTEGER VARIABLE. --P SHOULD BE BETWEEN 0.0 ( INCLUSIVELY ) AND 1.0 ( EXCLUSIVELY ).

OTHER DATAPAC SUBROUTINES NEEDED--NONE.

FORTAN LIBRARY SUBROUTINES NEEDED--DEXP, DLOG.

MODE OF INTERNAL OPERATIONS--DOUBLE PRECISION.

LANGUAGE--ANSI FORTRAN.

ACCURACY--(ON THE UNIVAC 1108, EXEC 8 SYSTEM AT NBS)

COMPARED TO THE KNOWN NU = 2 (EXPONENTIAL)

RESULTS, AGREEMENT WAS HAD OUT TO 6 SIGNIFICANT

DIGITS FOR ALL TESTED P IN THE RANGE P = .001 TO

P = .999. FOR P = .95 AND SMALLER, THE AGREEMENT

WAS EVEN BETTER--7 SIGNIFICANT DIGITS.

(NOTE THAT THE TABULATED VALUES GIVEN IN THE WILK,

GNANADESIKAN, AND HUYETT REFERENCE BELOW, PAGE 20,

ARE IN ERROR FOR AT LEAST THE GAMMA = 1 CASE--

THE WORST DETECTED ERROR WAS AGREEMENT TO ONLY 3

SIGNIFICANT DIGITS ( IN THEIR 8 SIGNIFICANT DIGIT TABLE)

FOR P = .999.)

REFERENCES--WILK, GNANADESIKAN, AND HUYETT, 'PROBABILITY

PLOTS FOR THE GAMMA DISTRIBUTION',

TECHNOMETRICS, 1962, PAGES 1-15,

ESPECIALLY PAGES 3-5.

--NATIONAL BUREAU OF STANDARDS APPLIED MATHEMATICS

SERIES 55, 1964, PAGE 257, FORMULA 6.1.41,

AND PAGES 940-943.

--JOHNSON AND KOTZ, CONTINUOUS UNIVARIATE

DISTRIBUTIONS--1, 1970, PAGES 166-206.

--EASTINGS AND PEACOCK, STATISTICAL

DISTRIBUTIONS--A HANDBOOK FOR

STUDENTS AND PRACTITIONERS, 1975,

CHSP001  
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 CHSP114  
 CHSP115

WRITTEN BY--JAMES J. FILLIBEN  
 STATISTICAL ENGINEERING LABORATORY (205.03)  
 NATIONAL BUREAU OF STANDARDS  
 WASHINGTON, D. C. 20234  
 PHONE: 301-921-2315  
 ORIGINAL VERSION--SEPTEMBER 1975.  
 UPDATED --NOVEMBER 1975.

DOUBLE PRECISION DP, DCAMMA  
 DOUBLE PRECISION Z, Z2, Z3, Z4, Z5, DEN, A, B, C, D, C  
 DOUBLE PRECISION XMIN0, XMIN, AI, XMAX, DX, PCALC, XMID  
 DOUBLE PRECISION XLOWER, XUPPER, XDEL  
 DOUBLE PRECISION SUM, TERM, CUT1, CUT2, AJ, CUTOFF, T  
 DIMENSION D(10)  
 DATA C / .918938533204672741D0/  
 DATA D(1), D(2), D(3), D(4), D(5) / +.83333333333333333333333333333333D-1,  
 2 - .27777777777777777777778D-2, +.793650793650793651D-3,  
 3 - .595238095238095238D-3, +.841750841750841751D-3/  
 DATA D(6), D(7), D(8), D(9), D(10) / -.191752691752691753D-2,  
 2 +.641025641025641025D-2, -.295506535947712418D-1,  
 3 +.17964432368830573D0, -.139243221690590111D1/

IPR=6  
 CHECK THE INPUT ARGUMENTS FOR ERRORS

IF (P.LT.0.0.OR.P.GE.1.0) GO TO 10  
 IF (NU.LT.1) GO TO 20

GO TO 30  
 WRITE (IPR, 40)  
 WRITE (IPR, 60) P  
 PPF=0.0  
 RETURN  
 WRITE (IPR, 50)  
 WRITE (IPR, 70) NU  
 PPF=0.0  
 RETURN

CONTINUE  
 FORMAT (1H, 115H\*\*\*\* FATAL ERROR--THE FIRST INPUT ARGUMENT TO THE  
 2E CHSPPF SUBROUTINE IS OUTSIDE THE ALLOWABLE (0,1) INTERVAL \*\*\*\*\*) CHSP101  
 FORMAT (1H, 91H\*\*\*\* FATAL ERROR--THE SECOND INPUT ARGUMENT TO THE  
 2 CHSPPF SUBROUTINE IS NON-POSITIVE \*\*\*\*\*)  
 FORMAT (1H, 35H\*\*\*\* THE VALUE OF THE ARGUMENT IS, E15.8, 6H \*\*\*\*\*) CHSP104  
 FORMAT (1H, 35H\*\*\*\* THE VALUE OF THE ARGUMENT IS, I8, 6H \*\*\*\*\*)

START POINT-----  
 EXPRESS THE CHI-SQUARED DISTRIBUTION PERCENT POINT  
 FUNCTION IN TERMS OF THE EQUIVALENT GAMMA  
 DISTRIBUTION PERCENT POINT FUNCTION,  
 AND THEN EVALUATE THE LATTER.

ANU=NU  
 GAMMA=ANU/2.0

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 CHSPP117  
 CHSPP118  
 CHSPP119  
 CHSPP120  
 CHSPP121  
 CHSPP122  
 CHSPP123  
 CHSPP124  
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 CHSPP171  
 CHSPP172  
 CHSPP173

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DP=P
DNU=NU
DCAMMA=DNU/2.0D0
MAXIT=10000

C COMPUTE THE GAMMA FUNCTION USING THE ALGORITHM IN THE
C NBS APPLIED MATHEMATICS SERIES REFERENCE.
C THIS GAMMA FUNCTION NEED BE CALCULATED ONLY ONCE.
C IT IS USED IN THE CALCULATION OF THE CDF BASED ON
C THE TENTATIVE VALUE OF THE PPF IN THE ITERATION.
C
Z=DCAMMA
DER=1.0D0
IF (Z.GE.10.0D0) GO TO 90
DER=DEN*Z
Z=Z+1.0D0
GO TO 80
90 Z2=Z*Z
Z3=Z*Z2
Z4=Z2*Z2
Z5=Z2*Z3
A=(Z-0.5D0)*DLOG(Z)-Z+C
B=D(1)/Z+D(2)/Z3+D(3)/Z5+D(4)/(Z2*Z5)+D(5)/(Z4*Z5)+D(6)/(Z*Z3*Z5)+
2D(7)/(Z3*Z5*Z5)+D(8)/(Z5*Z5*Z5)+D(9)/(Z2*Z5*Z5*Z5)
C=DEXP(A+B)/DEN
C DETERMINE LOWER AND UPPER LIMITS ON THE DESIRED 100%
C PERCENT POINT.
C
ILOOP=1
XMIN=(DP*DCAMMA*C)**(1.0D0/DCAMMA)
XMIN=XMIN0
ICOUNT=1
AI=ICOUNT
XMAX=AI*XMIN0
DX=XMAX
GO TO 180
IF (PCALC.GE.DP) GO TO 120
XMIN=XMAX
ICOUNT=ICOUNT+1
IF (ICOUNT.LE.30000) GO TO 100
XMIN=(XMIN+XMAX)/2.0D0
C NOW ITERATE BY BISECTION UNTIL THE DESIRED ACCURACY IS ACHIEVED.
C
ILOOP=2
XLOWER=XMIN
XUPPER=XMAX
ICOUNT=0
DX=XMIN
GO TO 180
IF (PCALC.EQ.DP) GO TO 170
IF (PCALC.GT.DP) GO TO 150
XLOWER=XMIN
XMIN=(XMIN+XUPPER)/2.0D0
GO TO 160
XUPPER=XMIN
XMIN=(XMIN+XLOWER)/2.0D0
  
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174 XDEL=XMID-XLOWER
175 IF (XDEL.LT.0.0D0) XDEL=-XDEL
176 ICOUNT=ICOUNT+1
177 IF (XDEL.LT.0.0000000001D0.OR.ICOUNT.GT.100) GO TO 170
178 GO TO 130
179 PPF=2.0D0*XMID
180 RETURN
181
182 C*****
183 C THIS SECTION BELOW IS LOGICALLY SEPARATE FROM THE ABOVE.
184 C THIS SECTION COMPUTES A CDF VALUE FOR ANY GIVEN TENTATIVE
185 C PERCENT POINT X VALUE AS DEFINED IN EITHER OF THE 2
186 C ITERATION LOOPS IN THE ABOVE CODE.
187
188 C COMPUTE T-SUB-Q AS DEFINED ON PAGE 4 OF THE WILK, GNANADESIKAN,
189 C AND HUYEIT REFERENCE
190 C
191 C SUM=1.0D0/DCAMMA
192 C TERN=1.0D0/DCAMMA
193 C CUT1=DX-DCAMMA
194 C CUT2=DX*1000000000.0D0
195 C DO 190 J=1,MAXIT
196 C AJ=J
197 C TERM=DX*TERM/(DCAMMA+AJ)
198 C SUM=SUM+TERM
199 C CUTOFF=CUT1+(CUT2*TERM/SUM)
200 C IF (AJ.GT.CUTOFF) GO TO 200
201 C CONTINUE
202 C WRITE (IPR,210) MAXIT
203 C WRITE (IPR,220) P
204 C WRITE (IPR,230) NU
205 C WRITE (IPR,240)
206 C PPF=0.0
207 C RETURN
208
209 C T-SUM
210 C PCALC=(DX**DCAMMA)*(DEXP(-DX))*T/G
211 C IF (ILOOP.EQ.1) GO TO 110
212 C GO TO 140
213
214 C FORMAT (1H,48H****ERROR IN INTERNAL OPERATIONS IN THE CHSPPF,
215 C 2 45HROUTINE--THE NUMBER OF ITERATIONS EXCEEDS ,17)
216 C FORMAT (1H,33H THE INPUT VALUE OF P IS ,E15.8)
217 C FORMAT (1H,33H THE INPUT VALUE OF NU IS ,18)
218 C FORMAT (1H,48H THE OUTPUT VALUE OF PPF HAS BEEN SET TO 0.0)
219 C
220 C

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CHSP174
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CPR=NS(1).CIYFIN(6)

```
1 SUBROUTINE CIYFIN (XF, YF, YFSD, NF, RSD, AL, DL, C, NRS, NB, YFL, YFU, IP) CIYFIN01
2 C----- CIYFIN CIYFIN02
3 C CIYFIN WRITTEN BY CHARLES P. REEVE, STATISTICAL ENGINEERING CIYFIN03
4 C DIVISION, NATIONAL BUREAU OF STANDARDS, WASHINGTON, D. C. CIYFIN04
5 C AS PART OF THE FIXED-KNOT SPLINE PACKAGE FOR CALIBRATION CIYFIN05
6 C FOR: COMPUTING CONFIDENCE INTERVALS FOR PREDICTED Y-VALUES ON A CIYFIN06
7 C CALIBRATION CURVE USING SCHEFFE'S TECHNIQUE CIYFIN07
8 C CIYFIN08
9 C REFERENCE: SCHEFFE, HENRY, 'A STATISTICAL THEORY OF CALIBRATION' CIYFIN09
10 C THE ANNALS OF STATISTICS, VOLUME 1, NUMBER 1 CIYFIN10
11 C JANUARY 1973, PP. 1-37 CIYFIN11
12 C CIYFIN12
13 C SUBPROGRAMS CALLED: CHSPFF, FPPF, NORPPF CIYFIN13
14 C CURRENT VERSION COMPLETED MARCH 17, 1980 CIYFIN14
15 C----- CIYFIN15
16 C DIMENSION XF(NF), YF(NF), YFSD(NF), YFL(NF), YFU(NF) CIYFIN16
17 C WRITE FORMATS CIYFIN17
18 C FORMAT (15X, 2HZ(, F7.5, 3H) =, F11.5) CIYFIN18
19 C FORMAT (6X, 6HCHISQ(, F7.5, 1H, 14, 3H) =, F11.5) CIYFIN19
20 C FORMAT (5X, 2HF(, F7.5, 1H, 14, 1H, 14, 3H) =, F11.5) CIYFIN20
21 C FORMAT (/1X, 75(1H-)/1X, 26H* CONFIDENCE INTERVALS FOR, 15, 1X, CIYFIN21
22 C 2 43HEVENLY SPACED POINTS WITHIN THE KNOT SPAN */1X, 75(1H-)/5X, CIYFIN22
23 C 3 7HALPHA =, F8.5, 5X, 7HDELTA =, F8.5, 5X, 3HC =, F5.2/) CIYFIN23
24 C FORMAT (1X, 14, 5G13.6) CIYFIN24
25 C FORMAT (/20X, 9HPREDICTED, 5X, 7HSTD DEV, 6X, 19HCONFIDENCE INTERVAL/ CIYFIN25
26 C 2 4X, 1H1, 5X, 4HX(1), 9X, 4HY(1), 6X, 9HPRED Y(1), 6X, 5HLOWER, 8X, 5HUPPER/) CIYFIN26
27 C WRITE (6, 40) NF, AL, DL, C CIYFIN27
28 C COMPUTE Z(1-AL/2) CRITICAL POINT FOR N(0, 1) P. D. F. CIYFIN28
29 C P=1.0-AL/2.0 CIYFIN29
30 C CALL NORPPF (P, ZAL) CIYFIN30
31 C WRITE (6, 10) P, ZAL CIYFIN31
32 C ARTIFICIALLY SET NEXT TWO CRITICAL POINTS IF DELTA=1 CIYFIN32
33 C CDL=NRS CIYFIN33
34 C FDL=0 CIYFIN34
35 C P=1.0-DL CIYFIN35
36 C IF (DL.EQ.1.0) GO TO 70 CIYFIN36
37 C COMPUTE CHISQ(DL) CRITICAL POINT FOR CHI-SQUARED(NRS) P. D. F. CIYFIN37
38 C CALL CHSPFF (DL, NRS, CDL) CIYFIN38
39 C WRITE (6, 20) DL, NRS, CDL CIYFIN39
40 C COMPUTE F(1-DL) CRITICAL POINT FOR F(NB, NRS) P. D. F. CIYFIN40
41 C CALL FPPF (P, NB, NRS, FDL) CIYFIN41
42 C WRITE (6, 30) P, NB, NRS, FDL CIYFIN42
43 C COMPUTE CONFIDENCE INTERVAL FOR EACH Y VALUE CIYFIN43
44 C C1=ZAL*SQRT(FLOAT(NRS)/CDL) CIYFIN44
45 C C2=SQRT(FLOAT(NB)*FDL) CIYFIN45
46 C C3=C*NRS CIYFIN46
47 C DO 80 I=1, NF CIYFIN47
48 C WIDTH=C3*(C1+C2*YFSD(I)) CIYFIN48
49 C YFL(I)=YF(I)-WIDTH CIYFIN49
50 C YFU(I)=YF(I)+WIDTH CIYFIN50
51 C CONTINUE CIYFIN51
52 C CHECK WHETHER TO PRINT OUT EACH Y VALUE AND ITS STANDARD DEVIATION CIYFIN52
53 C IF (IP.LT.2) GO TO 100 CIYFIN53
54 C PRINT OUT EACH Y VALUE AND ITS STANDARD DEVIATION CIYFIN54
55 C WRITE (6, 60) CIYFIN55
56 C DO 90 I=1, NF CIYFIN56
57 C WRITE (6, 50) I, XF(I), YF(I), YFSD(I), YFL(I), YFU(I) CIYFIN57
```

CIYFIN58  
CIYFIN59  
CIYFIN60  
CIYFIN61  
CIYFIN62  
CIYFIN63  
CIYFIN64

90 CONTINUE  
RETURN  
100 WRITE (6,110)  
110 FORMAT (/IX,43H\*\*\*\*\* PRINTOUT OF Y CONFIDENCE INTERVALS ,  
2 18HSUPPRESSED \*\*\*\*\*)  
RETURN  
END

58  
59  
60  
61  
62  
63  
64

CFR\*NS(1).COVAR(2)

1 C SUBROUTINE COVAR (NMX,N,KMX,K,Q,CI)  
2 C INTEGER NMX,N,KMX,K  
3 C REAL Q(KMX,N),CI(NMX,N)  
4 C  
5 C THIS FORTRAN SUBROUTINE COMPUTES AND RETURNS THE N X N UNSCALED  
6 C COVARIANCE MATRIX CI OBTAINED BY INVERTING THE GRAMIAN MATRIX C. THE  
7 C CHOLESKY FACTOR L OF C IS ASSUMED TO BE STORED IN Q ON INPUT.  
8 C SUBROUTINE BCHSLV IS USED TO SOLVE FOR EACH COLUMN OF THE INVERSE.  
9 C ON INPUT.  
10 C  
11 C NMX IS THE ROW DIMENSION OF CI.  
12 C  
13 C N IS THE DIMENSION OF THE SPACE OF SPLINES OF ORDER  
14 C K.  
15 C  
16 C KMX IS THE ROW DIMENSION OF Q.  
17 C  
18 C K IS THE ORDER OF THE SPLINES = DEGREE + 1  
19 C  
20 C Q(\*,\*) HAS ROW DIMENSION KMX AND COLUMN DIMENSION AT LEAST  
21 C N. THE CHOLESKY FACTOR L OF C IS STORED IN THE  
22 C FIRST K ROWS OF THE MATRIX.  
23 C  
24 C ON OUTPUT.  
25 C  
26 C CI(\*,\*) HAS ROW DIMENSION NMX AND COLUMN DIMENSION AT LEAST  
27 C N. IT CONTAINS THE UNSCALED COVARIANCE MATRIX IN  
28 C STANDARD ROW, COLUMN FORM.  
29 C  
30 C AND THE REST OF THE VARIABLES ARE UNCHANGED.  
31 C  
32 C ADDITIONAL ROUTINES REQUIRED.  
33 C  
34 C BCHSLV  
35 C  
36 C BY.  
37 C  
38 C MARTIN CORDES  
39 C CENTER FOR APPLIED MATHEMATICS, NBS  
40 C VERSION 1 - OCT 1979  
41 C  
42 C  
43 C  
44 C-----  
45 C INTEGER I, J  
46 C  
47 C DO 20 J=1,N  
48 C DO 10 I=1,N  
49 C CI(I,J)=0.0  
50 C CONTINUE  
51 C CI(J,J)=1.0  
52 C CALL BCHSLV (Q,KMX,K,N,CI(1,J))  
53 C CONTINUE  
54 C  
55 C RETURN  
56 C END

1 C SUBROUTINE FCDF (X, NU1, NU2, CDF)  
 2 C  
 3 C PURPOSE--THIS SUBROUTINE COMPUTES THE CUMULATIVE DISTRIBUTION  
 4 C FUNCTION VALUE FOR THE F DISTRIBUTION  
 5 C WITH INTEGER DEGREES OF FREEDOM  
 6 C PARAMETERS = NU1 AND NU2.  
 7 C THIS DISTRIBUTION IS DEFINED FOR ALL NON-NEGATIVE X.  
 8 C THE PROBABILITY DENSITY FUNCTION IS GIVEN  
 9 C IN THE REFERENCES BELOW.  
 10 C INPUT ARGUMENTS--X = THE SINGLE PRECISION VALUE AT  
 11 C WHICH THE CUMULATIVE DISTRIBUTION  
 12 C FUNCTION IS TO BE EVALUATED.  
 13 C X SHOULD BE NON-NEGATIVE.  
 14 C = THE INTEGER DEGREES OF FREEDOM  
 15 C FOR THE NUMERATOR OF THE F RATIO.  
 16 C NU1 SHOULD BE POSITIVE.  
 17 C = THE INTEGER DEGREES OF FREEDOM  
 18 C FOR THE DENOMINATOR OF THE F RATIO.  
 19 C NU2 SHOULD BE POSITIVE.  
 20 C OUTPUT ARGUMENTS--CDF = THE SINGLE PRECISION CUMULATIVE  
 21 C DISTRIBUTION FUNCTION VALUE.  
 22 C OUTPUT--THE SINGLE PRECISION CUMULATIVE DISTRIBUTION  
 23 C FUNCTION VALUE CDF FOR THE F DISTRIBUTION  
 24 C WITH DEGREES OF FREEDOM  
 25 C PARAMETERS = NU1 AND NU2.  
 26 C PRINTING--NONE UNLESS AN INPUT ARGUMENT ERROR CONDITION EXISTS.  
 27 C RESTRICTIONS--X SHOULD BE NON-NEGATIVE.  
 28 C ---NU1 SHOULD BE A POSITIVE INTEGER VARIABLE.  
 29 C ---NU2 SHOULD BE A POSITIVE INTEGER VARIABLE.  
 30 C OTHER DATAPAC SUBROUTINES NEEDED--NORCDF, CHSCDF.  
 31 C FORTRAN LIBRARY SUBROUTINES NEEDED--DSQRT, DATAN.  
 32 C MODE OF INTERNAL OPERATIONS--DOUBLE PRECISION.  
 33 C LANGUAGE--ANSI FORTRAN.  
 34 C REFERENCES--NATIONAL BUREAU OF STANDARDS APPLIED MATHEMATICS  
 35 C SERIES 55, 1964, PAGES 946-947,  
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 48 C STATISTICAL ENGINEERING LABORATORY (205.03)  
 49 C NATIONAL BUREAU OF STANDARDS  
 50 C WASHINGTON, D. C. 20234  
 51 C PHONE: 301-921-2315  
 52 C ORIGINAL VERSION--AUGUST 1972.  
 53 C UPDATED --SEPTEMBER 1975.  
 54 C UPDATED --NOVEMBER 1975.  
 55 C UPDATED --OCTOBER 1976.  
 56 C  
 57 C

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58 C DOUBLE PRECISION DX,PI,ANU1,ANU2,Z,SUM,TERM,AI,COEF1,COEF2,ARG
59 C DOUBLE PRECISION COEF
60 C DOUBLE PRECISION THETA,SINTH,COSTH,A,B
61 C DOUBLE PRECISION DSQRT,DATAN
62 C DOUBLE PRECISION DFACT1,DFACT2,DNUM,DEN
63 C DOUBLE PRECISION DPOW1,DPOW2
64 C DOUBLE PRECISION DNU1,DNU2
65 C DOUBLE PRECISION TERMI,TERM2,TERM3
66 C DATA PI /3.14159265358979D0/
67 C DATA DPOW1,DPOW2 /0.333333333333333D0,0.666666666666667D0/
68 C DATA NUCUT1,NUCUT2 /100,1000/
69 C
70 C IPR=6
71 C
72 C CHECK THE INPUT ARGUMENTS FOR ERRORS
73 C
74 C
75 C IF (NU1.LE.0) GO TO 10
76 C IF (NU2.LE.0) GO TO 20
77 C IF (X.LT.0) GO TO 30
78 C GO TO 40
79 C WRITE (IPR,60)
80 C WRITE (IPR,90) NU1
81 C CDF=0.0
82 C RETURN
83 C WRITE (IPR,70)
84 C WRITE (IPR,90) NU2
85 C CDF=0.0
86 C RETURN
87 C WRITE (IPR,50)
88 C WRITE (IPR,80) X
89 C CDF=0.0
90 C RETURN
91 C CONTINUE
92 C FORMAT (1H ,96H*** NON-FATAL DIAGNOSTIC--THE FIRST INPUT ARGUMENT
93 C 2NT TO THE FCDF SUBROUTINE IS NEGATIVE *****)
94 C FORMAT (1H ,91H*** FATAL ERROR--THE SECOND INPUT ARGUMENT TO THE
95 C 2 FCDF SUBROUTINE IS NON-POSITIVE *****)
96 C FORMAT (1H ,91H*** FATAL ERROR--THE THIRD INPUT ARGUMENT TO THE
97 C 2 FCDF SUBROUTINE IS NON-POSITIVE *****)
98 C FORMAT (1H ,35H*** THE VALUE OF THE ARGUMENT IS ,E15.8,6H *****)
99 C FORMAT (1H ,35H*** THE VALUE OF THE ARGUMENT IS ,I8,6H *****)
100 C
101 C-----START POINT-----
102 C
103 C DX=X
104 C M=NU1
105 C N=NU2
106 C ANU1=NU1
107 C ANU2=NU2
108 C DNU1=NU1
109 C DNU2=NU2
110 C
111 C IF X IS NON-POSITIVE, SET CDF = 0.0 AND RETURN.
112 C IF NU2 IS 5 THROUGH 9 AND X IS MORE THAN 3000
113 C STANDARD DEVIATIONS BELOW THE MEAN,
114 C SET CDF = 0.0 AND RETURN.
115 C IF NU2 IS 10 OR LARGER AND X IS MORE THAN 150

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FCDF0101
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FCDF0103
FCDF0104
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FCDF0109
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FCDF0113
FCDF0114
FCDF0115

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116 C STANDARD DEVIATIONS BELOW THE MEAN.
117 C SET CDF = 0.0 AND RETURN.
118 C IF NU2 IS 5 THROUGH 9 AND X IS MORE THAN 3000
119 C STANDARD DEVIATIONS ABOVE THE MEAN,
120 C SET CDF = 1.0 AND RETURN.
121 C IF NU2 IS 10 OR LARGER AND X IS MORE THAN 150
122 C STANDARD DEVIATIONS ABOVE THE MEAN,
123 C SET CDF = 1.0 AND RETURN.
124 C
125 C IF (X.LE.0.0) GO TO 100
126 C IF (NU2.LE.4) GO TO 120
127 C T1=2.0/ANU1
128 C T2=ANU2/(ANU2-2.0)
129 C T3=(ANU1+ANU2-2.0)/(ANU2-4.0)
130 C AMEAN=T2
131 C SD=SQRT(T1*T2*T3)
132 C ZRATIO=(X-AMEAN)/SD
133 C IF (NU2.LT.10.AND.ZRATIO.LT.-3000.0) GO TO 100
134 C IF (NU2.GE.10.AND.ZRATIO.LT.-150.0) GO TO 100
135 C IF (NU2.LT.10.AND.ZRATIO.GT.3000.0) GO TO 110
136 C IF (NU2.GE.10.AND.ZRATIO.GT.150.0) GO TO 110
137 C GO TO 120
138 C CDF=0.0
139 C RETURN
140 C CDF=1.0
141 C RETURN
142 C CONTINUE
143 C
144 C
145 C DISTINGUISH BETWEEN 6 SEPARATE REGIONS
146 C OF THE (NU1,NU2) SPACE.
147 C BRANCH TO THE PROPER COMPUTATIONAL METHOD
148 C DEPENDING ON THE REGION.
149 C NUCUT1 HAS THE VALUE 100.
150 C NUCUT2 HAS THE VALUE 1000.
151 C
152 C IF (NU1.LT.NUCUT2.AND.NU2.LT.NUCUT2) GO TO 140
153 C IF (NU1.GE.NUCUT2.AND.NU2.GE.NUCUT2) GO TO 310
154 C IF (NU1.LT.NUCUT1.AND.NU2.GE.NUCUT2) GO TO 320
155 C IF (NU1.GE.NUCUT1.AND.NU2.GE.NUCUT2) GO TO 310
156 C IF (NU1.GE.NUCUT2.AND.NU2.LT.NUCUT1) GO TO 330
157 C IF (NU1.GE.NUCUT2.AND.NU2.GE.NUCUT1) GO TO 310
158 C IBRAN=5
159 C WRITE (IPR,130) IBRAN
160 C FORMAT (1H,42H***INTERNAL ERROR IN FCDF SUBROUTINE--
161 C 2 46HIMPOSSIBLE BRANCH CONDITION AT BRANCH POINT = ,18)
162 C RETURN
163 C
164 C TREAT THE CASE WHEN NU1 AND NU2
165 C ARE BOTH SMALL OR MODERATE
166 C (THAT IS, BOTH ARE SMALLER THAN 1000).
167 C METHOD UTILIZED--EXACT FINITE SUM
168 C (SEE AMS 55, PAGE 946, FORMULAE 26.6.4, 26.6.5,
169 C AND 26.6.8).
170 C CONTINUE
171 C Z=ANU2/(ANU2+ANU1*DX)
172 C IFLAG1=NU1-2*(NU1/2)
173 C IFLAG2=NU2-2*(NU2/2)

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FCDF0123
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FCDF0125
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FCDF0127
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220 CONTINUE  
 C  
 230 SUM=SUM+1.0D0  
 SUM=SUM\*SINTH\*COSTH  
 C  
 240 A=(2.0D0/PI)\*(THETA+SUM  
 SUM=0.0D0  
 TERM=1.0D0  
 IF (M.EQ.1) B=0.0D0  
 IF (M.EQ.1) GO TO 300  
 IF (M.EQ.3) GO TO 260  
 IMAX=M-3  
 DO 250 I=1, IMAX, 2  
 AI=I  
 COEF1=AI  
 COEF2=AI+2.0D0  
 TERM=TERM\*((ANU2+COEF1)/COEF2)\*(SINTH\*SINTH)  
 SUM=SUM+TERM  
 CONTINUE  
 250  
 C  
 260 SUM=SUM+1.0D0  
 SUM=SUM\*SINTH\*(COSTH\*\*N)  
 COEF=1.0D0  
 IEVODD=N-2\*(N/2)  
 IMIN=3  
 IF (IEVODD.EQ.0) IMIN=2  
 IF (IMIN.GT.N) GO TO 280  
 DO 270 I=IMIN, N, 2  
 AI=I  
 COEF=((AI-1.0D0)/AI)\*COEF  
 CONTINUE  
 270  
 C  
 280 COEF=COEF\*ANU2  
 IF (IEVODD.EQ.0) GO TO 290  
 COEF=COEF\*(2.0D0/PI)  
 C  
 290 B=COEF\*SUM  
 C  
 300 CDF=A-B  
 RETURN  
 C  
 C TREAT THE CASE WHEN NU1 AND NU2  
 ARE BOTH LARGE  
 (THAT IS, BOTH ARE EQUAL TO OR LARGER THAN 1000);  
 OR WHEN NU1 IS MODERATE AND NU2 IS LARGE  
 (THAT IS, WHEN NU1 IS EQUAL TO OR GREATER THAN 100  
 BUT SMALLER THAN 1000,  
 AND NU2 IS EQUAL TO OR LARGER THAN 1000);  
 OR WHEN NU2 IS MODERATE AND NU1 IS LARGE  
 (THAT IS WHEN NU2 IS EQUAL TO OR GREATER THAN 100  
 BUT SMALLER THAN 1000,  
 AND NU1 IS EQUAL TO OR LARGER THAN 1000).  
 METHOD UTILIZED--PAULSON APPROXIMATION  
 (SEE AMS 55, PAGE 947, FORMULA 26.6.15).  
 CONTINUE  
 DFACT1=1.0D0/(4.5D0\*DNU1)  
 DFACT2=1.0D0/(4.5D0\*DNU2)  
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290 DNUM=((1.0D0-DFACT2)*(DX**DPOW1))-((1.0D0-DFACT1)
291 DDEN=DSQRT((DFACT2*(DX**DPOW2))+DFACT1)
292 U=DNUM/DDEN
293 CALL NORCDF (U,CCDF)
294 CDF=CCDF
295 RETURN
296
297 C
298 C TREAT THE CASE WHEN NU1 IS SMALL
299 C AND NU2 IS LARGE
300 C (THAT IS, WHEN NU1 IS SMALLER THAN 100,
301 C AND NU2 IS EQUAL TO OR LARGER THAN 1000).
302 C METHOD UTILIZED--SHEFFE-TUKEY APPROXIMATION
303 C (SEE JOHNSON AND KOTZ, VOLUME 2, PAGE 84, THIRD FORMULA).
304 C
305 C 320
306 C CONTINUE
307 C TERM1=DNU1
308 C TERM2=(DNU1/DNU2)*(0.5D0*DNU1-1.0D0)
309 C TERM3=-((DNU1/DNU2)*0.5D0
310 C U=((TERM1+TERM2)/((1.0D0/DX)-TERM3)
311 C CALL CHSCDF (U,NU1,CCDF)
312 C CDF=CCDF
313 C RETURN
314 C
315 C TREAT THE CASE WHEN NU2 IS SMALL
316 C AND NU1 IS LARGE
317 C (THAT IS, WHEN NU2 IS SMALLER THAN 100,
318 C AND NU1 IS EQUAL TO OR LARGER THAN 1000).
319 C METHOD UTILIZED--SHEFFE-TUKEY APPROXIMATION
320 C (SEE JOHNSON AND KOTZ, VOLUME 2, PAGE 84, THIRD FORMULA).
321 C
322 C 330
323 C CONTINUE
324 C TERM1=DNU2
325 C TERM2=(DNU2/DNU1)*(0.5D0*DNU2-1.0D0)
326 C TERM3=-((DNU2/DNU1)*0.5D0
327 C U=((TERM1+TERM2)/((DX)-TERM3)
328 C CALL CHSCDF (U,NU2,CCDF)
329 C CDF=1.0-CCDF
330 C RETURN
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1 SUBROUTINE FPPF (P, NU1, NU2, PPF)  
2  
3 PURPOSE--THIS SUBROUTINE COMPUTES THE PERCENT POINT  
4 FOR THE F DISTRIBUTION  
5 WITH INTEGER DEGREES OF FREEDOM  
6 PARAMETERS = NU1 AND NU2.  
7 THIS DISTRIBUTION IS DEFINED FOR ALL NON-NEGATIVE X.  
8 THE PROBABILITY DENSITY FUNCTION IS GIVEN  
9 IN THE REFERENCES BELOW.  
10 INPUT ARGUMENTS--P = THE SINGLE PRECISION VALUE  
11 (BETWEEN 0.0 AND 1.0)  
12 AT WHICH THE PERCENT POINT  
13 FUNCTION IS TO BE EVALUATED.  
14 --NU1 = THE INTEGER DEGREES OF FREEDOM  
15 FOR THE NUMERATOR OF THE F RATIO.  
16 NU1 SHOULD BE POSITIVE.  
17 --NU2 = THE INTEGER DEGREES OF FREEDOM  
18 FOR THE DENOMINATOR OF THE F RATIO.  
19 NU2 SHOULD BE POSITIVE.  
20 OUTPUT ARGUMENTS--PPF = THE SINGLE PRECISION PERCENT POINT  
21 FUNCTION VALUE.  
22 OUTPUT--THE SINGLE PRECISION PERCENT POINT  
23 FUNCTION VALUE PPF FOR THE F DISTRIBUTION  
24 WITH DEGREES OF FREEDOM  
25 PARAMETERS = NU1 AND NU2.  
26 PRINTING--NONE UNLESS AN INPUT ARGUMENT ERROR CONDITION EXISTS.  
27 RESTRICTIONS--P SHOULD BE BETWEEN  
28 0.0 (INCLUSIVELY) AND 1.0 (EXCLUSIVELY).  
29 --NU1 SHOULD BE A POSITIVE INTEGER VARIABLE.  
30 --NU2 SHOULD BE A POSITIVE INTEGER VARIABLE.  
31 OTHER DATAPAC SUBROUTINES NEEDED--FCDF, NORCDF, CHSCDF, NORPPF.  
32 FORTRAN LIBRARY SUBROUTINES NEEDED--DSQRT, DATAN.  
33 MODE OF INTERNAL OPERATIONS--DOUBLE PRECISION.  
34 LANGUAGE--ANSI FORTRAN.  
35 REFERENCES--NATIONAL BUREAU OF STANDARDS APPLIED MATHEMATICS  
36 SERIES 55, 1964, PAGES 946-947.  
37 FORMULAE 26.6.4, 26.6.5, 26.6.8, AND 26.6.15.  
38 --JOHNSON AND KOTZ, CONTINUOUS UNIVARIATE  
39 DISTRIBUTIONS--2, 1970, PAGE 83, FORMULA 20,  
40 AND PAGE 84, THIRD FORMULA.  
41 --PAULSON, AN APPROXIMATE NORMALIZATION  
42 OF THE ANALYSIS OF VARIANCE DISTRIBUTION,  
43 ANNALS OF MATHEMATICAL STATISTICS, 1942,  
44 NUMBER 13, PAGES 233-135.  
45 --SCHEFFE AND TUKEY, A FORMULA FOR SAMPLE SIZES  
46 FOR POPULATION TOLERANCE LIMITS, 1944,  
47 NUMBER 15, PAGE 217.  
48 WRITTEN BY--JAMES J. FILLIBEN  
49 STATISTICAL ENGINEERING LABORATORY (205.03)  
50 NATIONAL BUREAU OF STANDARDS  
51 WASHINGTON, D. C. 20234  
52 PHONE: 301-921-2315  
53 ORIGINAL VERSION--MAY 1978.  
54 UPDATED --AUGUST 1979.  
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58 FFFF0058
59 FFFF0059
60 FFFF0060
61 FFFF0061
62 FFFF0062
63 FFFF0063
64 FFFF0064
65 FFFF0065
66 FFFF0066
67 FFFF0067
68 FFFF0068
69 FFFF0069
70 FFFF0070
71 FFFF0071
72 FFFF0072
73 FFFF0073
74 FFFF0074
75 FFFF0075
76 FFFF0076
77 FFFF0077
78 FFFF0078
79 FFFF0079
80 FFFF0080
81 FFFF0081
82 FFFF0082
83 FFFF0083
84 FFFF0084
85 FFFF0085
86 FFFF0086
87 FFFF0087
88 FFFF0088
89 FFFF0089
90 FFFF0090
91 FFFF0091
92 FFFF0092
93 FFFF0093
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95 FFFF0095
96 FFFF0096
97 FFFF0097
98 FFFF0098
99 FFFF0099
100 FFFF0100
101 FFFF0101
102 FFFF0102
103 FFFF0103
104 FFFF0104
105 FFFF0105
106 FFFF0106
107 FFFF0107
108 FFFF0108
109 FFFF0109
110 FFFF0110
111 FFFF0111
112 FFFF0112
113 FFFF0113
114 FFFF0114
115 FFFF0115

IPR=6
CHECK THE INPUT ARGUMENTS FOR ERRORS
PPF=0.0
IF (NU1.LE.0) GO TO 10
IF (NU2.LE.0) GO TO 20
IF (P.LT.0.0.OR.P.GE.1.0) GO TO 30
GO TO 40
WRITE (IPR,60)
WRITE (IPR,90) NU1
PPF=0.0
RETURN
WRITE (IPR,70)
WRITE (IPR,90) NU2
PPF=0.0
RETURN
WRITE (IPR,50)
WRITE (IPR,80) P
PPF=0.0
RETURN
CONTINUE
FORMAT (1H ,113H***** FATAL ERROR--THE FIRST INPUT ARGUMENT TO THE
50 2E FPPF SUBROUTINE IS OUTSIDE THE ALLOWABLE (0,1) INTERVAL ***** FPPF0081
60 FORMAT (1H ,91H***** FATAL ERROR--THE SECOND INPUT ARGUMENT TO THE
2 FPPF SUBROUTINE IS NON-POSITIVE ***** FPPF0083
70 FORMAT (1H ,91H***** FATAL ERROR--THE THIRD INPUT ARGUMENT TO THE
2 FCDF SUBROUTINE IS NON-POSITIVE ***** FPPF0085
80 FORMAT (1H ,35H***** THE VALUE OF THE ARGUMENT IS ,E15.8,6H ***** FPPF0086
90 FORMAT (1H ,35H***** THE VALUE OF THE ARGUMENT IS ,I8,6H ***** FPPF0087
C-----START POINT-----
C
C IBUC=0.0
TOL=0.000001
MAXIT=100
XMIN=0.0
XMAX=10.0**30
XLOW=XMIN
XUP=XMAX
ANU1=NU1
ANU2=NU2
EXP=0.5*((1.0/ANU2)-(1.0/ANU1))
SDF=SQRT(0.5*((1.0/ANU2)+(1.0/ANU1)))
CALL NORPPF (P,ZN)
XN=EXP+ZN*SDF
XNID=EXP(2.0**XN)
IF (IBUC.EQ.1) WRITE (6,100) XNID
FORMAT (1H ,7HXNID = ,E15.7)
100 IF (P.EQ.0.0) GO TO 110
C
GO TO 120
CONTINUE
PPF=XMIN
RETURN
110

```

FPPF0116  
 FPPF0117  
 FPPF0118  
 FPPF0119  
 FPPF0120  
 FPPF0121  
 FPPF0122  
 FPPF0123  
 FPPF0124  
 FPPF0125  
 FPPF0126  
 FPPF0127  
 FPPF0128  
 FPPF0129  
 FPPF0130  
 FPPF0131  
 FPPF0132  
 FPPF0133  
 FPPF0134  
 FPPF0135  
 FPPF0136  
 FPPF0137  
 FPPF0138  
 FPPF0139  
 FPPF0140  
 FPPF0141  
 FPPF0142  
 FPPF0143  
 FPPF0144  
 FPPF0145  
 FPPF0146  
 FPPF0147  
 FPPF0148  
 FPPF0149  
 FPPF0150  
 FPPF0151  
 FPPF0152  
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 FPPF0154  
 FPPF0155  
 FPPF0156  
 FPPF0157  
 FPPF0158  
 FPPF0159  
 FPPF0160  
 FPPF0161  
 FPPF0162  
 FPPF0163  
 FPPF0164  
 FPPF0165  
 FPPF0166

120 CONTINUE  
 C ICOUNT=0  
 C CONTINUE  
 130 X=XMID  
 CALL FPDF ( X, NU1, NU2, PCALC )  
 IF ( PCALC.EQ.P ) GO TO 190  
 IF ( PCALC.GT.P ) GO TO 160  
 C  
 140 CONTINUE  
 XLOW=XMID  
 X=XMID\*2.0  
 IF ( X.CE.XUP ) GO TO 150  
 XMID=X  
 IF ( IBUG.EQ.1 ) WRITE ( 6,100 ) XMID  
 CALL FPDF ( X, NU1, NU2, PCALC )  
 IF ( PCALC.EQ.P ) GO TO 190  
 IF ( PCALC.LT.P ) GO TO 140  
 XUP=X  
 CONTINUE  
 150 XMID=( XLOW+XUP )/2.0  
 IF ( IBUG.EQ.1 ) WRITE ( 6,100 ) XMID  
 GO TO 180  
 C  
 160 CONTINUE  
 XUP=XMID  
 X=XMID/2.0  
 IF ( X.LE.XLOW ) GO TO 170  
 XMID=X  
 IF ( IBUG.EQ.1 ) WRITE ( 6,100 ) XMID  
 CALL FPDF ( X, NU1, NU2, PCALC )  
 IF ( PCALC.EQ.P ) GO TO 190  
 IF ( PCALC.GT.P ) GO TO 160  
 XLOW=X  
 CONTINUE  
 170 XMID=( XLOW+XUP )/2.0  
 IF ( IBUG.EQ.1 ) WRITE ( 6,100 ) XMID  
 GO TO 180  
 C  
 180 CONTINUE  
 XDEL=ABS(XMID-XLOW)  
 ICOUNT=ICOUNT+1  
 IF ( XDEL.LT.TOL.OR.ICOUNT.GT.MAXIT ) GO TO 190  
 GO TO 130  
 C  
 190 CONTINUE  
 PPF=XMID  
 C RETURN  
 END

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CPR\*NS(1).GETX(2)

```
1 SUBROUTINE GETX (XF, YF, NF, Y, L, M, X, I, KS, KL)
2
3 C-----
4 C GETX WRITTEN BY CHARLES P. REEVE, STATISTICAL ENGINEERING
5 C DIVISION, NATIONAL BUREAU OF STANDARDS, WASHINGTON, D. C.
6 C AS PART OF THE FIXED-KNOT SPLINE PACKAGE FOR CALIBRATION
7 C FOR: THE INVERSE INTERPOLATION OF A CALIBRATION CURVE OR ITS
8 C UPPER OR LOWER CONFIDENCE LIMIT WHEREBY AN X-VALUE IS
9 C COMPUTED FOR A GIVEN Y-VALUE
10 C SUBPROGRAMS CALLED: -NONE-
11 C CURRENT VERSION COMPLETED JUNE 18, 1980
12 C-----
13 DIMENSION XF(NF), YF(NF)
14 IF (Y.LT.YF(L+1)) GO TO 20
15 IF (L+1.EQ.NF) GO TO 30
16 L=L+1
17 GO TO 10
18 IF (L.EQ.0) GO TO 40
19 C=(Y-YF(L))/(YF(L+1)-YF(L))
20 X=C*(XF(L+1)-XF(L))+XF(L)
21 I=1
22 RETURN
23 X=XF(NF)
24 I=(5+M)/2
25 KL=KL+1
26 RETURN
27 X=XF(1)
28 I=(5-M)/2
29 KS=KS+1
30 RETURN
31 END
```

GETX0001  
GETX0002  
GETX0003  
GETX0004  
GETX0005  
GETX0006  
GETX0007  
GETX0008  
GETX0009  
GETX0010  
GETX0011  
GETX0012  
GETX0013  
GETX0014  
GETX0015  
GETX0016  
GETX0017  
GETX0018  
GETX0019  
GETX0020  
GETX0021  
GETX0022  
GETX0023  
GETX0024  
GETX0025  
GETX0026  
GETX0027  
GETX0028  
GETX0029  
GETX0030



CPR\*NS(1) . INTERV(1)

```

SUBROUTINE INTERV (XT,LXT,X,LEFT,MFLAG)
C FROM * A PRACTICAL GUIDE TO SPLINES * BY C. DE BOOR
COMPUTES LEFT = MAX( I , 1 .LE. I .LE. LXT .AND. XT(I) .LE. X )
C
C***** I N P U T *****
C XT...A REAL SEQUENCE, OF LENGTH LXT, ASSUMED TO BE NONDECREASING
C LXT...NUMBER OF TERMS IN THE SEQUENCE XT
C X...THE POINT WHOSE LOCATION WITH RESPECT TO THE SEQUENCE XT IS
C TO BE DETERMINED.
C
C***** O U T P U T *****
C LEFT, MFLAG....BOTH INTEGERS, WHOSE VALUE IS
C
C -1 IF X .LT. XT(I)
C 1 IF XT(I) .LE. X .LT. XT(I+1)
C LXT 1 IF XT(LXT) .LE. X
C
IN PARTICULAR, MFLAG = 0 IS THE 'USUAL' CASE, MFLAG .NE. 0
INDICATES THAT X LIES OUTSIDE THE HALFOPEN INTERVAL
XT(1) .LE. Y .LT. XT(LXT) . THE ASYMMETRIC TREATMENT OF THE
INTERVAL IS DUE TO THE DECISION TO MAKE ALL PP FUNCTIONS CONT-
INUOUS FROM THE RIGHT.
C
C***** M E T H O D *****
C THE PROGRAM IS DESIGNED TO BE EFFICIENT IN THE COMMON SITUATION THAT
C IT IS CALLED REPEATEDLY, WITH X TAKEN FROM AN INCREASING OR DECREA-
C SING SEQUENCE. THIS WILL HAPPEN, E.G., WHEN A PP FUNCTION IS TO BE
C GRAPHED. THE FIRST GUESS FOR LEFT IS THEREFORE TAKEN TO BE THE VAL-
C UE RETURNED AT THE PREVIOUS CALL AND STORED IN THE L O C A L VARIA-
C BLE ILO . A FIRST CHECK ASCERTAINS THAT ILO .LT. LXT (THIS IS NEC-
C ESSARY SINCE THE PRESENT CALL MAY HAVE NOTHING TO DO WITH THE PREVI-
C OUS CALL) . THEN, IF XT(ILO) .LE. X .LT. XT(ILO+1), WE SET LEFT =
C ILO AND ARE DONE AFTER JUST THREE COMPARISONS.
C OTHERWISE, WE REPEATEDLY DOUBLE THE DIFFERENCE ISTEP = IHI - ILO
C WHILE ALSO MOVING ILO AND IHI IN THE DIRECTION OF X , UNTIL
C XT(ILO) .LE. X .LT. XT(IHI)
C AFTER WHICH WE USE BISECTION TO GET, IN ADDITION, ILO+1 = IHI .
C LEFT = ILO IS THEN RETURNED.
C
INTEGER LEFT,LXT,MFLAG,IHI,ILO,ISTEP,MIDDLE
REAL X,XT(LXT)
DATA ILO /1/
SAVE ILO (A VALID FORTRAN STATEMENT IN THE NEW 1977 STANDARD)
IHI = ILO+1
IF (IHI.LT.LXT) GO TO 10
IF (X.GE.XT(LXT)) GO TO 110
IF (LXT.LE.1) GO TO 90
ILO=LXT-1
IHI=LXT
C
10 IF (X.GE.XT(IHI)) GO TO 40
IF (X.GE.XT(ILO)) GO TO 100
C
C ***** NOW X .LT. XT(ILO) . DECREASE ILO TO CAPTURE X .
C ISTEP=1
C IHI=ILO
C ILO=IHI-ISTEP

```

INTERV01  
INTERV02  
INTERV03  
INTERV04  
INTERV05  
INTERV06  
INTERV07  
INTERV08  
INTERV09  
INTERV10  
INTERV11  
INTERV12  
INTERV13  
INTERV14  
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INTERV16  
INTERV17  
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INTERV48  
INTERV49  
INTERV50  
INTERV51  
INTERV52  
INTERV53  
INTERV54  
INTERV55  
INTERV56  
INTERV57

```

58 IF (ILO.LE.1) GO TO 30
59 IF (X.GE.XT(ILO)) GO TO 70
60 ISTEP=ISTEP*2
61 GO TO 20
62 ILO=1
63 IF (X.LT.XT(1)) GO TO 90
64 GO TO 70
65 ***** NOW X .GE. XT(IHI) . INCREASE IHI TO CAPTURE X .
66 ISTEP=1
67 ILO=IHI
68 IHI=ILO+ISTEP
69 IF (IHI.GE.LXT) GO TO 60
70 IF (X.LT.XT(IHI)) GO TO 70
71 ISTEP=ISTEP*2
72 GO TO 50
73 IF (X.GE.XT(LXT)) GO TO 110
74 IHI=LXT
75 C
76 C
77 ***** NOW XT(ILO) .LE. X .LT. XT(IHI) . NARROW THE INTERVAL.
78 MIDDLE=(ILO+IHI)/2
79 IF (MIDDLE.EQ.ILO) GO TO 100
80 NOTE. IT IS ASSUMED THAT MIDDLE = ILO IN CASE IHI = ILO+1 .
81 IF (X.LT.XT(MIDDLE)) GO TO 80
82 ILO=MIDDLE
83 GO TO 70
84 IHI=MIDDLE
85 GO TO 70
86 C***** SET OUTPUT AND RETURN.
87 MFLAG=-1
88 LEFT=1
89 RETURN
90 MFLAG=0
91 LEFT=ILO
92 RETURN
93 MFLAG=1
94 LEFT=LXT
95 RETURN
END
INTERV58
INTERV59
INTERV60
INTERV61
INTERV62
INTERV63
INTERV64
INTERV65
INTERV66
INTERV67
INTERV68
INTERV69
INTERV70
INTERV71
INTERV72
INTERV73
INTERV74
INTERV75
INTERV76
INTERV77
INTERV78
INTERV79
INTERV80
INTERV81
INTERV82
INTERV83
INTERV84
INTERV85
INTERV86
INTERV87
INTERV88
INTERV89
INTERV90
INTERV91
INTERV92
INTERV93
INTERV94
INTERV95

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58 L2APP058
59 L2APP059
60 L2APP060
61 L2APP061
62 L2APP062
63 L2APP063
64 L2APP064
65 L2APP065
66 L2APP066
67 L2APP067
68 L2APP068
69 L2APP069
70 L2APP070
71 L2APP071
72 L2APP072
73 L2APP073
74 L2APP074
75 L2APP075
76 L2APP076
77 L2APP077
78 L2APP078
79 L2APP079
80 L2APP080
81 L2APP081
82 L2APP082
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84 L2APP084
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87 L2APP087
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104 L2APP104
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109 L2APP109
110 L2APP110
111 L2APP111
112 L2APP112
113 L2APP113
114 L2APP114
115 L2APP115

```

AND THE REST OF THE VARIABLES ARE UNCHANGED.

```

C***** M E T H O D *****
C THE B-SPLINE COEFFICIENTS OF THE L2-APPR. ARE DETERMINED AS THE SOL-
C UTION OF THE NORMAL EQUATIONS
C SUM ( (B(I),B(J))*BCOEF(J) : J=1,...,N) = (B(I),G),
C I = 1, ..., N.
C HERE, B(I) DENOTES THE I-TH B-SPLINE, G DENOTES THE FUNCTION TO
C BE APPROXIMATED, AND THE I N N E R P R O D U C T OF TWO FUNCT-
C IONS F AND G IS GIVEN BY
C (F,G) := SUM ( F(TAU(I))*G(TAU(I))*WEIGHT(I) : I=1,...,NTAU) .
C THE ARRAYS T A U AND W E I G H T ARE GIVEN IN COMMON BLOCK
C D A T A , AS IS THE ARRAY G T A U CONTAINING THE SEQUENCE
C G(TAU(I)), I=1,...,NTAU.
C THE RELEVANT FUNCTION VALUES OF THE B-SPLINES B(I), I=1,...,N, ARE
C SUPPLIED BY THE SUBPROGRAM B S P L V B .
C THE COEFF.MATRIX C, WITH
C C(I,J) := (B(I),B(J)), I,J=1,...,N,
C OF THE NORMAL EQUATIONS IS SYMMETRIC AND (2*K-1)-BANDED, THEREFORE
C CAN BE SPECIFIED BY GIVING ITS K BANDS AT OR BELOW THE DIAGONAL. FOR
C I=1,...,N, WE STORE
C (B(I),B(J)) = C(I,J) IN Q(I-J+1,J), J=1,...,MIN0(I+K-1,N)
C AND THE RIGHT SIDE
C (B(I),G) IN BCOEF(I) .
C SINCE B-SPLINE VALUES ARE MOST EFFICIENTLY GENERATED BY FINDING SIM-
C ULTANEOUSLY THE VALUE OF E V E R Y NONZERO B-SPLINE AT ONE POINT,
C THE ENTRIES OF C (I.E., OF Q), ARE GENERATED BY COMPUTING, FOR
C EACH LL, ALL THE TERMS INVOLVING TAU(LL) SIMULTANEOUSLY AND ADDING
C THEM TO ALL RELEVANT ENTRIES.
C ADDITIONAL ROUTINES REQUIRED.
C
C B SPLV B B C H F A C B C H S L V
C M O D I F I C A T I O N B Y .
C
C M A R T I N C O R D E S
C C E N T E R F O R A P P L I E D M A T H E M A T I C S , N B S
C V E R S I O N 1
C O C T 1 9 7 9

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```

REAL BIATX(20)
REAL DW
INTEGER I, J, JJ, LEFT, LEFTMK, LL, MM
FORMAT (/5X,5H<<<<<14,1X,22HB-SPLINE COEFFICIENTS ,
2 14HCOMPUTED >>>>)
DO 20 J=1,N
BCOEF(J)=0.
DO 20 I=1,K
Q(I,J)=0.
LEFT=K
LEFTMK=0
DO 50 LL=1,NTAU
LOCATE LEFT S.T. TAU(LL) IN (T(LEFT),T(LEFT+1))

```



```

CPR*NS(1).NORCDF(1)
1 SUBROUTINE NORCDF (X,CDF)
2
3 C
4 C
5 C
6 C
7 C
8 C
9 C
10 C
11 C
12 C
13 C
14 C
15 C
16 C
17 C
18 C
19 C
20 C
21 C
22 C
23 C
24 C
25 C
26 C
27 C
28 C
29 C
30 C
31 C
32 C
33 C
34 C
35 C
36 C
37 C
38 C
39 C
40 C
41 C
42 C
43 C
44 C
45 C
46 C
47 C
48 C
49 C
50 C
51 C
52 C
53 C
54 C
55 C
56 C

PURPOSE--THIS SUBROUTINE COMPUTES THE CUMULATIVE DISTRIBUTION
FUNCTION VALUE FOR THE NORMAL (GAUSSIAN)
DISTRIBUTION WITH MEAN = 0 AND STANDARD DEVIATION = 1.
THIS DISTRIBUTION IS DEFINED FOR ALL X AND HAS
THE PROBABILITY DENSITY FUNCTION
 $F(X) = (1/\sqrt{2*\pi}) * \exp(-X*X/2)$ .
INPUT ARGUMENTS--X = THE SINGLE PRECISION VALUE AT
WHICH THE CUMULATIVE DISTRIBUTION
FUNCTION IS TO BE EVALUATED.
OUTPUT ARGUMENTS--CDF = THE SINGLE PRECISION CUMULATIVE
DISTRIBUTION FUNCTION VALUE.
OUTPUT--THE SINGLE PRECISION CUMULATIVE DISTRIBUTION
FUNCTION VALUE CDF.
PRINTING--NONE.
RESTRICTIONS--NONE.
OTHER DATAPAC SUBROUTINES NEEDED--NONE.
FORTRAN LIBRARY SUBROUTINES NEEDED--EXP.
MODE OF INTERNAL OPERATIONS--SINGLE PRECISION.
LANGUAGE--ANSI FORTRAN.
REFERENCES--NATIONAL BUREAU OF STANDARDS APPLIED MATHEMATICS
SERIES 55, 1964, PAGE 932, FORMULA 26.2.17.
--JOHNSON AND KOITZ, CONTINUOUS UNIVARIATE
DISTRIBUTIONS--1, 1970, PAGES 40-111.
WRITTEN BY--JAMES J. FILLIBEN
STATISTICAL ENGINEERING LABORATORY (205.03)
NATIONAL BUREAU OF STANDARDS
WASHINGTON, D. C. 20234
PHONE: 301-921-2315
ORIGINAL VERSION--JUNE 1972.
UPDATED --SEPTEMBER 1975.
UPDATED --NOVEMBER 1975.

DATA B1,B2,B3,B4,B5,P / .319381530,-0.356563782,1.781477937,
2 -1.821255978,1.330274429,.2316419/

IPR=6

CHECK THE INPUT ARGUMENTS FOR ERRORS.
NO INPUT ARGUMENT ERRORS POSSIBLE
FOR THIS DISTRIBUTION.

START POINT-----
Z=X
IF (X.LT.0.0) Z=-Z
T=1.0/(1.0+P*Z)
CDF=1.0-(0.39894228040143)*EXP(-0.5*Z*Z)*(B1*T+B2*T**2+B3*T**3+B
24*T**4+B5*T**5)
IF (X.LT.0.0) CDF=1.0-CDF

RETURN
END

```

NORPP001  
NORPP002  
NORPP003  
NORPP004  
NORPP005  
NORPP006  
NORPP007  
NORPP008  
NORPP009  
NORPP010  
NORPP011  
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PURPOSE--THIS SUBROUTINE COMPUTES THE PERCENT POINT  
FUNCTION VALUE FOR THE NORMAL (GAUSSIAN)  
DISTRIBUTION WITH MEAN = 0 AND STANDARD DEVIATION = 1.  
THIS DISTRIBUTION IS DEFINED FOR ALL X AND HAS  
THE PROBABILITY DENSITY FUNCTION  
 $F(X) = (1/\sqrt{2*\pi}) * \exp(-X*X/2)$ .

NOTE THAT THE PERCENT POINT FUNCTION OF A DISTRIBUTION  
IS IDENTICALLY THE SAME AS THE INVERSE CUMULATIVE  
DISTRIBUTION FUNCTION OF THE DISTRIBUTION.  
INPUT ARGUMENTS--P = THE SINGLE PRECISION VALUE  
(BETWEEN 0.0 AND 1.0)  
AT WHICH THE PERCENT POINT  
FUNCTION IS TO BE EVALUATED.

OUTPUT ARGUMENTS--PPF = THE SINGLE PRECISION PERCENT  
POINT FUNCTION VALUE.  
OUTPUT--THE SINGLE PRECISION PERCENT POINT  
FUNCTION VALUE PPF.

PRINTING--NONE UNLESS AN INPUT ARGUMENT ERROR CONDITION EXISTS.  
RESTRICTIONS--P SHOULD BE BETWEEN 0.0 AND 1.0, EXCLUSIVELY.  
OTHER DATAPAC SUBROUTINES NEEDED--NONE.

FORTRAN LIBRARY SUBROUTINES NEEDED--SQRT, ALOG.  
MODE OF INTERNAL OPERATIONS--SINGLE PRECISION.  
LANGUAGE--ANSI FORTRAN.

REFERENCES--ODEH AND EVANS, THE PERCENTAGE POINTS  
OF THE NORMAL DISTRIBUTION, ALGORITHM 70,  
APPLIED STATISTICS, 1974, PAGES 96-97.

--EVANS, ALGORITHMS FOR MINIMAL DEGREE  
POLYNOMIAL AND RATIONAL APPROXIMATION,  
M. SC. THESIS, 1972, UNIVERSITY  
OF VICTORIA, B. C., CANADA.

--HASTINGS, APPROXIMATIONS FOR DIGITAL  
COMPUTERS, 1955, PAGES 113, 191, 192.  
--NATIONAL BUREAU OF STANDARDS APPLIED MATHEMATICS  
SERIES 55, 1964, PAGE 933, FORMULA 26.2.23.

--FILLIBEN, SIMPLE AND ROBUST LINEAR ESTIMATION  
OF THE LOCATION PARAMETER OF A SYMMETRIC  
DISTRIBUTION (UNPUBLISHED PH.D. DISSERTATION,  
PRINCETON UNIVERSITY), 1969, PAGES 21-44, 229-231.

--FILLIBEN, 'THE PERCENT POINT FUNCTION',  
(UNPUBLISHED MANUSCRIPT), 1970, PAGES 28-31.  
--JOHNSON AND KOTZ, CONTINUOUS UNIVARIATE  
DISTRIBUTIONS--1, 1970, PAGES 40-111.

--THE KELLEY STATISTICAL TABLES, 1948.  
--OWEN, HANDBOOK OF STATISTICAL TABLES,  
1962, PAGES 3-16.  
--PEARSON AND HARTLEY, BIOMETRIKA TABLES  
FOR STATISTICIANS, VOLUME 1, 1954,  
PAGES 104-113.

COMMENTS--THE CODING AS PRESENTED BELOW  
IS ESSENTIALLY IDENTICAL TO THAT  
PRESENTED BY ODEH AND EVANS  
AS ALGORITHM 70 OF APPLIED STATISTICS.  
THE PRESENT AUTHOR HAS MODIFIED THE  
ORIGINAL ODEH AND EVANS CODE WITH ONLY  
MINOR STYLISTIC CHANGES.

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58 C --AS POINTED OUT BY ODEH AND EVANS
59 C IN APPLIED STATISTICS,
60 C THEIR ALGORITHM REPRESENTS A
61 C SUBSTANTIAL IMPROVEMENT OVER THE
62 C PREVIOUSLY EMPLOYED
63 C HASTINGS APPROXIMATION FOR THE
64 C NORMAL PERCENT POINT FUNCTION--
65 C THE ACCURACY OF APPROXIMATION
66 C BEING IMPROVED FROM 4.5*(10**-4)
67 C TO 1.5*(10**-8).
68 C WRITTEN BY--JAMES J. FILLIBEN
69 C STATISTICAL ENGINEERING LABORATORY (205.03)
70 C NATIONAL BUREAU OF STANDARDS
71 C WASHINGTON, D. C. 20234
72 C PHONE: 301-921-2315
73 C ORIGINAL VERSION--JUNE 1972.
74 C UPDATED --SEPTEMBER 1975.
75 C UPDATED --NOVEMBER 1975.
76 C UPDATED --OCTOBER 1976.
77 C
78 C -----
79 C
80 C DATA P0,P1,P2,P3,P4 /-.322232431088,-1.0,-.342242088547,
81 C 2 -.204231210245E-1,-.453642210148E-4/
82 C DATA Q0,Q1,Q2,Q3,Q4 / .993484626060E-1,.586581570495,.531103462366,
83 C 2 .103537752850,.38560700634E-2/
84 C
85 C IPR=6
86 C
87 C CHECK THE INPUT ARGUMENTS FOR ERRORS
88 C
89 C IF (P.LE.0.0.OR.P.GE.1.0) GO TO 10
90 C GO TO 20
91 C WRITE (IPR,30)
92 C WRITE (IPR,40) P
93 C RETURN
94 C CONTINUE
95 C 30 FORMAT (1H,115H***** FATAL ERROR--THE FIRST INPUT ARGUMENT TO THINORPF095
96 C 2E NORPPF SUBROUTINE IS OUTSIDE THE ALLOWABLE (0,1) INTERVAL *****NORPP096
97 C 40 FORMAT (1H,35H***** THE VALUE OF THE ARGUMENT IS ,E15.8,6H *****NORPP097
98 C
99 C -----START POINT-----
100 C
101 C IF (P.NE.0.5) GO TO 50
102 C PPF=0.0
103 C RETURN
104 C
105 C 50 R=P
106 C IF (P.GT.0.5) R=1.0-R
107 C T=SQR((-2.0*ALOG(R))
108 C ANUM=((T*P4+P3)*T+P2)*T+P1)*T+P0)
109 C ADEN=((T*Q4+Q3)*T+Q2)*T+Q1)*T+Q0)
110 C PPF=T+(ANUM/ADEN)
111 C IF (P.LT.0.5) PPF=-PPF
112 C RETURN
113 C
114 C

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SUBROUTINE PLOT (Y,X,CHAR,N, ITYPE)  
 PURPOSE--THIS SUBROUTINE YIELDS A ONE-PAGE PRINTER PLOT OF Y(I) VERSUS X(I) WITH SPECIAL PLOTTING CHARACTERS.  
 THIS 'SPECIAL PLOTTING CHARACTER' CAPABILITY ALLOWS THE DATA ANALYST TO INCORPORATE INFORMATION FROM A THIRD VARIABLE (ASIDE FROM Y AND X) INTO THE PLOT.  
 THE PLOT CHARACTER USED AT THE I-TH PLOTTING POSITION (THAT IS, AT THE COORDINATE (X(I),Y(I))) WILL BE  
 1 IF CHAR(1) IS BETWEEN 0.5 AND 1.5  
 2 IF CHAR(1) IS BETWEEN 1.5 AND 2.5  
 .  
 .  
 9 IF CHAR(1) IS BETWEEN 8.5 AND 9.5  
 . IF CHAR(1) IS BETWEEN 9.5 AND 10.5  
 A IF CHAR(1) IS BETWEEN 10.5 AND 11.5  
 B IF CHAR(1) IS BETWEEN 11.5 AND 12.5  
 C IF CHAR(1) IS BETWEEN 12.5 AND 13.5  
 .  
 .  
 W IF CHAR(1) IS BETWEEN 32.5 AND 33.5  
 X IF CHAR(1) IS BETWEEN 33.5 AND 34.5  
 Y IF CHAR(1) IS BETWEEN 34.5 AND 35.5  
 Z IF CHAR(1) IS BETWEEN 35.5 AND 36.5  
 X IF CHAR(1) IS ANY VALUE OUTSIDE THE RANGE 0.5 TO 36.5.  
 INPUT ARGUMENTS--Y = THE SINGLE PRECISION VECTOR OF (UNSORTED OR SORTED) OBSERVATIONS TO BE PLOTTED VERTICALLY.  
 --X = THE SINGLE PRECISION VECTOR OF (UNSORTED OR SORTED) OBSERVATIONS TO BE PLOTTED HORIZONTALLY.  
 --CHAR = THE SINGLE PRECISION VECTOR OF OBSERVATIONS WHICH CONTROL THE VALUE OF EACH INDIVIDUAL PLOT CHARACTER.  
 --N = THE INTEGER NUMBER OF OBSERVATIONS IN THE VECTOR Y.  
 OUTPUT--A ONE-PAGE PRINTER PLOT OF Y(I) VERSUS X(I) WITH SPECIAL PLOT CHARACTERS.  
 PRINTING--YES.  
 RESTRICTIONS--THERE IS NO RESTRICTION ON THE MAXIMUM VALUE OF N FOR THIS SUBROUTINE.  
 OTHER DATAPAC SUBROUTINES NEEDED--NONE.  
 FORTRAN LIBRARY SUBROUTINES NEEDED--NONE.  
 MODE OF INTERNAL OPERATIONS--SINGLE PRECISION.  
 LANGUAGE--ANSI FORTRAN.  
 COMMENT--VALUES IN THE VERTICAL AXIS VECTOR (Y), THE HORIZONTAL AXIS VECTOR (X), OR THE PLOT CHARACTER VECTOR (CHAR) WHICH ARE EQUAL TO OR IN EXCESS OF 10.0\*\*10 WILL NOT BE PLOTTED.

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58 C THIS CONVENTION GREATLY SIMPLIFIES THE PROBLEM PLOT058  
59 C OF PLOTTING WHEN SOME ELEMENTS IN THE VECTOR Y PLOT059  
60 C (OR X, OR CHAR) ARE 'MISSING DATA', OR WHEN WE PURPOSELY PLOT060  
61 C WANT TO IGNORE CERTAIN ELEMENTS IN THE VECTOR Y PLOT061  
62 C (OR X, OR CHAR) FOR PLOTTING PURPOSES (THAT IS, WE DO NOT PLOT062  
63 C WANT CERTAIN ELEMENTS IN Y (OR X, OR CHAR) TO BE PLOT063  
64 C PLOTTED). PLOT064  
65 C TO CAUSE SPECIFIC ELEMENTS IN Y (OR X, OR CHAR) TO BE PLOT065  
66 C IGNORED, WE REPLACE THE ELEMENTS BEFOREHAND PLOT066  
67 C (BY, FOR EXAMPLE, USE OF THE REPLAC SUBROUTINE) PLOT067  
68 C BY SOME LARGE VALUE (LIKE, SAY, 10.0\*\*10) AND PLOT068  
69 C THEY WILL SUBSEQUENTLY BE IGNORED IN THE PLOT PLOT069  
70 C SUBROUTINE. PLOT070  
71 C REFERENCES--FILLIBEN, 'STATISTICAL ANALYSIS OF INTERLAB PLOT071  
72 C FATIGUE TIME DATA', UNPUBLISHED MANUSCRIPT PLOT072  
73 C (AVAILABLE FROM AUTHOR) PLOT073  
74 C PRESENTED AT THE 'COMPUTER-ASSISTED DATA PLOT074  
75 C ANALYSIS' SESSION AT THE NATIONAL MEETING PLOT075  
76 C OF THE AMERICAN STATISTICAL ASSOCIATION, PLOT076  
77 C NEW YORK CITY, DECEMBER 27-30, 1973. PLOT077  
78 C WRITTEN BY--JAMES J. FILLIBEN PLOT078  
79 C NATIONAL ENGINEERING LABORATORY (205.03) PLOT079  
80 C STATISTICAL BUREAU OF STANDARDS PLOT080  
81 C WASHINGTON, D. C. 20234 PLOT081  
82 C PHONE--301-921-2315 PLOT082  
83 C ORIGINAL VERSION--OCTOBER 1974. PLOT083  
84 C UPDATED --NOVEMBER 1974. PLOT084  
85 C --JANUARY 1975. PLOT085  
86 C --JULY 1975. PLOT086  
87 C --SEPTEMBER 1975. PLOT087  
88 C --OCTOBER 1975. PLOT088  
89 C --NOVEMBER 1975. PLOT089  
90 C --FEBRUARY 1976. PLOT090  
91 C --FEBRUARY 1977. PLOT091  
92 C MINOR UPDATES --APRIL 1980 BY CHARLES P. REEVE. PLOT092  
93 C PLOT093  
94 C PLOT094  
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96 C PLOT096  
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5, IPL0TC(25), IPL0TC(26), IPL0TC(27), IPL0TC(28), IPL0TC(29), IPL0TC(30) PLOTCl16
6, IPL0TC(31), IPL0TC(32), IPL0TC(33), IPL0TC(34), IPL0TC(35), IPL0TC(36) PLOTCl17
7, IPL0TC(37) /IH1, IH2, IH3, IH4, IH5, IH6, IH7, IH8, IH9, IH., IHA, IHB, IHC, PLOTCl18
8 IHD, IHE, IHF, IHG, IHH, IHI, IHJ, IHK, IHL, IHM, IHN, IHO, IHP, IHQ, IHR, IHS, PLOTCl19
9 IHT, IHU, IHV, IHW, IHX, IHY, IHZ, IHX/ PLOTCl20
C IPR=6 PLOTCl21
CUTOFF=(10.0**10)-1000.0 PLOTCl22
C CHECK THE INPUT ARGUMENTS FOR ERRORS PLOTCl23
C PLOTCl24
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IF ( ITYPE.EQ.1 ) WRITE ( IPR,520)
IF ( ITYPE.EQ.2 ) WRITE ( IPR,530)
IF (N.LT.1) GO TO 10
GO TO 20
WRITE ( IPR,200)
WRITE ( IPR,210)
WRITE ( IPR,230) ( ALPHA4(L), L=1,6), ( SBNAME(L), L=1,6)
WRITE ( IPR,260) N
WRITE ( IPR,200)
RETURN
CONTINUE
IF (N.EQ.1) GO TO 30
GO TO 40
WRITE ( IPR,200)
WRITE ( IPR,210)
WRITE ( IPR,230) ( ALPHA4(L), L=1,6), ( SBNAME(L), L=1,6)
WRITE ( IPR,270) N
RETURN
CONTINUE
HOLD=Y(1)
DO 50 I=2,N
IF (Y(I).NE.HOLD) GO TO 60
CONTINUE
WRITE ( IPR,200)
WRITE ( IPR,210)
WRITE ( IPR,230) ( ALPHA1(L), L=1,6), ( SBNAME(L), L=1,6)
WRITE ( IPR,280) HOLD
RETURN
CONTINUE
HOLD=X(1)
DO 70 I=2,N
IF (X(I).NE.HOLD) GO TO 80
CONTINUE
WRITE ( IPR,200)
WRITE ( IPR,210)
WRITE ( IPR,230) ( ALPHA2(L), L=1,6), ( SBNAME(L), L=1,6)
WRITE ( IPR,280) HOLD
RETURN
CONTINUE
HOLD=CHAR(1)
DO 90 I=2,N
IF (CHAR(I).NE.HOLD) GO TO 100
CONTINUE

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174 WRITE (IPR, 200)
175 WRITE (IPR, 220)
176 WRITE (IPR, 230) (ALPHA3(L), L=1, 6), (SBNAME(L), L=1, 6)
177 WRITE (IPR, 280) HOLD
178 WRITE (IPR, 200)
179 CONTINUE
180
181 DO 110 I=1, N
182 IF (Y(I).LT.CUTOFF) GO TO 120
183 CONTINUE
184 WRITE (IPR, 200)
185 WRITE (IPR, 210)
186 WRITE (IPR, 230) (ALPHA1(L), L=1, 6), (SBNAME(L), L=1, 6)
187 WRITE (IPR, 290) CUTOFF
188 WRITE (IPR, 300)
189 WRITE (IPR, 200)
190 RETURN
191 CONTINUE
192 DO 130 I=1, N
193 IF (X(I).LT.CUTOFF) GO TO 140
194 CONTINUE
195 WRITE (IPR, 200)
196 WRITE (IPR, 210)
197 WRITE (IPR, 230) (ALPHA2(L), L=1, 6), (SBNAME(L), L=1, 6)
198 WRITE (IPR, 290)
199 WRITE (IPR, 300) CUTOFF
200 WRITE (IPR, 200)
201 RETURN
202 CONTINUE
203 DO 150 I=1, N
204 IF (CHAR(I).LT.CUTOFF) GO TO 160
205 CONTINUE
206 WRITE (IPR, 200)
207 WRITE (IPR, 210)
208 WRITE (IPR, 230) (ALPHA3(L), L=1, 6), (SBNAME(L), L=1, 6)
209 WRITE (IPR, 290)
210 WRITE (IPR, 300) CUTOFF
211 WRITE (IPR, 200)
212 RETURN
213 CONTINUE
214
215 N2=0
216 DO 180 I=1, N
217 IF (Y(I).LT.CUTOFF.AND.X(I).LT.CUTOFF.AND.CHAR(I).LT.CUTOFF) GO TO 170
218
219 GO TO 180
220 N2=N2+1
221 IF (N2.GE.2) GO TO 190
222 CONTINUE
223 WRITE (IPR, 200)
224 WRITE (IPR, 210)
225 WRITE (IPR, 240) (ALPHA1(L), L=1, 6), (ALPHA2(L), L=1, 6), (ALPHA3(L), L=1, 6)
226
227 WRITE (IPR, 250) (SBNAME(L), L=1, 6)
228 WRITE (IPR, 310)
229 WRITE (IPR, 320) N2
230 WRITE (IPR, 200)
231 RETURN

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290 IF (CHAR(I).GE.CUTOFF) GO TO 390
291 IF (X(I).LT.XMIN) XMIN=X(I)
292 IF (X(I).GT.XMAX) XMAX=X(I)
293 CONTINUE
294
295 X MID=(XMIN+XMAX)/2.0
296 X25=0.75*XMIN+0.25*XMAX
297 X75=0.25*XMIN+0.75*XMAX
298
299 BLANK OUT THE GRAPH
300
301 DO 410 I=1,45
302 DO 400 J=1,109
303 IGRAPH(I,J)=BLANK
304 CONTINUE
305 CONTINUE
306
307 PRODUCE THE VERTICAL AXES
308
309 DO 420 I=3,43
310 IGRAPH(I,5)=ALPHA
311 IGRAPH(I,109)=ALPHA
312 CONTINUE
313
314 DO 430 I=3,43,5
315 IGRAPH(I,5)=HYPHEN
316 IGRAPH(I,109)=HYPHEN
317 CONTINUE
318
319 IGRAPH(3,1)=EQUAL
320 IGRAPH(3,2)=ALPHAM
321 IGRAPH(3,3)=ALPHAM
322 IGRAPH(3,4)=ALPHAA
323 IGRAPH(3,4)=ALPHAX
324 IGRAPH(23,1)=EQUAL
325 IGRAPH(23,2)=ALPHAM
326 IGRAPH(23,3)=ALPHA
327 IGRAPH(23,4)=ALPHAD
328 IGRAPH(43,1)=EQUAL
329 IGRAPH(43,2)=ALPHAM
330 IGRAPH(43,3)=ALPHA
331 IGRAPH(43,4)=ALPHAN
332
333 PRODUCE THE HORIZONTAL AXES
334
335 DO 440 J=7,107
336 IGRAPH(1,J)=HYPHEN
337 IGRAPH(45,J)=HYPHEN
338 CONTINUE
339
340 DO 450 J=7,107,25
341 IGRAPH(1,J)=ALPHA
342 IGRAPH(45,J)=ALPHA
343 CONTINUE
344
345 DO 460 J=20,107,25
346 IGRAPH(1,J)=ALPHA
347 IGRAPH(45,J)=ALPHA
348 CONTINUE
349
350 DETERMINE THE (X,Y) PLOT POSITIONS
351
352 RATIOY=40.0/(YMAX-YMIN)
353 RATIOX=100.0/(XMAX-XMIN)
354
355 PLOT C290
356 PLOT C291
357 PLOT C292
358 PLOT C293
359 PLOT C294
360 PLOT C295
361 PLOT C296
362 PLOT C297
363 PLOT C298
364 PLOT C299
365 PLOT C300
366 PLOT C301
367 PLOT C302
368 PLOT C303
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376 PLOT C311
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380 PLOT C315
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402 PLOT C337
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405 PLOT C340
406 PLOT C341
407 PLOT C342
408 PLOT C343
409 PLOT C344
410 PLOT C345
411 PLOT C346
412 PLOT C347

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348 DO 470 I=1,N
349 IF (Y(I).GE.CUTOFF) GO TO 470
350 IF (X(I).GE.CUTOFF) GO TO 470
351 IF (CHAR(I).GE.CUTOFF) GO TO 470
352 MX=RATIOX*(X(I)-XMIN)+0.5
353 MY=RATIOY*(Y(I)-YMIN)+0.5
354 MY=43-MY
355 IARG=37
356 IF (0.5.LT.CHAR(I).AND.CHAR(I).LT.36.5) IARG=CHAR(I)+0.5
357 IGRAPH(MY,MX)=IPLOT(IARG)
358 CONTINUE
359
360 WRITE OUT THE GRAPH
361
362 DO 480 I=1,45
363 IP2=I+2
364 IFLAG=IP2-(IP2/5)*5
365 K=IP2/5
366 IF (IFLAG.NE.0) WRITE (IPR,490) (IGRAPH(I,J),J=1,109)
367 IF (IFLAG.EQ.0) WRITE (IPR,500) YLABLE(K),(IGRAPH(I,J),J=1,109)
368 CONTINUE
369 WRITE (IPR,510) XMIN,X25,XMID,X75,XMAX
370 WRITE (IPR,540)
371
372 C
373 FORMAT (1H,20X,109A1)
374 FORMAT (1H,F20.7,109A1)
375 FORMAT (1H,14X,F20.7,5X,F20.7,5X,F20.7,1X,F20.7)
376 FORMAT (1H1,59X,34HRESIDUALS VS. INDEPENDENT VARIABLE//)
377 FORMAT (1H1,53X,47HSTANDARDIZED RESIDUALS VS. INDEPENDENT VARIABLE//)
378 2//)
379 FORMAT (//55X,44HKNOT LOCATIONS ARE INDICATED BY THE SYMBOL X/)
380 C
381 RETURN
382 END

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PLOT382

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CPR*NS(1).PLOTSR(1)
1 SUBROUTINE PLOTSR ( X, N, NX, HOR, RES, CHAR, NKX, T, K, KX)
2
3 PLOTSR WRITTEN BY CHARLES P. REEVE, STATISTICAL ENGINEERING
4 DIVISION, NATIONAL BUREAU OF STANDARDS, WASHINGTON, D.C.
5 AS PART OF THE FIXED-KNOT SPLINE PACKAGE FOR CALIBRATION
6 FOR: PLOTTING KNOT LOCATIONS AND RESIDUALS/STANDARDIZED RESIDUALS
7 VS. INDEPENDENT VARIABLE
8 SUBPROGRAMS CALLED: PLOTG
9 CURRENT VERSION COMPLETED MARCH 14, 1980
10
11 DIMENSION X(NX), HOR(NKX), RES(NKX), CHAR(NKX), T(KX)
12 CREATE SUB-VECTORS OF INDEPENDENT VARIABLE AND STANDARDIZED
13 RESIDUALS
14 DO 10 I=1,N
15 SWITCH INDEPENDENT VARIABLE AND STANDARD DEVIATIONS OF RESIDUALS
16 Q=HOR(I)
17 HOR(I)=X(I)
18 X(I)=Q
19 CHAR(I)=10.0
20 CONTINUE
21 ADD KNOT LOCATIONS TO SUB-VECTORS
22 DO 20 I=1,K
23 L=I+N
24 HOR(L)=T(I)
25 RES(L)=0.0
26 CHAR(L)=0.0
27 CONTINUE
28 GENERATE PLOT OF RESIDUALS VS. INDEPENDENT VARIABLE
29 NK=N+K
30 CALL PLOTG (RES, HOR, CHAR, NK, I)
31 CREATE SUB-VECTOR OF STANDARDIZED RESIDUALS
32 DO 30 I=1,N
33 IF (X(I).LE.0.0) GO TO 30
34 RES(I)=RES(I)/X(I)
35 CONTINUE
36 GENERATE PLOT OF STANDARDIZED RESIDUALS VS. INDEPENDENT VARIABLE
37 CALL PLOTG (RES, HOR, CHAR, NK, 2)
38 RETURN
39 END

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PLOTSR01  
PLOTSR02  
PLOTSR03  
PLOTSR04  
PLOTSR05  
PLOTSR06  
PLOTSR07  
PLOTSR08  
PLOTSR09  
PLOTSR10  
PLOTSR11  
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PLOTSR39



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CPR*NS(1).PPREP(2)
1 SUBROUTINE PPREP (T,BCOEF,SCRITCH,BREAK,COEF,KX,JX,NB,MO,IP) PPREP001
2 C----- PPREP002
3 C WRITTEN BY CHARLES P. REEVE, STATISTICAL ENGINEERING PPREP003
4 C DIVISION, NATIONAL BUREAU OF STANDARDS, WASHINGTON, D.C. PPREP004
5 C AS PART OF THE FIXED-KNOT SPLINE PACKAGE FOR CALIBRATION PPREP005
6 C FOR: CONVERTING THE B-REPRESENTATION OF THE SPLINE INTO THE PPREP006
7 C PIECEWISE POLYNOMIAL REPRESENTATION PPREP007
8 C SUBPROGRAMS CALLED: BSPLPP PPREP008
9 C CURRENT VERSION COMPLETED APRIL 3, 1980 PPREP009
10 C----- PPREP010
11 C DIMENSION T(KX),BCOEF(KX),SCRITCH(JX,JX),BREAK(KX),COEF(JX,KX), PPREP011
12 C 2 II(20) PPREP012
13 C 2 FORMAT (/1X,50(1H-)/1X,38H* PIECEWISE POLYNOMIAL REPRESENTATION , PPREP013
14 C 2 12HOF SPLINES */1X,50(1H-)//9X,16H...INTERVAL...9X, PPREP014
15 C 3 27HCOEFFICIENTS OF (X-X(I))**P//3X,1HI,6X,4HX(I),7X,6HX(I+1),5X, PPREP015
16 C 4 3HP = 8(14,8X)/35X,8(14,8X)/35X,4(14,8X) PPREP016
17 C 20 FORMAT (1X,13,2X,2C12.5,3X,8C12.5/33X,8C12.5/33X,4C12.5) PPREP017
18 C 30 FORMAT ( ) PPREP018
19 C 40 FORMAT (/1X,42H***** PRINTOUT OF PIECEWISE POLYNOMIALS , PPREP019
20 C 2 18HSUPPRESSED ***** PPREP020
21 C--- COMPUTE PIECEWISE POLYNOMIAL REPRESENTATION OF SPLINE PPREP021
22 C CALL BSPLPP (T,BCOEF,NB,MO,SCRITCH,BREAK,COEF,L,JX) PPREP022
23 C--- DIVIDE EACH COEF(J,I) BY (J-1) FACTORIAL TO NORMALIZE PPREP023
24 C IF (MO.LT.3) GO TO 80 PPREP024
25 C DO 70 I=1,L PPREP025
26 C DO 60 J=3,MO PPREP026
27 C DO 50 K=3,J PPREP027
28 C COEF(J,I)=COEF(J,I)/FLOAT(K-1) PPREP028
29 C CONTINUE PPREP029
30 C CONTINUE PPREP030
31 C CONTINUE PPREP031
32 C IF (IP.EQ.0) GO TO 110 PPREP032
33 C DO 90 I=1,MO PPREP033
34 C II(I)=I-1 PPREP034
35 C CONTINUE PPREP035
36 C WRITE (6,10) (II(I),I=1,MO) PPREP036
37 C WRITE (6,30) PPREP037
38 C DO 100 I=1,L PPREP038
39 C WRITE (6,20) I,BREAK(I),BREAK(I+1),(COEF(J,I),J=1,MO) PPREP039
40 C CONTINUE PPREP040
41 C RETURN PPREP041
42 C WRITE (6,40) PPREP042
43 C RETURN PPREP043
44 C END PPREP044

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CPR*NS(1).RESSD(1)
1 SUBROUTINE RESSD ( X,Y,W,N,NX,NKX,NRSD,T,BCOEF,XXI,K,KX,NB,MO,YHAT,RESSD001
2 RES,RSD,BIATX,JX,IP)
3
4 RESSD WRITTEN BY CHARLES P. REEVE, STATISTICAL ENGINEERING
5 DIVISION, NATIONAL BUREAU OF STANDARDS, WASHINGTON, D.C.
6 AS PART OF THE FIXED-KNOT SPLINE PACKAGE FOR CALIBRATION
7 FOR: COMPUTING PREDICTED Y-VALUES, STANDARD DEVIATIONS OF
8 PREDICTED Y-VALUES, AND THE RESIDUAL STANDARD DEVIATION
9 SUBPROGRAMS CALLED: BVALUE, INTERV, BSPLVB
10 CURRENT VERSION COMPLETED MARCH 24, 1980
11
12 DIMENSION X(NX),Y(NX),W(NX),T(NX),BCOEF(KX),YHAT(NKX),RES(NKX),
13 BIATX(JX),XXI(KX,KX)
14
15 10 FORMAT (//1X,25(1H-)/1X,25H* ANALYSIS OF RESIDUALS */1X,25(1H-)//
16 2 9X,6HWEIGHT,20X,8HOBERVED,5X,9HPREDICTED,20X,10HSTD DEV OF/4X,
17 3 1H1,5X,4HW(1),9X,4HX(1),10X,4HY(1),10X,11HRESIDUAL(1),
18 4 3X,14HPREDICTED Y(1)/
19
20 20 FORMAT (1X,14,2X,G11.5,3G14.7,G12.5,G16.7)
21
22 30 FORMAT (//5X,16HRESIDUAL STD DEV,5X,13HRESIDUAL D.F./7X,G12.6,9X,
23 2 15)
24
25 40 FORMAT (/1X,48H***** PRINTOUT OF RESIDUALS SUPPRESSED *****
26 C--- INITIALIZE SUMMING VARIABLE
27 SUM=0.0
28 IF (IP.EQ.0) WRITE (6,40)
29 IF (IP.NE.0) WRITE (6,10)
30
31 C--- COMPUTE PREDICTED VALUES AND RESIDUALS
32 DO 50 I=1,N
33 XX=X(I)
34 YHAT(I)=BVALUE(T,BCOEF,NB,MO,XX,0)
35 RES(I)=Y(I)-YHAT(I)
36 SUM=SUM+W(I)*RES(I)**2
37 CONTINUE
38
39 50 COMPUTE RESIDUAL STANDARD DEVIATION
40 RSD=SQRT(SUM/FLOAT(NRSD))
41
42 C--- COMPUTE STANDARD DEVIATIONS OF PREDICTED VALUES
43 DO 90 L=1,N
44 XX=X(L)
45
46 FIND INDEX OF FIRST KNOT TO LEFT OF X-VALUE
47 CALL INTERV (T,K,XX,LEFT,MFLAG)
48 CHECK WHETHER X-VALUE LIESE WITHIN KNOT SPAN
49 IF (MFLAG.EQ.0) GO TO 60
50 SET RESIDUAL TO ZERO FOR X-VALUE OUTSIDE KNOT SPAN
51 RES(L)=0.0
52 SET STANDARD DEVIATION OF RESIDUAL TO ZERO
53 YHAT(L)=0.0
54 GO TO 90
55
56 EVALUATE POSSIBLY NON-ZERO B-SPLINES AT X-VALUE
57 CALL BSPLVB (T,MO,1,XX,LEFT,BIATX)
58
59 COMPUTE VARIANCE COEFFICIENT (BIATX)'(XXI)(BIATX) OF
60 PREDICTED Y-VALUE
61 NLOW=LEFT-MO
62 Q1=0.0
63 DO 80 I=1,MO
64 Q2=0.0
65 NI=NLOW+I
66 DO 70 J=1,MO
67 NJ=NLOW+J

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RESSD058  
RESSD059  
RESSD060  
RESSD061  
RESSD062  
RESSD063  
RESSD064  
RESSD065  
RESSD066  
RESSD067  
RESSD068  
RESSD069  
RESSD070  
RESSD071  
RESSD072

70 Q2=Q2+BIATX(J)\*XXI(NJ,NI)  
CONTINUE  
Q1=Q1+Q2\*BIATX(I)  
80 CONTINUE  
C--- COMPUTE STANDARD DEVIATION OF PREDICTED Y-VALUE  
YHATSD=RSD\*SQRT(Q1)  
IF (IP.EQ.0) GO TO 90  
WRITE (6,20) L, W(L), X(L), Y(L), YHAT(L), RES(L), YHATSD  
66 COMPUTE STANDARD DEVIATION OF EACH RESIDUAL AND STORE IN  
C--- VECTOR \*YHAT\*  
YHAT(L)=SQRT(RSD\*\*2-YHATSD\*\*2)  
90 CONTINUE  
WRITE (6,30) RSD, NRSD  
RETURN  
END

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CPR\*NS(1).RSQ(3)

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1 SUBROUTINE RSQ (RSD, NRSD, Y, W, N, NX, NNZ)
2
3 C-----
4 C  RSQ  WRITTEN BY CHARLES P. REEVE, STATISTICAL ENGINEERING
5 C  DIVISION, NATIONAL BUREAU OF STANDARDS, WASHINGTON, D.C.
6 C  AS PART OF THE FIXED-KNOT SPLINE PACKAGE FOR CALIBRATION
7 C  FOR: COMPUTING THE MULTIPLE CORRELATION COEFFICIENT R SQUARE
8 C  SUBPROGRAMS CALLED: -NONE-
9 C  CURRENT VERSION COMPLETED JUNE 11, 1980
10 C-----
11 C  DIMENSION Y(NX), W(NX)
12 C  FORMAT (/7X, 8HR SQUARE, 7X, 26HNUMBER OF NON-ZERO WEIGHTS/4X, F11.8,
13 C  2 16X, 15)
14 C--- COMPUTE RESIDUAL SUM OF SQUARES
15 C  RSS=FLOAT(NRSD)*RSD**2
16 C--- INITIALIZE SUMMING VARIABLE
17 C  TSS=0.0
18 C  DO 20 I=1, N
19 C  TSS=TSS+Y(I)*SQRT(W(I))
20 C  CONTINUE
21 C  YW=TSS/FLOAT(NNZ)
22 C--- INITIALIZE SUMMING VARIABLE
23 C  TSS=0.0
24 C--- COMPUTE TOTAL SUM OF SQUARES
25 C  DO 30 I=1, N
26 C  IF (W(I).EQ.0.0) GO TO 30
27 C  TSS=TSS+(Y(I)*SQRT(W(I)))-YD**2
28 C  CONTINUE
29 C--- COMPUTE R**2
30 C  R2=1.0-RSS/TSS
31 C--- TO PRINT OUT R-SQUARED CHANGE THE 'C' IN THE FOLLOWING LINE
32 C  WRITE (6, 10) R2, NNZ
33 C  RETURN
34 C  END

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RSQ000001
RSQ000002
RSQ000003
RSQ000004
RSQ000005
RSQ000006
RSQ000007
RSQ000008
RSQ000009
RSQ000010
RSQ000011
RSQ000012
RSQ000013
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RSQ000029
RSQ000030
RSQ000031
RSQ000032
RSQ000033
RSQ000034

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CPR*NS(1).SDYFIN(1)
1 SUBROUTINE SDYFIN (XF,YFSD,NF,T,K,MO,XXI,KX,RSD,BIATX,JX) SDYFIN01
2 SDYFIN02
3 SDYFIN03
4 SDYFIN04
5 SDYFIN05
6 SDYFIN06
7 SDYFIN07
8 SDYFIN08
9 SDYFIN09
10 SDYFIN10
11 SDYFIN11
12 SDYFIN12
13 SDYFIN13
14 SDYFIN14
15 SDYFIN15
16 SDYFIN16
17 SDYFIN17
18 SDYFIN18
19 SDYFIN19
20 SDYFIN20
21 SDYFIN21
22 SDYFIN22
23 SDYFIN23
24 SDYFIN24
25 SDYFIN25
26 SDYFIN26
27 SDYFIN27
28 SDYFIN28
29 SDYFIN29
30 SDYFIN30
31 SDYFIN31
32 SDYFIN32
33 SDYFIN33
34 SDYFIN34
35 SDYFIN35
36 SDYFIN36
37 SDYFIN37
38 SDYFIN38

C-----
C SDYFIN WRITTEN BY CHARLES P. REEVE, STATISTICAL ENGINEERING
C DIVISION, NATIONAL BUREAU OF STANDARDS, WASHINGTON, D.C.
C AS PART OF THE FIXED-KNOT SPLINE PACKAGE FOR CALIBRATION
C FOR: COMPUTING THE STANDARD DEVIATION OF THE PREDICTED
C Y-VALUES IN THE FINE MESH
C SUBPROGRAMS CALLED: INTERV, BSPLVB
C CURRENT VERSION COMPLETED OCTOBER 9, 1979
C-----
10 DIMENSION XF(NF),YFSD(NF),T(KX),BIATX(JX),XXI(KX,KX)
11 FORMAT (/5X,18H<<<<< STD. DEV. OF,15,1X,11HPREDICTED Y,1X,
12 2 21HVALUES COMPUTED >>>>>)
13 DO 40 L=1,NF
14 XX=XF(L)
15
16 C--- FIND INDEX OF FIRST KNOT TO LEFT OF X-VALUE
17 CALL INTERV (T,K,XX,LEFT,MFLAG)
18 EVALUATE POSSIBLY NON-ZERO B-SPLINES AT X-VALUE
19 CALL BSPLVB (T,MO,1,XX,LEFT,BIATX)
20 COMPUTE VARIANCE COEFFICIENT (BIATX)'(XXI)(BIATX) OF
21 PREDICTED Y-VALUE
22 NLOW=LEFT-MO
23 Q1=0.0
24 DO 30 I=1,MO
25 Q2=0.0
26 NI=NLOW+I
27 DO 20 J=1,MO
28 NJ=NLOW+J
29 Q2=Q2+BIATX(J)*XXI(NJ,NI)
30 CONTINUE
31 Q1=Q1+Q2*BIATX(I)
32 CONTINUE
33 COMPUTE STANDARD DEVIATION OF PREDICTED Y-VALUE
34 YFSD(L)=RSD*SQR(Q1)
35 CONTINUE
36 WRITE (6,10) NF
37 RETURN
38 END

```

CPR\*NS(1).SORT1(2)

SUBROUTINE SORT1 (X, M, N, NX)

C SORT1 OBTAINED BY CHARLES P. REEVE FROM DR. D. A. ZAHN AT  
 C THE FLORIDA STATE UNIVERSITY, TALLAHASSEE, FLORIDA  
 C UNDER THE NAME \*FTASORT\*. SEVERAL MINOR CORRECTIONS  
 C WERE MADE TO THE ORIGINAL VERSION AFTER LINE 61.  
 C FOR: SORTING THE SEGMENT OF A REAL ARRAY BETWEEN ENTRIES  
 C M AND N FROM SMALLEST TO LARGEST  
 C SUBROUTINES CALLED: -NONE-  
 C CURRENT VERSION COMPLETED JANUARY 30, 1978  
 C NOTE: ARRAYS LP(K) AND LQ(K) PERMIT SORTING UP TO 2\*\*(K+1)-1  
 C ELEMENTS, I.E., FOR K=25 YOU MAY SORT 67,108,863 ELEMENTS.

----- DIMENSION LP(25), LQ(25), X(NX)

I=1

KN=M

KN=N

IF (KM.GE.KN) GO TO 70

J=KM

K=(KN+KM)/2

A=X(K)

IF (X(KM).LE.A) GO TO 20

X(K)=X(KM)

X(KM)=A

A=X(K)

L=KN

IF (X(KN).GE.A) GO TO 40

X(K)=X(KN)

X(KN)=A

A=X(K)

IF (X(KM).LE.A) GO TO 40

X(K)=X(KM)

X(KM)=A

A=X(K)

GO TO 40

X(L)=X(J)

X(J)=B

L=L-1

IF (X(L).GT.A) GO TO 40

B=X(L)

J=J+1

IF (X(J).LT.A) GO TO 50

IF (J.LE.L) GO TO 30

IF (L-KM.LE.KN-J) GO TO 60

LP(I)=KM

LQ(I)=L

KN=J

I=I+1

GO TO 80

LP(I)=J

LQ(I)=KN

KN=L

I=I+1

GO TO 80

I=I-1

IF (I.EQ.0) RETURN

KM=LP(I)

SORT1001  
 SORT1002  
 SORT1003  
 SORT1004  
 SORT1005  
 SORT1006  
 SORT1007  
 SORT1008  
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69 SORT1069  
70 SORT1070  
71 SORT1071  
72 SORT1072

KN=LQ(I)  
80 IF (KN-KM.CE.11) GO TO 10  
KM=KM-1  
90 KM=KM+1  
IF (KM.EQ.KN) GO TO 70  
A=X(KM+1)  
IF (X(KM).LE.A) GO TO 90  
J=KM  
100 X(J+1)=X(J)  
J=J-1  
IF (J.EQ.M-1) GO TO 110  
IF (A.LT.X(J)) GO TO 100  
110 X(J+1)=A  
GO TO 90  
END

```

1 SUBROUTINE SORT2 ( X, Y, M, N, NX)
2 C-----
3 C SORT2 OBTAINED BY CHARLES P. REEVE FROM DR. D. A. ZAHN AT
4 C THE FLORIDA STATE UNIVERSITY, TALLAHASSEE, FLORIDA
5 C UNDER THE NAME *FTASORT*. SEVERAL MINOR CORRECTIONS
6 C WERE MADE TO THE ORIGINAL VERSION AFTER LINE 61.
7 C THE PROGRAM HAS BEEN ALTERED SO THAT A SECOND ARRAY IS
8 C CARRIED ALONG AND SORTED IDENTICALLY AS THE FIRST
9 C FOR: SORTING THE SEGMENT OF A REAL ARRAY BETWEEN ENTRIES
10 C M AND N FROM SMALLEST TO LARGEST
11 C SUBROUTINES CALLED: -NONE-
12 C CURRENT VERSION COMPLETED MARCH 24, 1980
13 C NOTE: ARRAYS LP(K) AND LQ(K) PERMIT SORTING UP TO 2**(K+1)-1
14 C ELEMENTS, I.E., FOR K=25 YOU MAY SORT 67,108,863 ELEMENTS.
15 C-----
16 C DIMENSION LP(25),LQ(25),X(NX),Y(NX)
17 C I=1
18 C KN=M
19 C KN=N
20 C IF (KM.GE.KN) GO TO 70
21 C J=KM
22 C K=(KN+KM)/2
23 C A=X(K)
24 C B=Y(K)
25 C IF (X(KM).LE.A) GO TO 20
26 C X(K)=X(KM)
27 C Y(K)=Y(KM)
28 C X(KM)=A
29 C Y(KM)=B
30 C A=X(K)
31 C B=Y(K)
32 C L=KN
33 C IF (X(KN).GE.A) GO TO 40
34 C X(K)=X(KN)
35 C Y(K)=Y(KN)
36 C X(KN)=A
37 C Y(KN)=B
38 C A=X(K)
39 C B=Y(K)
40 C IF (X(KM).LE.A) GO TO 40
41 C X(K)=X(KM)
42 C Y(K)=Y(KM)
43 C X(KM)=A
44 C Y(KM)=B
45 C A=X(K)
46 C B=Y(K)
47 C GO TO 40
48 C X(L)=X(J)
49 C Y(L)=Y(J)
50 C X(J)=C
51 C Y(J)=H
52 C L=L-1
53 C IF (X(L).GT.A) GO TO 40
54 C G=X(L)
55 C H=Y(L)
56 C J=J+1
57 C IF (X(J).LT.A) GO TO 50

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SORT2001  
 SORT2002  
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 SORT2090

58 IF (J.LE.L) GO TO 30  
 59 IF (L-KM.LE.KN-J) GO TO 60  
 60 LP(I)=KM  
 61 LQ(I)=L  
 62 KM=J  
 63 I=I+1  
 64 GO TO 80  
 65 LP(I)=J  
 66 LQ(I)=KN  
 67 KN=L  
 68 I=I+1  
 69 GO TO 80  
 70 I=I-1  
 71 IF (I.EQ.0) RETURN  
 72 KM=LP(I)  
 73 KN=LQ(I)  
 74 IF (KN-KM.GE.11) GO TO 10  
 75 KM=KM-1  
 76 KM=KM+1  
 77 IF (KM.EQ.KN) GO TO 70  
 78 A=X(KM+1)  
 79 B=Y(KM+1)  
 80 IF (X(KM).LE.A) GO TO 90  
 81 J=KM  
 82 X(J+1)=X(J)  
 83 Y(J+1)=Y(J)  
 84 J=J-1  
 85 IF (J.EQ.M-1) GO TO 110  
 86 IF (A.LT.X(J)) GO TO 100  
 87 X(J+1)=A  
 88 Y(J+1)=B  
 89 GO TO 90  
 90 END

CPR\*NS(1) . SPLLEN(8)

1 SUBROUTINE SPLLEN (H, X, Y, W, R1, R2, RES, N, NX, NKX, T, BCOEF, XXI, Q, DIAG, KSPLEE001  
2 2, KX, YY, NY, NYX, MD, SCRICH, JX, AL, DL, C, IP)

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SPLEEN WRITTEN BY CHARLES P. REEVE, STATISTICAL ENGINEERING  
DIVISION, NATIONAL BUREAU OF STANDARDS, WASHINGTON, D. C.  
  
\* \* \* \* \*  
\* FIXED-KNOT SPLINE PACKAGE FOR CALIBRATION \*  
\* \* \* \* \*

THIS PACKAGE OF SUBROUTINES WAS WRITTEN FOR THE FOLLOWING  
CALIBRATION PROCEDURES:

1) A MONOTONIC SEQUENCE OF RESPONSES Y(1), Y(2), ..., Y(N)  
EACH CONTAINING SOME ERROR ARE OBSERVED AT KNOWN POINTS  
X(1), X(2), ..., X(N) WHERE X(1) < X(2) < ... < X(N).

2) A SPLINE OF SPECIFIED DEGREE WITH A SPECIFIED SEQUENCE OF  
FIXED KNOTS IS FIT TO THE Y-VALUES WHICH MAY BE WEIGHTED.

3) THE RESIDUAL STANDARD DEVIATION IS COMPUTED IN ORDER TO  
MEASURE THE GOODNESS OF THE SPLINE FIT.

4) PREDICTED RESPONSE VALUES ARE COMPUTED AT A LARGE NUMBER  
OF UNIFORMLY SPACED X-VALUES BETWEEN THE EXTREME KNOTS.  
A CONFIDENCE INTERVAL FOR EACH PREDICTED RESPONSE IS  
COMPUTED BASED ON SPECIFIED CONSTANTS ALPHA, BETA, AND C  
IN ACCORDANCE WITH REFERENCE PAPER BY SCHEFFE GIVEN BELOW.

5) FOR SPECIFIED Y-VALUES, INVERSE INTERPOLATION IS APPLIED  
TO THE CALIBRATION CURVE AND ITS CONFIDENCE BAND TO GIVE  
PREDICTED X-VALUES WITH CORRESPONDING UPPER AND LOWER  
CONFIDENCE LIMITS.

PASSED PARAMETERS (AND DIMENSIONS):

\* H(80) = UP TO 80 CHARACTERS IN 80A1 FORMAT IDENTIFYING THE  
DATA

\* X(NX) = VECTOR (LENGTH N) OF X-VALUES WHERE OBSERVATIONS  
WERE MADE (INDEPENDENT VARIABLE)

\* Y(NX) = VECTOR (LENGTH N) OF OBSERVATIONS

\* W(NX) = VECTOR (LENGTH N) OF WEIGHTS FOR OBSERVATIONS

R1(NKX) = VECTOR (LENGTH N+K) FOR SCRATCH AREA

R2(NKX) = VECTOR (LENGTH N+K) FOR SCRATCH AREA

RES(NKX) = VECTOR (LENGTH N+K) OF RESIDUALS FROM SPLINE FIT

\* N = NUMBER OF OBSERVATIONS

\* NX = DIMENSION (>=N) OF VECTORS X, Y, W

\* NKX = DIMENSION (>=N+K) OF VECTORS R1, R2, RES

SPLEE002  
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SPLEE057

58 C \* T(KX) = VECTOR (LENGTH K+2\*MD) OF KNOT LOCATIONS  
 59 C  
 60 C BCOEF(KX) = VECTOR (LENGTH K+MD-1) OF B-SPLINE COEFFICIENTS  
 61 C  
 62 C XXI(KX, KX) = VARIANCE-COVARIANCE MATRIX (SIZE [K+MD-1] X [K+MD-1])  
 63 C OF B-SPLINE COEFFICIENTS  
 64 C  
 65 C Q(JX, KX) = MATRIX (SIZE [MD+1] X [K+MD-1]) FOR SCRATCH AREA  
 66 C  
 67 C DIAG(KX) = VECTOR (LENGTH K+MD-1) FOR SCRATCH AREA  
 68 C  
 69 C \* K = NUMBER OF KNOTS SPECIFIED BY USER (LATER INCREASED  
 70 C TO K+2\*MD BY PROGRAM)  
 71 C  
 72 C \* KX = DIMENSION (>=K+2\*MD) OF VECTORS T, BCOEF, DIAG AND  
 73 C MATRICES XXI AND Q (COLUMN ONLY)  
 74 C  
 75 C \* YY(NYX) = VECTOR (LENGTH NY) OF Y-VALUES FOR WHICH PREDICTED  
 76 C X-VALUES (WITH CONFIDENCE INTERVALS) ARE TO BE  
 77 C COMPUTED  
 78 C  
 79 C \* NY = NUMBER OF Y-VALUES FOR WHICH PREDICTED X-VALUES  
 80 C ARE TO BE COMPUTED  
 81 C  
 82 C \* NYX = DIMENSION (>=NY) OF VECTOR YY  
 83 C  
 84 C \* MD = DEGREE OF SPLINE (<=19); FOR EXAMPLE, 1=LINEAR,  
 85 C 2=QUADRATIC, 3=CUBIC  
 86 C  
 87 C SCRTCH(JX, JX) = MATRIX (SIZE [MD+1] X [MD+1]) FOR SCRATCH AREA  
 88 C  
 89 C \* JX = DIMENSION OF SQUARE MATRIX SCRATCH AND ROW  
 90 C DIMENSION OF MATRIX Q = 20  
 91 C  
 92 C \* AL = ALPHA LEVEL OF SIGNIFICANCE (SEE REFERENCE BELOW)  
 93 C  
 94 C \* DL = DELTA LEVEL OF SIGNIFICANCE (SEE REFERENCE BELOW)  
 95 C  
 96 C \* C = CONSTANT IN THE INTERVAL (0.85, 1.25) ASSOCIATED  
 97 C WITH SCHEFFE'S CALIBRATION TECHNIQUE  
 98 C  
 99 C 0 FOR ABBREVIATED PRINTOUT (NO RESIDUALS)  
 100 C \* IP = 1 FOR FULL PRINTOUT (RESIDUALS, PP REPRESENTATION)  
 101 C 2 FOR FULL PRINTOUT PLUS Y-CONFIDENCE INTERVALS FOR  
 102 C 300 EVENLY SPACED X-VALUES OVER KNOT SPAN  
 103 C  
 104 C \* INDICATES THAT AN INPUT VALUE IS REQUIRED FOR THIS VARIABLE  
 105 C  
 106 C NOTE: THE USER IS NOT REQUIRED TO ORDER THE ELEMENTS OF ANY INPUT  
 107 C VECTOR. THE PROGRAM WILL AUTOMATICALLY ORDER THOSE VECTORS  
 108 C WHICH NEED TO BE ORDERED.  
 109 C  
 110 C REFERENCE: SCHEFFE, HENRY, 'A STATISTICAL THEORY OF CALIBRATION',  
 111 C THE ANNALS OF STATISTICS, VOLUME 1, NUMBER 1,  
 112 C JANUARY 1973, PP. 1-37  
 113 C  
 114 C SUBPROGRAMS CALLED: ADKNTS, CHECK1, CHECK2, CIFYN, COVAR, L2APPR,  
 115 C

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116 C C PLOTSR, PPREP, RESSD, RSQ, SDYFIN, SORT1, SPLEE116
117 C C SORT2, XYFINE, YTOXCI SPLEE117
118 C C CURRENT VERSION COMPLETED JUNE 11, 1980 SPLEE118
119 C C----- SPLEE119
120 C C--- SET DIMENSIONS OF VECTORS AND MATRIX SPLEE120
121 DIMENSION X(NX), Y(NX), W(NX), R1(NKX), R2(NKX), RES(NKX) SPLEE121
122 DIMENSION T(KX), Q(JX, KX), DIAG(KX), BCOEF(KX), XX1(KX, KX) SPLEE122
123 DIMENSION YY(NYX), SCRATCH(JX, JX), BIATX(20), H(80) SPLEE123
124 C C PARAMETER NF=300 SPLEE124
125 DIMENSION XF(300), YF(300), YFL(300), YFU(300), YFSD(300) SPLEE125
126 FORMAT (1H1/1X, 45(1H*)/1X, 32H* FIXED-KNOT SPLINE PACKAGE FOR , SPLEE126
127 2 13CALIBRATION */1X, 45(1H*)) SPLEE127
128 20 FORMAT (//1X, 39(1H-)/1X, 25H* ESTIMATION OF B-SPLINE , SPLEE128
129 2 14HCOEFFICIENTS */1X, 39(1H-)) SPLEE129
130 30 FORMAT (/9X, 8HB-SPLINE/4X, 1H1, 5X, 4HCOEF, 10X, 7HSTD DEV/) SPLEE130
131 40 FORMAT (1X, 14, 2C15.8) SPLEE131
132 50 FORMAT (/1X, 42H***** PRINTOUT OF B-SPLINE COEFFICIENTS , SPLEE132
133 2 18SUPPRESSED ***** SPLEE133
134 60 FORMAT (//1X, 42(1H-)/1X, 37H* PARAMETERS OF LEAST SQUARES SPLINE , SPLEE134
135 2 5FIT */1X, 42(1H-)/13X, 18HDEGREE OF SPLINE =, 14//3X, SPLEE135
136 3 28NUMBER OF OBSERVATIONS =, 14/3X, SPLEE136
137 4 28NUMBER OF ZERO WEIGHTS =, 14/3X, 19HNUMBER OF NON-ZERO , SPLEE137
138 5 9HWEIGHTS =, 14/3X, 28HNUMBER OF KNOTS =, 14/3X, SPLEE138
139 6 28NUMBER OF B-SPLINES =, 14//11X, 18HNUMBER OF Y-VALUES/7X SPLEE139
140 7, 24HFOR WHICH X CONFIDENCE =, 14/3X, 18HINTERVAL IS TO BE , SPLEE140
141 8 8HCOMPUTED) SPLEE141
142 70 FORMAT (//5X, 25H----- FULL PRINTOUT -----/) SPLEE142
143 80 FORMAT (//5X, 32H----- ABBREVIATED PRINTOUT -----/) SPLEE143
144 90 FORMAT (//1X, 80A1) SPLEE144
145 100 FORMAT (//1X, 8(1H*)/1X, 8H* STOP */1X, 8(1H*)/) SPLEE145
146 C C--- DEFINE NUMBER OF POINTS IN FINE MESH SPLEE146
147 NF=300 SPLEE147
148 C C--- WRITE HEADING FOR HARDCOPY OUTPUT SPLEE148
149 WRITE (6, 10) SPLEE149
150 C C--- WRITE RUN IDENTIFICATION SPLEE150
151 WRITE (6, 90) (H(I), I=1, 80) SPLEE151
152 IF (IP.GE.1) WRITE (6, 70) SPLEE152
153 IF (IP.EQ.0) WRITE (6, 80) SPLEE153
154 C C--- COMPUTE ORDER OF SPLINE SPLEE154
155 MO=MD+1 SPLEE155
156 C C--- CHECK THAT INPUT PARAMETERS FALL WITHIN ALLOWABLE RANGES SPLEE156
157 CALL CHECK1 (W, N, NX, K, KX, NKX, NY, NYX, JX, MO, AL, DL, C, NZ) SPLEE157
158 C C--- SORT THE VECTOR OF KNOT LOCATIONS FROM LEAST TO GREATEST SPLEE158
159 SORT THE VECTOR OF KNOT LOCATIONS FROM LEAST TO GREATEST SPLEE159
160 CALL SORT1 (T, 1, K, KX) SPLEE160
161 C C--- SORT THE VECTOR OF X-VALUES FROM LEAST TO GREATEST AND CARRY SPLEE161
162 SORT THE VECTOR OF X-VALUES FROM LEAST TO GREATEST AND CARRY SPLEE162
163 ALONG THE CORRESPONDING Y-VALUES SPLEE163
164 CALL SORT2 (X, Y, 1, N, NX) SPLEE164
165 C C--- CHECK FOR OBSERVATIONS OUTSIDE KNOT SEQUENCE SPLEE165
166 CHECK FOR OBSERVATIONS OUTSIDE KNOT SEQUENCE SPLEE166
167 CALL CHECK2 (T, K, KX, X, W, N, NX, NZ, MO) SPLEE167
168 C C--- COMPUTE NUMBER OF NON-ZERO WEIGHTS SPLEE168
169 COMPUTE NUMBER OF NON-ZERO WEIGHTS SPLEE169
170 SPLEE170
171 SPLEE171
172 SPLEE172
173 SPLEE173

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174 NNZ=N-NZ  
175 C--- DEFINE NEW VECTOR OF KNOTS WITH END POINTS DUPLICATED  
176 C--- (MD) TIMES  
177 C  
178 CALL ADKNTS (T,K,KX,MO)  
179 C  
180 C--- COMPUTE NUMBER OF B-SPLINES  
181 NB=K-MO  
182 C--- COMPUTE NUMBER OF DEGREES OF FREEDOM FOR RESIDUALS  
183 NRSD=NNZ-NB  
184 WRITE (6,60) MD,N,NZ,NNZ,K,NB,NY  
185 C--- COMPUTE ESTIMATES OF B-SPLINE COEFFICIENTS  
186 C  
187 CALL L2APPR (T,NB,MO,Q,DIAG,BCOEF,JX,K,N,X,Y,W)  
188 C  
189 C--- COMPUTE UNSCALED VARIANCE-COVARIANCE MATRIX OF  
190 B-SPLINE COEFFICIENTS  
191 C  
192 CALL COVAR (KX,NB,JX,MO,Q,XXI)  
193 C  
194 C--- COMPUTE (PREDICTED Y-VALUES AND) RESIDUAL STANDARD DEVIATION  
195 C  
196 CALL RSDSD (X,Y,W,N,NX,NKX,NRSD,T,BCOEF,XXI,K,KX,NB,MO,R1,RES,RSD,  
197 2BIATX,JX,IP)  
198 C  
199 IF (IP.EQ.0) WRITE (6,50)  
200 IF (IP.EQ.0) GO TO 120  
201 C--- WRITE B-SPLINE COEFFICIENTS AND THEIR STANDARD DEVIATIONS  
202 WRITE (6,20)  
203 WRITE (6,30)  
204 DO 110 I=1,NB  
205 S=RSD\*SQRT(XXI(I,I))  
206 WRITE (6,40) I,BCOEF(I),S  
207 110 CONTINUE  
208 C--- COMPUTE MULTIPLE CORRELATION COEFFICIENT R-SQUARED (THIS VALUE IS  
209 NOT PRINTED. TO PRINT R-SQUARED MAKE A CHANGE IN SUBROUTINE RSQ.)  
210 C  
211 120 CALL RSQ (RSD,NRSD,Y,W,N,NX,NNZ)  
212 C  
213 C--- CREATE FINE MESH OF EVENLY SPACED X-VALUES BETWEEN END KNOTS  
214 C--- AND COMPUTE PREDICTED Y-VALUES THERE  
215 C  
216 CALL XYFINE (NF,T,BCOEF,K,KX,NB,MO,XF,YF)  
217 C  
218 C--- COMPUTE STANDARD DEVIATION OF PREDICTED Y-VALUES  
219 C  
220 CALL SDYFIN (XF,YFSD,NF,T,K,MO,XXI,KX,RSD,BIATX,JX)  
221 C  
222 C--- COMPUTE CONFIDENCE INTERVALS FOR PREDICTED Y-VALUES USING  
223 SCHEFFE'S TECHNIQUE (SEE REFERENCE IN SUBROUTINE CIYFIN)  
224 C  
225 CALL CIYFIN (XF,YF,YFSD,NF,RSD,AL,DL,C,NRSD,NB,YFL,YFU,IP)  
226 C  
227 C--- COMPUTE X CONFIDENCE INTERVALS FOR SPECIFIED Y-VALUES  
228 C  
229 CALL YTOXCI (XF,YFL,YF,YFU,NF,YY,NY,NYXO)  
230 C  
231 C--- COMPUTE PIECEWISE POLYNOMIAL REPRESENTATION OF SPLINE

232  
233  
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C CALL PPREP ( T, BCOEF, SCRITCH, DIAC, Q, KX, JX, NB, MO, IP )  
C  
C---- PLOT KNOT LOCATIONS AND RESIDUALS VS. INDEPENDENT VARIABLE  
C  
C CALL PLOTSR ( X, N, NX, R1, RES, R2, NKX, T, K, KX )  
C WRITE ( 6, 100 )  
RETURN  
END

SPLEE232  
SPLEE233  
SPLEE234  
SPLEE235  
SPLEE236  
SPLEE237  
SPLEE238  
SPLEE239  
SPLEE240  
SPLEE241

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CPR*NS(1).XYFINE(1)
1 SUBROUTINE XYFINE (NF, T, BCOEF, K, KX, NB, MO, XF, YF)
2
3 C
4 C XYFINE WRITTEN BY CHARLES P. REEVE, STATISTICAL ENGINEERING
5 C DIVISION, NATIONAL BUREAU OF STANDARDS, WASHINGTON, D.C.
6 C AS PART OF THE FIXED-KNOT SPLINE PACKAGE FOR CALIBRATION
7 C FOR: CREATING A FINE MESH OF VALUES OVER THE DOMAIN OF X-VALUES
8 C WHERE OBSERVATIONS WERE MADE AND COMPUTING CORRESPONDING
9 C PREDICTED Y-VALUES
10 C SUBPROGRAMS CALLED: BVALUE
11 C CURRENT VERSION COMPLETED MARCH 19, 1980
12 C
13 C-----
14 C DIMENSION T(KX), BCOEF(KX), XF(NF), YF(NF)
15 C--- CREATE FINE MESH OF X VALUES OVER INTERVAL SPANNED BY KNOTS
16 10 FORMAT (//5X,13H<<<<<< GRID OF,15,1X,24H EVENLY SPACED X VALUES ,
17 2 13HCREATED >>>>>)
18 C=(T(K)-T(1))/FLOAT(NF-1)
19 DO 20 I=1,NF
20 C CONTINUE
21 C--- COMPUTE PREDICTED Y VALUE AT EACH X VALUE
22 DO 30 I=1,NF
23 XX=XF(I)
24 YF(I)=BVALUE(T,BCOEF,NB,MO,XX,0)
25 CONTINUE
26 WRITE (6,10) NF
27 RETURN
28 END
XYFINE01
XYFINE02
XYFINE03
XYFINE04
XYFINE05
XYFINE06
XYFINE07
XYFINE08
XYFINE09
XYFINE10
XYFINE11
XYFINE12
XYFINE13
XYFINE14
XYFINE15
XYFINE16
XYFINE17
XYFINE18
XYFINE19
XYFINE20
XYFINE21
XYFINE22
XYFINE23
XYFINE24
XYFINE25
XYFINE26
XYFINE27

```

CPR\*NS(1).YTOXCI(8)

```

1 SUBROUTINE YTOXCI (XF, YFL, YF, YFU, NF, YY, NY, NYX)
2
3 YTOXCI WRITTEN BY CHARLES P. REEVE, STATISTICAL ENGINEERING
4 DIVISION, NATIONAL BUREAU OF STANDARDS, WASHINGTON, D.C.
5 AS PART OF THE FIXED-KNOT SPLINE PACKAGE FOR CALIBRATION
6 FOR: COMPUTING X CONFIDENCE INTERVALS FOR GIVEN Y-VALUES BY
7 INVERSE INTERPOLATION ON THE CALIBRATION CURVE AND ITS
8 UPPER AND LOWER BOUNDS
9 SUBPROGRAMS CALLED: GETX, SORT1
10 CURRENT VERSION COMPLETED SEPTEMBER 3, 1980
11
12 DIMENSION XF(NF), YFL(NF), YF(NF), YFU(NF), YY(NYX), IND(6)
13 DATA IND(1), IND(2), IND(3), IND(4), IND(5), IND(6) /1H, 1HS, 1HL, 1H*,
14 2 1H<, 1H>/
15
16 FORMAT (/5X, 40H<<<<< NO Y-VALUES SPECIFIED FOR INVERSE ,
17 2 19INTERPOLATION >>>>>)
18
19 FORMAT (/1X, 47H*** LOWER CONFIDENCE CURVE IS NOT MONOTONIC AT ,
20 2 4HYFL( , 14, 3H) = , G12.7/5X, 21HNO INTERPOLATION DONE)
21
22 FORMAT (/1X, 45H*** CALIBRATION CURVE IS NOT MONOTONIC AT YF( , 14,
23 2 3H) = , G12.7/5X, 21HNO INTERPOLATION DONE)
24
25 FORMAT (/1X, 47H*** UPPER CONFIDENCE CURVE IS NOT MONOTONIC AT ,
26 2 4HYFU( , 14, 3H) = , G12.7/5X, 21HNO INTERPOLATION DONE)
27
28 FORMAT (/1X, 65(1H-)/1X, 29H* COMPUTATION OF CALIBRATION ,
29 2 36HINTERVALS BY INVERSE INTERPOLATION */1X, 65(1H-)/24X,
30 3 11HLOWER LIMIT, 7X, 9HPREDICTED, 7X, 11HUPPER LIMIT/4X, 1H1, 6X, 4HY(1),
31 4 12X, 5HFOR X, 14X, 1HX, 14X, 5HFOR X/)
32
33 FORMAT (/1X, 14, G15.7, 3(3X, A1, G13.7) )
34
35 FORMAT (/1X, 46H*** OF AT LEAST ONE CALIBRATION CURVE
36 2 38***/1X, 49H*** DENOTES THE VALUE OF THE SMALLEST KNOT
37 2 38***/1X, 49H*** DENOTES THE VALUE OF THE LARGEST KNOT
38
39 FORMAT (/5X, 40HL DENOTES VALUES OUTSIDE THE RANGE OF THE,
40 2 22H CALIBRATION DATA - NO/7X, 29HVALID PREDICTION IS AVAILABLE)
41
42 FORMAT (/5X, 49H< INDICATES THAT NO VALID LOWER CALIBRATION LIMIT/
43 2 7X, 55HGREATER THAN THE MINIMUM POSSIBLE X-VALUE IS AVAILABLE.)
44
45 FORMAT (/5X, 49H> INDICATES THAT NO VALID UPPER CALIBRATION LIMIT/
46 2 7X, 55HSMALLER THAN THE MAXIMUM POSSIBLE X-VALUE IS AVAILABLE.)
47
48 WRITE (6, 50)
49 IF (NY.LT.1) GO TO 230
50 M=1
51 IF (YF(1).GT.YF(NF)) M=-1
52 NF=NF-1
53
54 C--- CHECK WHETHER CALIBRATION CURVE AND BOUNDS ARE MONOTONIC
55 DO 150 J=1, NF1
56 D=(YFL(J+1)-YFL(J))*FLOAT(M)
57 IF (D.GT.0.0) GO TO 130
58 J1=J+1
59 WRITE (6, 20) J1, YFL(J1)
60 RETURN
61
62 D=(YF(J+1)-YF(J))*FLOAT(M)
63 IF (D.GT.0.0) GO TO 140
64 J1=J+1
65 WRITE (6, 30) J1, YF(J1)
66 RETURN
67
68 D=(YFU(J+1)-YFU(J))*FLOAT(M)
69 IF (D.CT.0.0) GO TO 150
70 J1=J+1

```



```

58 WRITE (6,40) J1,YFU(J1)
59 RETURN
60 CONTINUE
61 ORDER VECTOR OF Y-VALUES FOR WHICH X CONFIDENCE LIMITS ARE TO
62 BE COMPUTED
63 CALL SORT1 (YY,1,NY,NYX)
64 L1=0
65 L2=0
66 L3=0
67 KS=0
68 KL=0
69
70 C--- IF CURVE IS MONOTONE DECREASING INVERT VECTORS ASSOCIATED
71 C--- WITH FINE MESH OF POINTS
72 IF (M.EQ.1) GO TO 170
73 NHALF=NF/2
74 DO 160 I=1,NHALF
75 J=NF+1-I
76 Q=XF(I)
77 XF(I)=XF(J)
78 Q=YFL(I)
79 YFL(I)=YFL(J)
80 YFL(J)=Q
81 Q=YF(I)
82 YF(I)=YF(J)
83 YF(J)=Q
84 Q=YFU(I)
85 YFU(I)=YFU(J)
86 YFU(J)=Q
87 CONTINUE
88 DO 220 J=1,NY
89 Y=YY(J)
90
91 C--- GET THREE (3) X-VALUES BY INVERSE INTERPOLATION
92 CALL GETX (XF,YFL,NF,Y,L1,M,XU,I3,KS,KL)
93 IF (I3.EQ.1) GO TO 180
94 I3=(3-15*M+2*I3+6*M*I3)/2
95 CALL GETX (XF,YF,NF,Y,L2,M,X,I2,KS,KL)
96 IF (I2.EQ.1) GO TO 190
97 I2=4
98 X=0.
99 CALL GETX (XF,YFU,NF,Y,L3,M,XL,I1,KS,KL)
100 IF (I1.EQ.1) GO TO 200
101 I1=(3+15*M+2*I1-6*M*I1)/2
102 IF CURVE IS MONOTONE DECREASING REVERSE LIMITS
200 IF (M.EQ.1) GO TO 210
103 D=XL
104 XL=XU
105 XU=D
106 I=I1
107 I1=I3
108 I3=I
109 WRITE (6,60) J,Y,IND(I1),XL,IND(I2),X,IND(I3),XU
110 CONTINUE
111 FLAG Y-VALUES WHICH GIVE INTERPOLATED X-VALUES OUTSIDE THE KNOT
112 C--- SPAN
113 IF (KS+KL.EQ.0) RETURN
114 WRITE (6,70)
115 WRITE (6,80)

```

YT0XC116  
YT0XC117  
YT0XC118  
YT0XC119  
YT0XC120  
YT0XC121  
YT0XC122  
YT0XC123

WRITE (6,90)  
WRITE (6,100)  
WRITE (6,110)  
WRITE (6,120)  
RETURN  
WRITE (6,10)  
RETURN  
END

230

116  
117  
118  
119  
120  
121  
122  
123

## References

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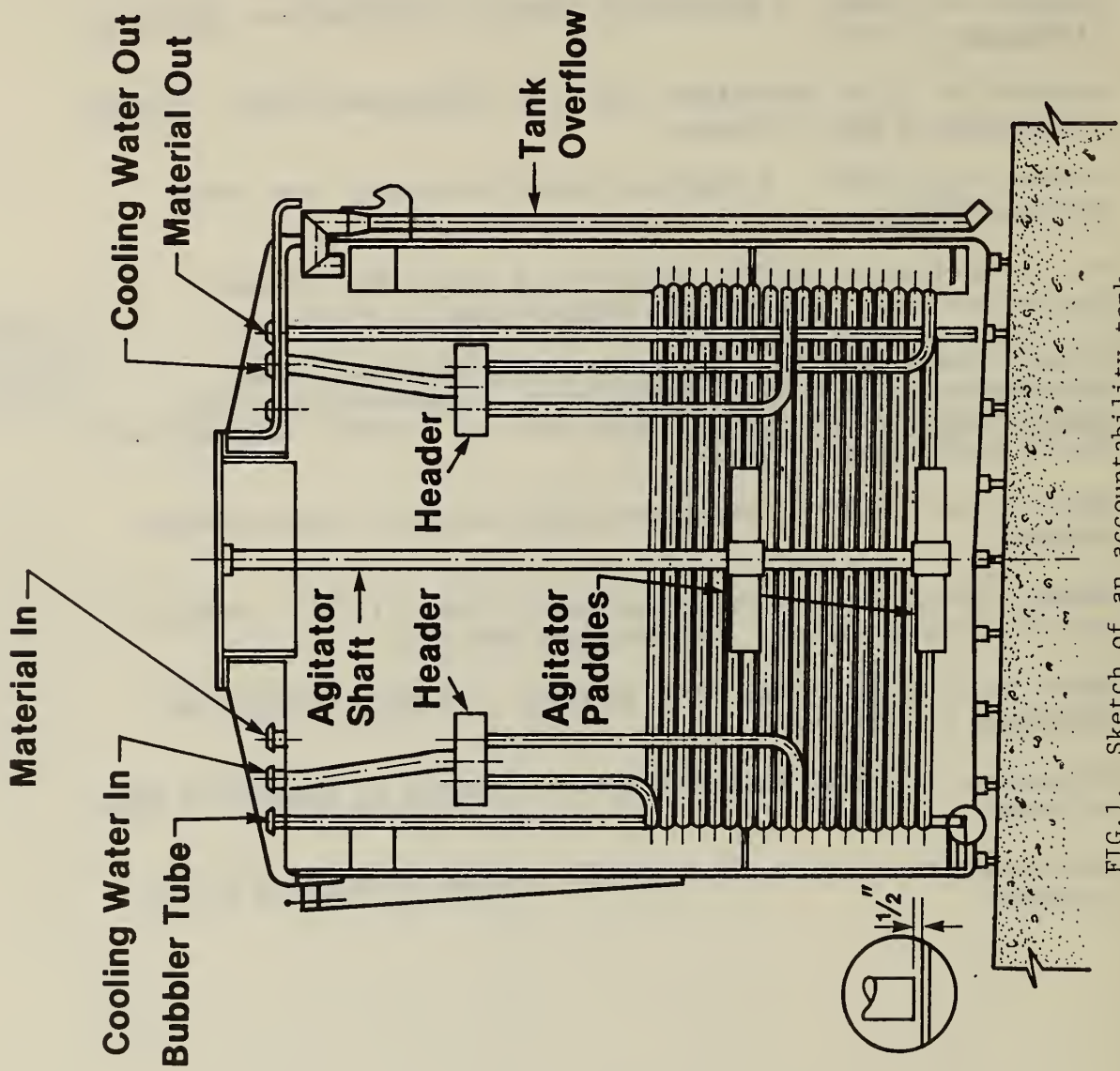


FIG.1. Sketch of an accountability tank.

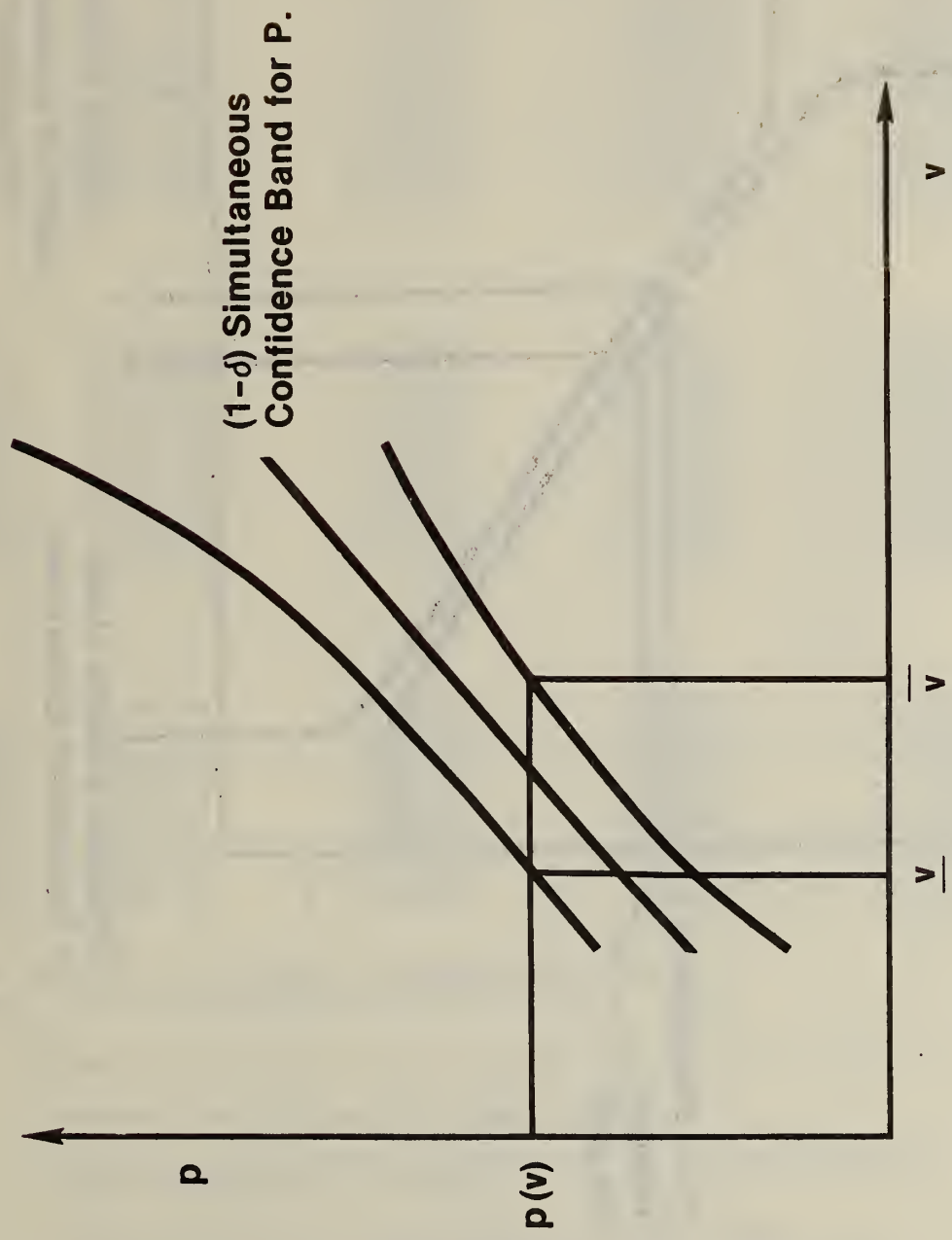


FIG. 2. Hypothetical Interval for  $v$  obtained from an exact value of  $p = p(v)$ .

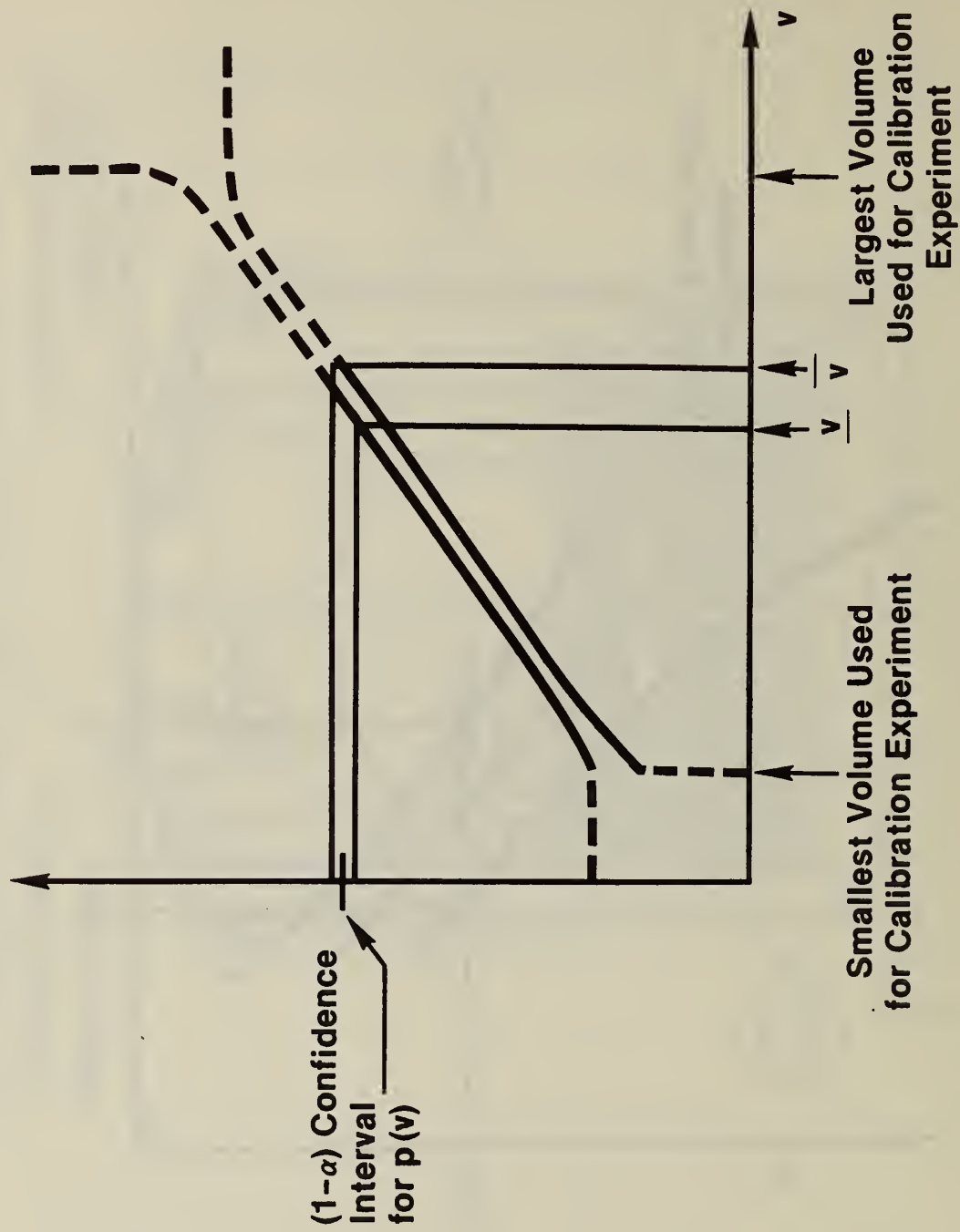


FIG. 3. Schematic for approximate construction of the calibration intervals.

\* COMPUTATION OF CALIBRATION INTERVALS BY INVERSE INTERPOLATION \*

I	Y(I)	LOWER LIMIT FOR X	PREDICTED X	UPPER LIMIT FOR X
1	3713.000	< 1.705250	1.705890	1.709779
2	3823.000	1.749691	1.753002	1.756223
3	3933.000	1.797422	1.800113	1.802745
4	4043.000	1.844952	1.847225	1.849473
5	4153.000	1.892090	1.894297	1.896511
6	4263.000	1.939002	1.941202	1.943401
7	4373.000	1.985893	1.988067	1.990239
8	4483.000	2.032783	2.034931	2.037077
9	4593.000	2.079673	2.081796	2.083916
10	4703.000	2.126563	2.128660	2.130755
.				
.				
.				
164	21643.00	9.704492	9.706814	9.709139
165	21753.00	9.755669	9.758022	9.760378
166	21863.00	9.806846	9.809230	9.811617
167	21973.00	9.858023	9.860439	9.862857
168	22083.00	9.909199	9.911647	9.914098
169	22193.00	9.960375	9.962855	9.965338
170	22303.00	10.01155	10.01406	10.01656
171	22413.00	10.06267	10.06506	10.06742
172	22523.00	10.11361	10.11578	10.11793
173	22633.00	10.16435	10.16651	10.16866
.				
.				
.				
234	29343.00	13.28631	13.28856	13.29082
235	29453.00	13.33740	13.33971	13.34203
236	29563.00	13.38849	13.39087	13.39325
237	29673.00	13.43957	13.44202	13.44447
238	29783.00	13.49066	13.49317	13.49570
239	29893.00	13.54174	13.54433	13.54692
240	30003.00	13.59281	13.59548	13.59815
241	30113.00	L 13.64334	* .0000000	> 13.64334
242	30223.00	L 13.64334	* .0000000	> 13.64334

\*\*\* AT LEAST ONE Y-VALUE IS OUTSIDE THE RANGE \*\*\*  
 \*\*\* OF AT LEAST ONE CALIBRATION CURVE \*\*\*

S DENOTES THE VALUE OF THE SMALLEST KNOT

L DENOTES THE VALUE OF THE LARGEST KNOT

\* DENOTES VALUES OUTSIDE THE RANGE OF THE CALIBRATION DATA - NO VALID PREDICTION IS AVAILABLE

< INDICATES THAT NO VALID LOWER CALIBRATION LIMIT GREATER THAN THE MINIMUM POSSIBLE X-VALUE IS AVAILABLE.

> INDICATES THAT NO VALID UPPER CALIBRATION LIMIT SMALLER THAN THE MAXIMUM POSSIBLE X-VALUE IS AVAILABLE.

Figure 4. Calibration chart. Y is pressure in pascals; X is volume in M<sup>3</sup>.

\*\*\*\*\*  
\* FIXED-KNOT SPLINE PACKAGE FOR CALIBRATION \*  
\*\*\*\*\*

REAL DATA FROM A TANK CALIBRATION (DATA IN FILE CPR\*NS.96)

----- FULL PRINTOUT -----

<<<< EACH END KNOT DUPLICATED 1 TIMES >>>>

-----  
\* SUMMARY OF KNOT LOCATIONS \*  
-----

I	KNOTS(I)
1	1.70525
2	1.70525
3	1.29466
4	4.54674
5	5.49482
6	5.87381
7	6.44156
8	7.13990
9	10.0425
10	10.2320
11	12.5044
12	13.6433
13	13.6433

-----  
\* PARAMETERS OF LEAST SQUARES SPLINE FIT \*  
-----

DEGREE OF SPLINE = 1  
NUMBER OF OBSERVATIONS = 172  
NUMBER OF ZERO WEIGHTS = 0  
NUMBER OF NON-ZERO WEIGHTS = 172  
NUMBER OF KNOTS = 13  
NUMBER OF B-SPLINES = 11  
NUMBER OF Y VALUES  
FOR WHICH X CONFIDENCE = 242  
INTERVAL IS TO BE COMPUTED

<<<< 11 B-SPLINE COEFFICIENTS COMPUTED >>>>

Figure 5. Preliminaries.



-----  
 \* ANALYSIS OF RESIDUALS \*  
 -----

I	WEIGHT W(I)	X(I)	OBSERVED Y(I)	PREDICTED Y(I)	RESIDUAL(I)	STD DEV OF PREDICTED Y(I)
1	1.0000	1.705250	3711.640	3711.505	.13455	1.052565
2	1.0000	1.705270	3711.420	3711.552	-.13223	1.052453
3	1.0000	1.894010	4152.240	4152.238	.18311-02	.4110981
4	1.0000	1.894140	4152.130	4152.542	-.41168	.4113765
5	1.0000	1.894580	4151.050	4153.569	-2.5190	.4123280
6	1.0000	1.894650	4151.910	4153.732	-1.8225	.4124807
7	1.0000	1.894660	4153.400	4153.756	-.35577	.4125026
8	1.0000	2.084060	4599.320	4598.315	1.0054	.3729185
9	1.0000	2.084110	4600.090	4598.432	1.6581	.3729083
10	1.0000	2.272720	5044.100	5041.136	2.9636	.3359134
11	1.0000	2.273020	5042.730	5041.841	.88947	.3358569
162	1.0000	13.07486	28884.68	28883.46	1.2214	.2921614
163	1.0000	13.26022	29282.92	29282.06	.86230	.3425575
164	1.0000	13.26158	29285.71	29284.98	.72754	.3430482
165	1.0000	13.26232	29284.50	29286.57	-2.0735	.3433159
166	1.0000	13.45198	29695.29	29694.42	.87061	.4235761
167	1.0000	13.45385	29699.14	29698.44	.69897	.4244610
168	1.0000	13.63914	30096.50	30096.89	-.38940	.5180907
169	1.0000	13.64052	30099.62	30099.86	-.23706	.5188241
170	1.0000	13.64133	30098.26	30101.60	-3.3391	.5192548
171	1.0000	13.64143	30102.36	30101.81	.54614	.5193080
172	1.0000	13.64333	30105.91	30105.90	.10254-01	.5203189

RESIDUAL STD DEV      RESIDUAL D.F.  
 1.48848                      161

-----  
 \* ESTIMATION OF B-SPLINE COEFFICIENTS \*  
 -----

I	B-SPLINE COEF	STD DEV
1	3711.5053	1.0525651
2	4153.7559	.41250259
3	10378.705	.41074148
4	12579.214	.57466792
5	13403.155	.74306913
6	14630.321	.62254084
7	16236.443	.41161732
8	22364.034	.44698178
9	22774.945	.43252287
10	27656.846	.39959609
11	30105.922	.52032419

<<<<< GRID OF 300 EVENLY SPACED X VALUES CREATED >>>>>

<<<<< STD. DEV. OF 300 PREDICTED Y VALUES COMPUTED >>>>>

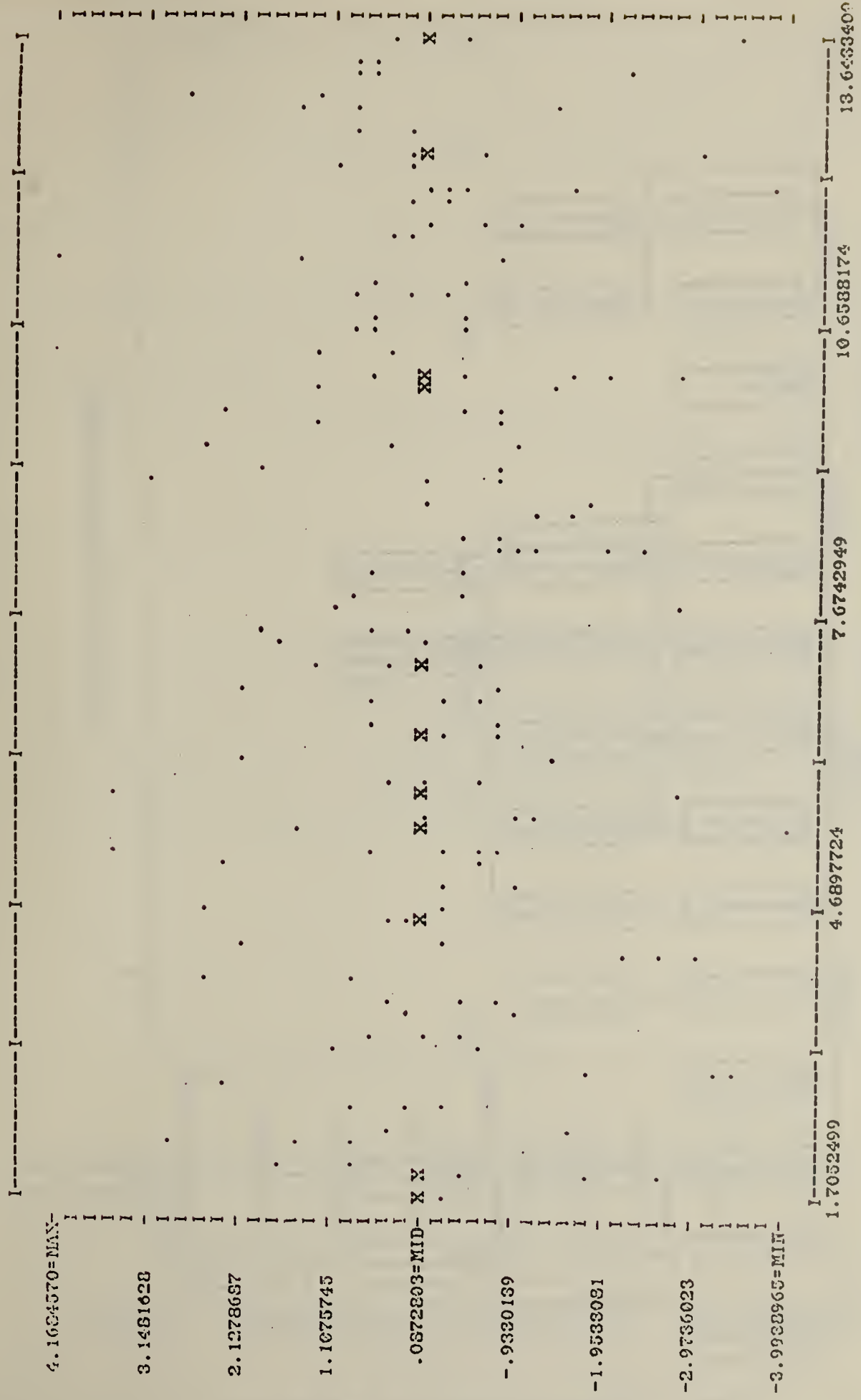
Figure 6. Regression fit.

-----  
 \* PIECEWISE POLYNOMIAL REPRESENTATION OF SPLINES \*  
 -----

I	..... INTERVAL.....		COEFFICIENTS OF (X-X(I))**P	
	X(I)	X(I+1)	P = 0	1
1	1.7052	1.8947	3711.5	2334.9
2	1.8947	4.5467	4152.8	2347.2
3	4.5467	5.4948	10379.	2321.0
4	5.4948	5.8738	12579.	2174.0
5	5.8738	6.4416	13403.	2161.5
6	6.4416	7.1899	14639.	2146.2
7	7.1899	10.043	16236.	2148.1
8	10.043	10.232	22364.	2168.6
9	10.232	12.504	22775.	2148.3
10	12.504	13.643	27657.	2150.4

Figure 7. Ordinary polynomial representation of the fitted spline.

Residuals (pascals) vs. independent variable ( $m^3$ ).



KNOT LOCATIONS ARE INDICATED BY THE SYMBOL X

Figure 8. Residual plot.

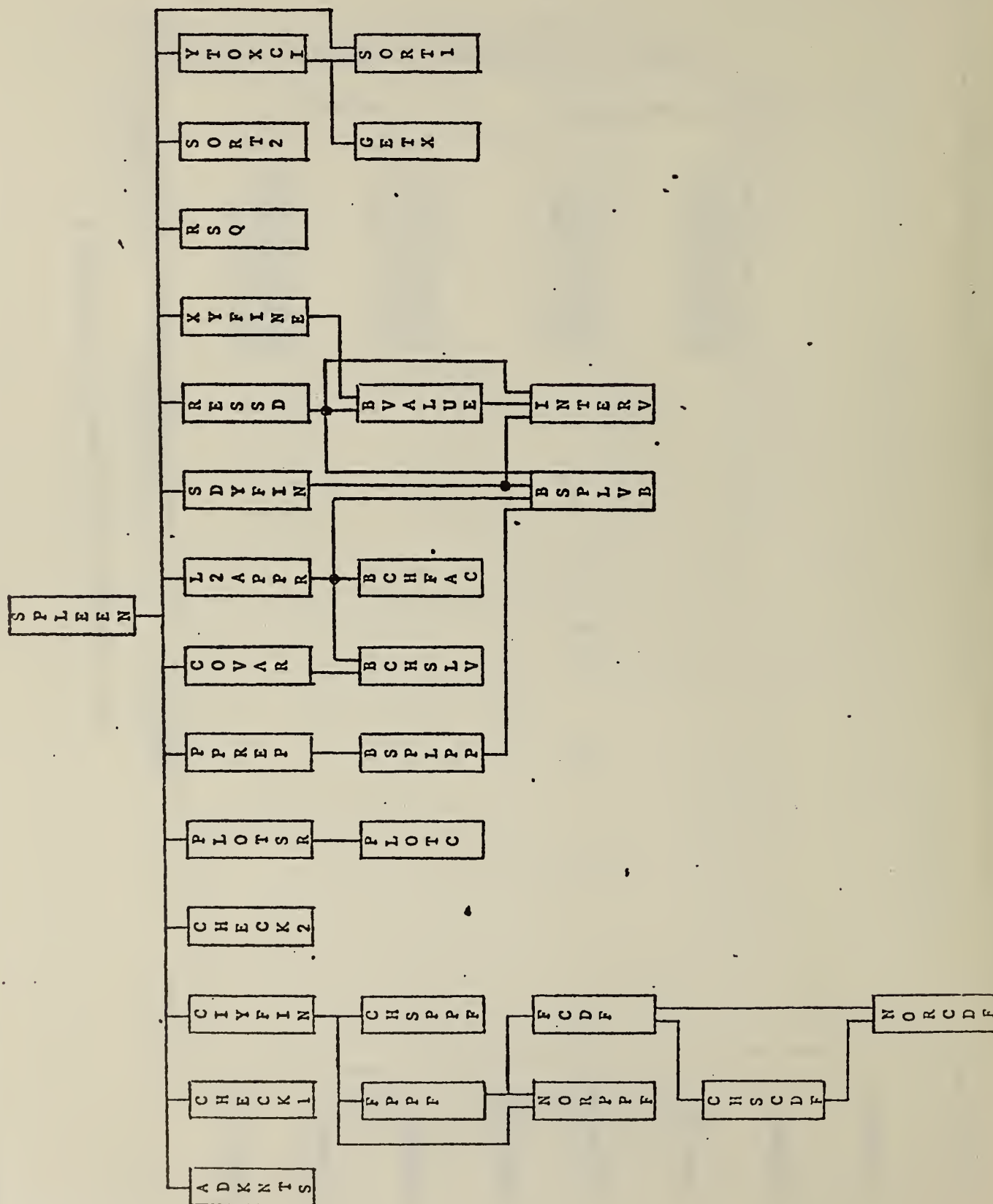
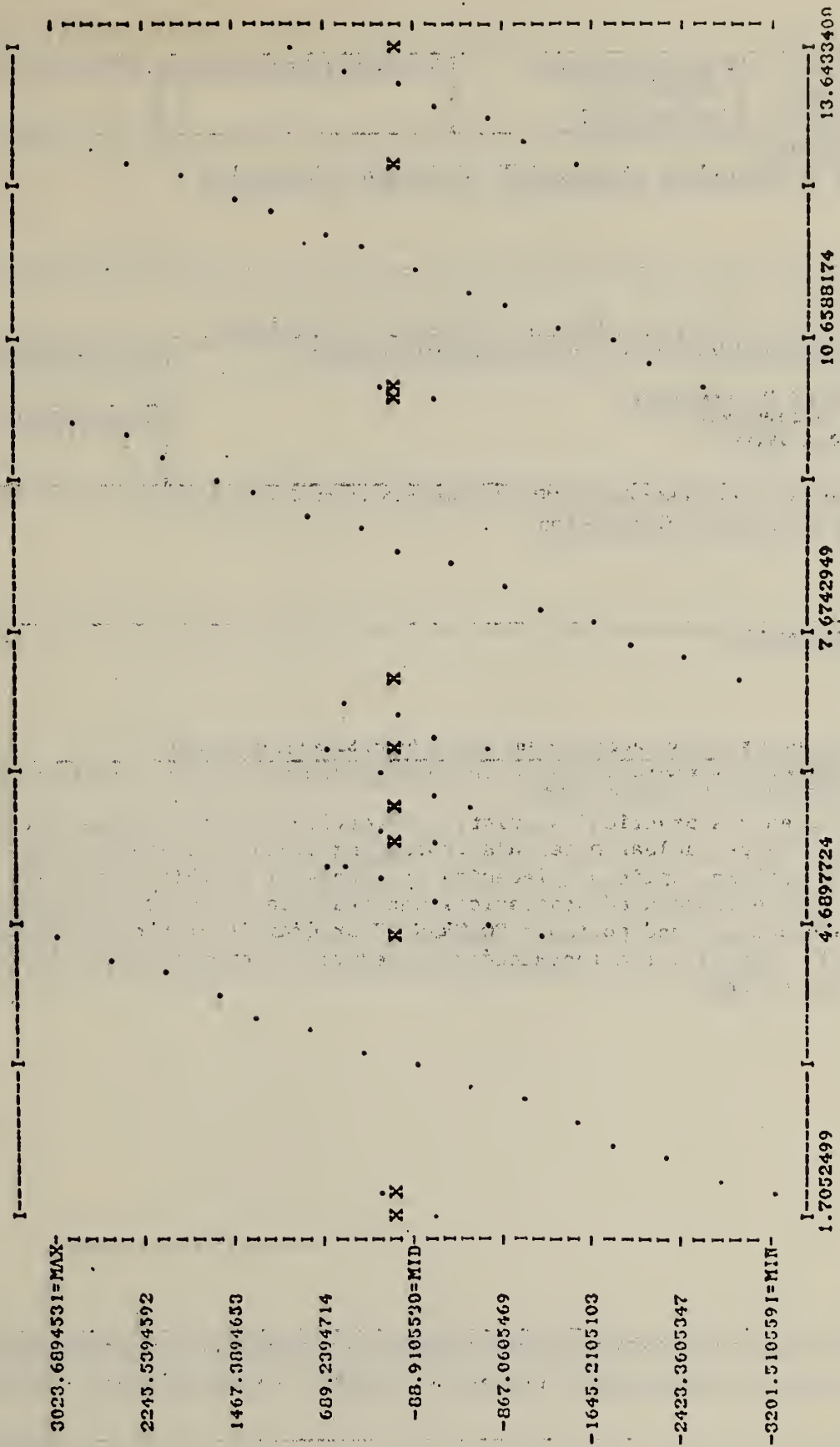


Figure 9. Diagram of subroutine interactions.

RESIDUALS VS. INDEPENDENT VARIABLE



KNOT LOCATIONS ARE INDICATED BY THE SYMBOL X

Figure 10: Diagnostic plot of residuals from a zero-degree spline fit (i.e., a step function).

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<b>4. TITLE AND SUBTITLE</b> A NEW METHOD OF ASSIGNING UNCERTAINTY IN VOLUME CALIBRATION			
<b>5. AUTHOR(S)</b> James A. Lechner, Charles P. Reeve, Clifford H. Spiegelman			
<b>6. PERFORMING ORGANIZATION</b> <i>(If joint or other than NBS, see instructions)</i>  <b>NATIONAL BUREAU OF STANDARDS</b> <b>DEPARTMENT OF COMMERCE</b> <b>WASHINGTON, D.C. 20234</b>		<b>7. Contract/Grant No.</b>	<b>8. Type of Report &amp; Period Covered</b>
<b>9. SPONSORING ORGANIZATION NAME AND COMPLETE ADDRESS</b> <i>(Street, City, State, ZIP)</i> U.S. Nuclear Regulatory Commission			
<b>10. SUPPLEMENTARY NOTES</b>  <input type="checkbox"/> Document describes a computer program; SF-185, FIPS Software Summary, is attached.			
<b>11. ABSTRACT</b> <i>(A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here)</i>  This paper presents a practical statistical overview of the pressure volume calibration curve for large nuclear materials processing tanks. It explains the appropriateness of applying splines (piecewise polynomials) to this curve, and it presents an overview of the associated statistical uncertainties. In order to implement these procedures a practical and portable FORTRAN IV program is provided along with its users' manual. Finally, the recommended procedure is demonstrated on actual tank data collected by NBS.			
<b>12. KEY WORDS</b> <i>(Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons)</i> Volume calibration; differential pressure; splines; accountability; statistics.			
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