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FORTRAN PROGRAMS FOR ANALYZING COLLABORATIVE TEST DATA

PART I: GENERAL STATISTICS

By

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METHODS DEVELOPMENT AND QUALITY ASSURANCE LABORATORY

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FOREWORD

Man and his environment must be protected from the adverse effects of pesticides, radiation, noise and other forms of pollution, and the unwise management of solid waste. Efforts to protect the environment require a focus that recognizes the interplay between the components of our physical environment--air, water, and land. The National Environment Research Centers provide this multidisciplinary focus through programs engaged in

studies on the effects of environmental contaminants on man and the biosphere, and

a search for ways to prevent contamination and to recycle valuable resources.

This work provides a method for understanding the deeper meaning of interlaboratory collaborations. This work also represents one effort to achieve a more complete knowledge of the effectiveness of various analytical methods.

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ABSTRACT

A FORTRAN program for IBM 1130 is described by which general statistics on interlaboratory studies of chemical analytical methods may be obtained. Data screening followed by a statistical t-test for identifying outliers is included. A histogram of data in ascending order is also provided.

PREFACE

These program systems for general statistics and plotting of data scatter diagrams were programmed in Fortran 1130. These program systems were designed to be executed on IBM 1130, Version 2, Modification 11, Core Size 16K.

General statistics were obtained on data from interlaboratory method studies. These statistical approaches are based on a procedure described by Youden (1). In his procedure, closely related pairs of samples, A and B, for example, are analyzed by each of the participating laboratories. The data from all of the participants for each of the samples is subjected to the statistical program, COLST.

The data from each sample pair was plotted, values of A versus values of B. In the application for this particular plot program, SCAT, the data from three pairs of samples, making three plots, or diagrams, were drawn on each page. This presentation of data provided a vivid visual display for purposes of comparison.

The general statistics program was adapted from a data summarization program written in Fortran IV (2). This program was adapted to the 1130 Model and expanded to provide for data input in any one of several forms of decimal expression, data screening, and the application of a statistical t-test to expose outliers and to leave a reduced vector of "retained" data. The plotter program, SCAT, utilized the plotter routines as supplied by IBM.

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REFERENCES

1. Youden, W.J.,Statistical Techniques for Collaborative Tests, AOAC, Washington, D.C.(1967).

2. Larson, K.E.,Ed.,The Summarization of Data, Journal of Quality Technology,1,68(1969).

INTRODUCTION

The program, COLST, is designed to provide elementary statistics on data obtained by an official test method. The program is designed to treat data from interlaboratory method studies.

USE

The data as obtained from the participants include missing values, censored values, wild values, and reasonable values. Furthermore, some of the participant's results had been obtained by using a different method instead of the official method of the test. The data as received, the input data, are screened to ignore missing and censored data, as well as data obtained by a different method. The data remaining after screening were termed "raw data."

After the standard deviation was obtained on the raw data vector, extreme data values equal to or greater than $\pm$ 4s are discarded. The symbol s is the estimated standard deviation on the raw data vector. These discarded values were termed "unacceptable data." The remaining values of the raw data vector are termed "acceptable data."

A statistical t-test is then applied to the acceptable data vector in order to identify and remove any "outliers." The outliers are marked with the letter R which indicates that the value is rejected as an outlier. The data vector remaining is termed "retained data." This t-test is applied in a rather conservative manner since an alpha of 0.0050 is used in a two-tailed test. That is, only 0.25% of a normal distribution was truncated from each extreme.

In reviewing, the input data are screened to produce raw data, which are tested for wild values to produce an acceptable data vector. The acceptable data vector is searched for outliers, which, when noted leave the retained data vector from which general statistics arecalculated. The statistics obtained are listed below:

number of data points
mean of acceptable data
accuracy based on retained data
range of retained data
variance of retained data
standard deviation on retained data
confidence limits, 95%, on a single determination of retained data
coefficient of variation on retained data
skewness of retained data
number of cells in the histogram

DESCRIPTION

The main program, COLST, utilizes sixteen subroutines by which input, calculations, editing and output are accomplished. This main program was developed from a program listing in a paper on the summarization of data by Thayer and Snyder of the Applied Statistics Group in the Engineering Research Center of the Western Electric Company (2).

Data input is accomplished by the subroutine, REALT, which is part of the data screening step. The acceptable data are subjected to the statistical t-test as described above. A histogram is developed using for the number of cells, the square root of the number of data points. This program accepts up to and including 120 data points. Appendix I shows the t-table at t(0.99).

In the following requirement lists, a variable like JOBS has a single location and a variable like NDF(I) is a one-dimension array or a vector.

INPUT REQUIREMENTS

Variable	Purpose	Format
JOBS	Number of sets of data to be evaluated	I4
NDF(I),CVT(I)	Degrees of freedom; critical value of t	I3,5X,F6.4
BLANK ASTER	A blank character; the character,'R'	2A1
EX	The character,'X'	A1
DA,TY	Date of evaluation, xx,xx,xx	2A4
AR1(I), AR2(I) AR3(I), AR41(I), AR42(I), AR43(I), AR44(I), AR5(I) BR1(I), BR2(I).	Text of heading, each	20A4
NR,NCELL, IZERO	Number of data points in raw data vector; specified number of cells. IZERO when greater than zero sets the lowest cell boundary to 0.0.	3I4
FN1(I).FN2(I)	Test of two footnotes	20A4
PAR1 thru PAR8, IJKL	Used as an extra blank line; inputs IJKL which designates the number of digits to the right of the decimal point	8A4,I1
TV	Designates the known, or 'true' value of the sample for which this test is run	F10.0
BR1(I)	Text printing the true value for the sample	20A4

OUTPUT VARIABLES

UNACCEPTABLE DATA LIST

Variable	Purpose	Format
KOR(I)	Numerical identification of laboratory	I3
KDER(I)	Numerical identification of analyst	A1
G(I)	Raw data element	F8.2
ANSA(I)	Symbol: D = Different method Blank = Official method of test	A1

HEADING

The heading is determined and printed by the subroutine, THEAD

ACCEPTABLE DATA LIST

The acceptable data vector is calculated and printed by the subroutine, DLIST.

STATISTICS ON RETAINED DATA

Variable	Purpose	Format
N	Number of data elements in retained data vector	I3
RANGE	Range of data elements in retained data vector	F11.5
COEFZ	Coefficient of variation of retained data vector	F11.5
TV	True, or known value of the sample	F6.2
VRZ	Variance of data elements of retained data vector	F11.5
SKEWZ	Skewness of the distribution of data elements of retained data vector	F11.5
XBAR	Mean of data elements in acceptable data vector	F11.5
SDZ1	Standard deviation of data elements in retained data vector	F11.5
NCELL	Number of cells used in planning and calculating the histogram	I4
ZAVE	Mean of data elements on retained data vector	F11.5
SZ196	Confidence limits on single determination of retained data, $\pm$ 95%	F11.5
ZMED	Median of data elements in retained data vector	F11.5
ACCZ	Accuracy of the mean, on retained data vector, based upon the true value	F11.5

RETAINED DATA IN ASCENDING ORDER: HISTOGRAM

Variable	Purpose	Format
X(I)	Data element	F8.2
W(I)	W = 'R', data element rejected by t-test alpha = 0.0050; two-tailed test W = ' ', data element retained	A1
N	Number of data elements in the acceptable data vector	I4

OUTPUT REQUIREMENTS

Variable	Purpose	Format
XBAR	Mean of retained data	F11.5
VAR	Variance on retained data	F11.5
VR	Sample variance on retained data	F11.5
SD	Standard deviation on retained data	F11.5
SD1	Sample standard deviation on retained data	F11.5
S196	Sample standard deviation * 1.96	F11.5
POINT(I)	Midpoint of any cell in histogram	F10.4
KKK	Frequency of data elements in any cell	I4
XIA(I)	Literal element,'X's, corresponding to frequency of data points in the cell but limited to 15 or less by space limi-limitations	A1

```
C          COLST
C               UP TO AND INCLUDING 121 DATA POINTS
C          INCLUDES T-TEST, IDENTIFICATION OF
C          OUTLIERS BY THE LETTER 'R'.  ACCURACY IS BASED UPON THE TRUE
C          VALUE VERSUS RETAINED DATA.
C          SUMMARY OF COLLABORATIVE TEST DATA/STATISTICS/HISTOGRAM
C          DATA INPUT, ONE VALUE PER DATA CARD
C          INPUT OF DATA THRU SUBROUTINE 'REALT'.
       INTEGER ANSA(120),ANA(120)
       DIMENSION X(120),NFREQ(120),GROUP(120),POINT(120),XIA(120),
      1KOR(120),KDER(120),XH(120),TE(120),TF(120),V(120),W(120)
       DIMENSION AR1(20),AR2(20),AR3(20),AR5(20),BR1(20),BR2(20)
       DIMENSION AR41(20),AR42(20),AR43(20),AR44(20)
       DIMENSION FN1(20),FN2(20)
       DIMENSION Z(120),G(120)
       DIMENSION NDF(120),CVT(120)
       DIMENDION KUR(120),KDUR(120),ANSB(120),ANS(120)
       IPUT=2
       IOUT=5
       READ(IPUT,7992) JOBS
       READ(IPUT,7991)(NDF(I),CVT(I),I=1,120)
C          INPUT SYMBOLS...BLANK,LETTER'R'
       READ(IPUT,901) BLANK,ASTER
```

```
C          INPUT LETTER'X'
           READ(IPUT,15) EX
C          INPUT DATE OF EVALUATION XX/XX/XX
           READ(IPUT,73) DA,TY
C          INPUT TEN LITERALS CARDS
           READ(IPUT,501) AR1
           READ(IPUT,501) AR2
           READ(IPUT,501) AR3
           READ(IPUT,501) AR41
           READ(IPUT,501) AR42
           READ(IPUT,501) AR43
           READ(IPUT,501) AR44
           READ(IPUT,501) AR5
           READ(IPUT,501) BR1
           READ(IPUT,501) BR2
C          SET IZERO = 1 FOR LOWEST CELL BOUNDARY TO BE ZERO.
C               OTHERWISE ENTER BLANK FIELD
C               NUMBER OF CELLS = SQUARE ROOT OF NR
           READ(IPUT,18) NR,NCELL,IZERO
           IF(NR) 402,500,402
C          READ IN TWO LINES OF FOOTNOTES
402        READ(IPUT,501) FN1
           READ(IPUT,501) FN2
C          DATA DESCRIPTION
           DO 7993 LOOP=1,JOBS
           WRITE(IOUT,30)
C          DIGIT CONTROL OF MANTISSA FOR DATA PRINTOUT, IJKL
           READ(IPUT,8) PAR1,PAR2,PAR3,PAR4,PAR5,PAR6,PAR7,PAR8,IJKL
           READ(IPUT,17) TV
           READ(IPUT,501) BR1
C          TEST FOR TOO MUCH DATA (MORE THAN 120)
           IF(NR-120) 21,21,22
22         WRITE(IOUT,24)
           WRITE(IOUT,30)
           GO TO 500
21         AN=NR
C          FOUR SIGMA SCREENING TEST TO ELIMINATE UNACCEPTABLE DATA
           MAC=1
           CALL THEAD(AR1,AR2,AR3,AR41,AR42,AR43,AR44,AR5,BR1,BR2,DA,TY,
          1 IOUT,MAC
           WRITE(IOUT,71)
           CALL REALT(KOR,KDER,G,ANSA,ANSB,NR)
           IF(TV) 503,500,503
C          GET STATISTICS ON RAW DATA (G(I))
503        CALL COLS1(G,NR,XBAR,SS,S)
C          CALCULATE 4*SIGMA
           FS = S*4.0
C          PRINT HEADING
           WRITE(IOUT,30)
           MAC=2
           CALL THEAD(AR1,AR2,AR3,AR41,AR42,AR43,AR44,AR5,BR1,BR2,DA,TY,
          1 IOUT,MAC
           WRITE(IOUT,71)
```

```
      WRITE(IOUT,7011)
C        ELIMINATE UNACCEPTABLE DATA, PRINT UNACCEPTABLE DATA LIST
C        REVISE THE VALUE OF N
      CALL COLT2(G,FS,NR,KDER,X,ANSA,ANSB,NA,IPUT,IOUT,KUR,KDUR,
     1 ANA,ANB,XBAR)
C        END OF FOUR SIGMA SCREENING TEST
C        SUBSTITUTE ACCEPTABLE DATA COUNT, NA, FOR N
      N=NA
C        SAVE ACCEPTABLE DATA VECTOR IN THE ORDER READ
      DO 510 I=1,N
      XH(I)=X(I)
510   CONTINUE
C        GET MEAN,SS,S,VR,SD1, ON ACCEPTABLE DATA
      CALL COLS3(X,N,XBAR,VAR,VR,SD,SD1,S196)
C        GET SKEWNESS ON DATA
      CALL COLS4(X,N,XBAR,SD,SKEW)
C        SORT DATA
      L=N-1
      DO 120 J=1,L
      LL=L-J+1
      DO 110 I=1,LL
      LG=I+1
      IF(X(I)-X(LG)) 110,111,111
111   A=X(I)
      X(I)=X(LG)
      X(LG)=A
      A=ANSA(I)
      ANSA(I)=ANSA(LG)
      ANSA(LG)=A
      A=ANSB(I)
      ANSB(I)=ANSB(LG)
      ANSB(LG)=A
110   CONTINUE
120   CONTINUE
C        T-TEST ON DATA, BOTH SORTED AND UNSORTED
C        OBTAIN T VALUE
      TL=0.
      KLM=0
      DO 610 I=1,N
      TE(I)=ABS((TV-XH(I))/SD1)
610   TF(I)=ABS((TV-X(I))/SD1)
C        READ CRITICAL VALUE OF T (CVT) FROM FILE
      KN=N-1
C        TEST SIGNIFICANCE OF THE T VALUE
      DO 621 I=1,N
      IF(TE(I)-CVT(KN)) 619,619,620
619   V(I)=BLANK
      GO TO 621
620   V(I)=ASTER
621   CONTINUE
C        OBTAIN RETAINED DATA VECTOR AND CALCULATE ITS STATISTICS
      DO 931 I=1,N
      IF(TF(I)-CVT(KN)) 929,929,930
```

```
929      W(I)=BLANK
         TL=TL+X(I)
         KLM=KLM+1
         Z(KLM)=X(I)
         GO TO 931
930      W(I)=ASTER
931      CONTINUE
         AN=KLM
         NCELL=SQRT(AN)
         IF(NCELL-1) 450,450,451
450      NCELL=2
C           CALCULATE RETAINED MEAN,VARIANCE AND STANDARD DEVIATION
451      CALL COLS3(Z,KLM,ZAVE,VARZ,VRZ,SDZ,SDZ1,SZ196)
C           GET SKEWNESS
         CALL COLS4(Z,KLM,ZAVE,SDZ,SKEWZ)
C           GET MEDIAN
         CALL COLS5(Z,KLM,ZMED)
C           GET COEFFICIENT OF VARIATION
         CALL COLS6(SDZ1,ZAVE,COEFZ)
C           GET RANGE
         CALL COLS7(Z,RANGE,KLM)
C           GET ACCURACY
         CALL COLS8(TV,ZAVE,ACCZ)
         WRITE(IOUT,30)
         MAC=3
         CALL THEAD(AR1,AR2,AR3,AR41,AR42,AR43,AR44,AR5,BR1,BR2,DA,TY,
        1 IOUT,MAC)
         WRITE(IOUT,71)
         WRITE(IOUT,993)
C           PRINT DATA LIST MARKING REJECTED DATA 'R'
         IF(N-35) 9000,9001,9002
9000     NDIF=35-N
         DO 9901 I=1,N
9901     CALL DLIST(IJKL,KUR,KDUR,XH,V,ANA,ANB,I,IOUT)
         DO 8901 MM=1,NDIF
8901     WRITE(IOUT,8800) BLANK
         WRITE(IOUT,502)  FN1
         WRITE(IOUT,502)  FN2
         GO TO 850
C
9001     DO 9902 I=1,N
9902     CALL DLIST(IJKL,KUR,KDUR,XH,V,ANA,ANB,I,IOUT)
         WRITE(IOUT,8800) BLANK
         WRITE(IOUT,502)  FN1
         WRITE(IOUT,502)  FN2
         GO TO 850
C
9002     IF(N-70) 9003,9004,9005
9003     DO 9903 I=1,35
9903     CALL DLIST(IJKL,KUR,KDUR,XH,V,ANA,ANB,I,IOUT)
         WRITE(IOUT,8800) BLANK
         WRITE(IOUT,502)  FN1
         WRITE(IOUT,502)  FN2
```

```
      NDIF=70-N
      WRITE(IOUT,30)
      CALL THEAD(AR1,AR2,AR3,AR41,AR42,AR43,AR44,AR5,BR1,BR2,DA,TY,
     1 IOUT,MAC)
      WRITE(IOUT,71)
      WRITE(IOUT,993)
      DO 9904 I=36,N
9904  CALL DLIST(IJKL,KUR,KDUR,XH,V,ANA,ANB,I,IOUT)
      DO 8903 MM=1,NDIF
8903  WRITE(IOUT,8800) BLANK
      WRITE(IOUT,502)  FN1
      WRITE(IOUT,502)  FN2
      GO TO 850
C
9004  DO 9905 I=1,35
9905  CALL DLIST(IJKL,KUR,KDUR,XH,V,ANA,ANB,I,IOUT)
      WRITE(IOUT,8800) BLANK
      WRITE(IOUT,502)  FN1
      WRITE(IOUT,502)  FN2
      WRITE(IOUT,30)
      CALL THEAD(AR1,AR2,AR3,AR41,AR42,AR43,AR44,AR5,BR1,BR2,DA,TY,
     1 IOUT,MAC)
      WRITE(IOUT,71)
      WRITE(IOUT,993)
      DO 9906 I=36,70
9906  CALL DLIST(IJKL,KUR,KDUR,XH,V,ANA,ANB,I,IOUT)
      WRITE(IOUT,8800) BLANK
      WRITE(IOUT,502)  FN1
      WRITE(IOUT,502)  FN2
      WRITE(IOUT,30)
C
9005  IF(N-105) 9006,9007,9008
9006  DO 9907 I=1,35
9907  CALL DLIST(IJKL,KUR,KDUR,XH,V,ANA,ANB,I,IOUT)
      WRITE(IOUT,8800) BLANK
      WRITE(IOUT,502)  FN1
      WRITE(IOUT,502)  FN2
      WRITE(IOUT,30)
      CALL THEAD(AR1,AR2,AR3,AR41,AR42,AR43,AR44,AR5,BR1,BR2,DA,TY,
     1 IOUT,MAC)
      WRITE(IOUT,71)
      WRITE(IOUT,993)
      DO 9908 I=36,70
9908  CALL DLIST(IJKL,KUR,KDUR,XH,V,ANA,ANB,I,IOUT)
      WRITE(IOUT,8800) BLANK
      WRITE(IOUT,502)  FN1
      WRITE(IOUT,502)  FN2
      NDIF=105-N
      WRITE(IOUT,30)
      CALL THEAD(AR1,AR2,AR3,AR41,AR42,AR43,AR44,AR5,BR1,BR2,DA,TY,
     1 IOUT,MAC)
      WRITE(IOUT,71)
      WRITE(IOUT,993)
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```
      DO 9909 I=71,N
9909  CALL DLIST(IJKL,KUR,KDUR,XH,V,ANA,ANB,I,IOUT)
      DO 8904 MM=1,NDIF
8904  WRITE(IOUT,71)
      WRITE(IOUT,502) FN1
      WRITE(IOUT,502) FN2
      GO TO 850
9007  DO 9910 I=1,35
9910  CALL DLIST(IJKL,KUR,KDUR,XH,V,ANA,ANB,I,IOUT)
      WRITE(IOUT,71)
      WRITE(IOUT,502) FN1
      WRITE(IOUT,502) FN2
      WRITE(IOUT,30)
      CALL THEAD(AR1,AR2,AR3,AR41,AR42,AR43,AR44,AR5,BR1,BR2,DA,TY,
     1 IOUT,MAC)
      WRITE(IOUT,71)
      WRITE(IOUT,993)
      DO 9911 I=36,70
9911  CALL DLIST(IJKL,KUR,KDUR,XH,V,ANA,ANB,I,IOUT)
      WRITE(IOUT,71)
      WRITE(IOUT,502) FN1
      WRITE(IOUT,502) FN2
      WRITE(IOUT,30)
      CALL THEAD(AR1,AR2,AR3,AR41,AR42,AR43,AR44,AR5,BR1,BR2,DA,TY,
     1 IOUT,MAC)
      WRITE(IOUT,71)
      WRITE(IOUT,993)
      DO 9912 I=71,105
9912  CALL DLIST(IJKL,KUR,KDUR,XH,V,ANA,ANB,I,IOUT)
      WRITE(IOUT,71)
      WRITE(IOUT,502) FN1
      WRITE(IOUT,502) FN2
      GO TO 850
9008  DO 9913 I=1,35
9913  CALL DLIST(IJKL,KUR,KDUR,XH,V,ANA,ANB,I,IOUT)
      WRITE(IOUT,71)
      WRITE(IOUT,502) FN1
      WRITE(IOUT,502) FN2
      WRITE(IOUT,30)
      CALL THEAD(AR1,AR2,AR3,AR41,AR42,AR43,AR44,AR5,BR1,BR2,DA,TY,
     1 IOUT,MAC)
      WRITE(IOUT,71)
      WRITE(IOUT,993)
      DO 9914 I=36,70
9914  CALL DLIST(IJKL,KUR,KDUR,XH,V,ANA,ANB,I,IOUT)
      WRITE(IOUT,71)
      WRITE(IOUT,502) FN1
      WRITE(IOUT,502) FN2
      WRITE(IOUT,30)
      CALL THEAD(AR1,AR2,AR3,AR41,AR42,AR43,AR44,AR5,BR1,BR2,DA,TY,
     1 IOUT,MAC)
      WRITE(IOUT,71)
      WRITE(IOUT,993)
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```
      DO 9915 I=71,105
9915  CALL DLIST(IJKL,KUR,KDUR,XH,V,ANA,ANB,I,IOUT)
      WRITE(IOUT,71)
      WRITE(IOUT,502) FN1
      WRITE(IOUT,502) FN2
      WRITE(IOUT,30)
      CALL THEAD(AR1,AR2,AR3,AR41,AR42,AR43,AR44,AR5,BR1,BR2,DA,TY,
     1 IOUT,MAC)
      WRITE(IOUT,71)
      WRITE(IOUT,993)
      DO 9916 I=106,N
9916  CALL DLIST(IJKL,KUR,KDUR,XH,V,ANA,ANB,I,IOUT)
      NDIF=140-N
      DO 8905 MM=1,NDIF
8905  WRITE(IOUT,71)
      WRITE(IOUT,502) FN1
      WRITE(IOUT,502) FN2
C
850   WRITE(IOUT,71)
C        GETREMAINDER OF STATISTICS ON ACCEPTABLE DATA
C             RANGE, MEDIAN, COEFFICIENT OF VARIATION
      CALL COLS5(X,N,XMED)
      CALL COLS6(SD1,XBAR,COEFV)
      CALL COLS7(X,RANGZ,N)
C        CALCULATE CELL BOUNDARIES, FREQUENCIES AND MIDPOINTS
      IF(NCELL) 113,112,113
112   NCELL = 15
113   DO 130 I=1,NCELL
130   NFREQ(I) = 0
      IF(IZERO-1) 141,140,140
141   WIDTH = RANGE/(NCELL-1)
      WIDTH = WIDTH + .00001
      RIDPT = WIDTH/2
      GROUP(1) = Z(1) + RIDPT
      POINT(1) = Z(1)
      GO TO 150
140   WIDTH = (Z(KLM)-0.)/(NCELL-0.5)
      WIDTH = WIDTH + .00001
      GROUP(1) = 0.0 + WIDTH
      POINT(1) = GROUP(1)/2
150   DO 160 I=2,NCELL
160   GROUP(I) = GROUP(I-1) + WIDTH
      DO 190 I=1,KLM
      DO 170 M=1,NCELL
      IF(Z(I) - GROUP(M)) 180,180,170
170   CONTINUE
180   NFREQ(M) = NFREQ(M) + 1
190   CONTINUE
      DO 200 I=2,NCELL
200   POINT(I) = POINT(I-1) + WIDTH
C        PRINT HEADING
      WRITE(IOUT,30)
      MAC=4
```

```
      CALL THEAD(AR1,AR2,AR3,AR41,AR42,AR43,AR44,AR5,BR1,BR2,DA,TY,
     1 IOUT,MAC)
      WRITE(IOUT,71)
C        PRINT STATISTICS
      WRITE(IOUT,40) N,RANGE,COEFZ
      IF(IJKL-1) 910,911,919
919   IF(IJKL-3) 912,913,914
910   WRITE(IOUT,410) TV
      GO TO 950
911   WRITE(IOUT,411) TV
      GO TO 950
912   WRITE(IOUT,412) TV
      GO TO 950
913   WRITE(IOUT,413) TV
      GO TO 950
914   WRITE(IOUT,414) TV
      GO TO 950
950   WRITE(IOUT,50) VRZ,SKEWZ
      WRITE(IOUT,60) XBAR,SDZ1,NCELL
      WRITE(IOUT,62) ZAVE,SZ196
      WRITE(IOUT,63) ZMED
      WRITE(IOUT,65) ACCZ
      WRITE(IOUT,71)
      WRITE(IOUT,66)
      WRITE(IOUT,71)
      MAX = NFREQ(1)
      DO 250 I = 2,NCELL
      IF(MAX - NFREQ(I)) 245,250,250
245   MAX = NFREQ(I)
250   CONTINUE
      LL = 0
      LM = 35
      LN = 70
      LP = 105
      DO 320 I=1,NCELL
      LL = LL+1
      LM = LM+1
      LN = LN+1
      LP = LP+1
      K = NFREQ(I)
      KKK = NFREQ(I)
      IF(NFREQ(I)) 322,321,322
322   IF(NFREQ(I) - 15) 323,323,324
324   NFREQ(I) = 15
      K = 15
323   DO 329 KIX=1,K
      XIA(KIX)=EX
329   CONTINUE
C
      CALL COL1(IJKL,X,W,LL,IOUT)
      IF(N-LM) 326,1325,1325
1325  CALL COL2(IJKL,X,W,LM,IOUT)
      IF(N-LN) 326,325,325
```

```
325      CALL COL3(IJKL,X,W,LN,IOUT)
         IF(N-LP) 326,927,927
927      CALL COL4(IJKL,X,W,LP,IOUT)
326      WRITE(IOUT,96) POINT(I),KKK,(XIA(KIX),KIX=1,K)
         GO TO 320
321      CALL COL1(IJKL,X,W,LL,IOUT)
         IF(N-LM) 328,1327,1327
1327     CALL COL2(IJKL,X,W,LM,IOUT)
         IF(N-LN) 328,327,327
327      CALL COL3(IJKL,X,W,LN,IOUT)
         IF(N-LP) 328,928,928
928      CALL COL4(IJKL,X,W,LP,IOUT)
328      WRITE(IOUT,96) POINT(I),KKK
320      CONTINUE
         J=LL+1
         DO 1120 I=J,35
         K=I+35
         L=I+70
         M=I+105
         IF(N-I) 1120,1121,1121
1121     CALL COL1(IJKL,X,W,I,IOUT)
         IF(N-K) 1120,1123,1123
1123     CALL COL2(IJKL,X,W,K,IOUT)
         IF(N-L) 1120,1126,1126
1126     CALL COL3(IJKL,X,W,L,IOUT)
         IF(N-M) 1120,1129,1129
1129     CALL COL4(IJKL,X,W,M,IOUT)
1120     CONTINUE
         WRITE(IOUT,30)
7993     CONTINUE
C           FORMAT STATEMENTS
8        FORMAT(8A4,I1)
15       FORMAT(A1)
17       FORMAT(F10.0)
18       FORMAT(3I4)
24       FORMAT(1H ,'INCORRECT SAMPLE SIZE.....TERMINATE JOB'////////)
30       FORMAT(1H1)
40       FORMAT(1H ,'N,ALL DATA',I3,8X,'RANGE',7X,F11.5,5X,
        1'COEF. VAR.',1X,F11.5)
50       FORMAT(1H+,21X,'VARIANCE',4X,F11.5,5X,'SKEWNESS',3X,F11.5)
60       FORMAT(1H ,'MEAN,ALL',F11.5,2X,'STD. DEV.',3X,F11.5,5X,
        1'NO. OF CELLS',I4)
62       FORMAT(1H ,'MEAN,RET.',F10.5,2X,'CONF. LIM.',2X,F11.5,1X,
        1'(95 PCT)')
63       FORMAT(1H ,'MEDIAN',2X,F11.5)
65       FORMAT(1H ,'ACCURACY',F11.5,2X,
        1'PCT RELATIVE ERROR, RETAINED DATA')
66       FORMAT(1H ,'ACCEPTABLE DATA IN ASCENDING ORDER',3X,
        1'MIDPOINT',2X,'FREQ.',4X,'HISTOGRAM'/1H ,42X,
        2'RETAINED DATA ONLY')
71       FORMAT(1H )
73       FORMAT(2A4)
96       FORMAT(1H+,35X,F10.4,2X,I4,4X,15A1)
```

```
C          NOTE: ALTER 'F' SPECS ACCORDING TO EDITORIAL REQUIREMENTS
410      FORMAT(1H ,'TRUE VAL.',F8.0)
411      FORMAT(1H ,'TRUE VAL.',F8.1)
412      FORMAT(1H ,'TRUE VAL.',F8.2)
413      FORMAT(1H ,'TRUE VAL.',F8.3)
414      FORMAT(1H ,'TRUE VAL.',F8.4)
501      FORMAT(20A4)
502      FORMAT(1H ,20A4)
901      FORMAT(2A1)
993      FORMAT(1H ,24X,'NUMBER OF     SAMPLE'/1H ,23X,
        1'LAB/ANALYST   RECOVERY'/1H ,38X,
        2'BY LAB.'/)
7011     FORMAT(1H ,'UNACCEPTABLE DATA LIST'///)
7991     FORMAT(I3,5X,F6.0)
7992     FORMAT(I4)
8800     FORMAT(1H ,A1)
500      CALL EXIT
         END
```

SUBROUTINE THEAD

This subroutine provides for the print of the heading upon demand by the main program. The input consists of a library of literal cards and a date card to be used in forming the specific heading. The actual format of the heading is controlled by an integer variable which activates a computed go to statement.

INPUT REQUIREMENTS

Variable	Purpose
AR1(I)	Literal card
AR2(I)	Literal card
DA,TY	Date card
BR2(I)	Literal card
AR3(I)	Literal card
MAC	Integer Variable assigned to select literal line specific for the current text.
AR41(I)	Literal card
AR42(I)	Literal card
AR43(I)	Literal card
AR44(I)	Literal card
AR5(I)	Literal card
BR2(I)	Literal card
BR1(I)	Literal card

```
      SUBROUTINE THEAD(AR1,AR2,AR3,AR41,AR42,AR43,AR44,AR5,BR1,BR2,
     1 DA,TY,IOUT,MAC)
      DIMENSION AR1(20),AR2(20),AR3(20),AR5(20),BR1(20),BR2(20)
      DIMENSION AR41(20),AR42(20),AR43(20),AR44(20)
      WRITE(IOUT,502) AR1
      WRITE(IOUT,502) AR2
      WRITE(IOUT,72) DA,TY
      WRITE(IOUT,502) BR2
      WRITE(IOUT,502) AR3
      GO TO (10,20,30,40),MAC
10    WRITE(IOUT,502) AR41
      GO TO 50
20    WRITE(IOUT,502) AR42
      GO TO 50
30    WRITE(IOUT,502) AR43
      GO TO 50
40    WRITE(IOUT,502) AR44
50    WRITE(IOUT,502) AR5
      WRITE(IOUT,502) BR2
      WRITE(IOUT,502) BR2
502   FORMAT(1H ,20A4)
72    FORMAT(1H ,80X,'EVALUATION DATE = ',2A4)
      RETURN
      END
```

SUBROUTINE REALT

The purpose of this subroutine is to screen the raw data as punched. The raw data may consist of censored data or blanks instead of data in valid form for this analysis. The number of data cards may be unknown. A card with numbers other than zero punched in card column 80 follows the data deck. Testing of fields such as censor sign or the absence of a decimal point is accomplished through character comparison. A valid raw data vector is created by this subroutine. This raw data vector is printed followed by count of input data and a count of output data. Subroutine CONV2 is used to convert the validated raw data into a real data vector, T.

INPUT REQUIREMENTS

Variable	Purpose	Format
ALAB(I)	Numerical identification of laboratory	I3
NNYL(I)	Numerical identification of analyst	A1
L(I)	Data censor (Greater than or less than)	A1
J(I)	Integer portion of data element	I4
M(I)	Decimal point of data element	A1
K(I)	Decimal portion of data element	I2
AN(I)	Symbol: D = Different method Blank = Official method of test	A1
ST(I)	Unused literal field	A2
KOUNT(I)	Field used for 'stop' card	I2

OUTPUT REQUIREMENTS

Variable	Purpose	Format
AL(I)	Numerical identification of laboratory	I3
NN(I)	Numerical identification of analyst	A1
T(I)	Element of the raw data vector	F10.2
ANA(I)	Method type, all blank	A2

```
      SUBROUTINE REALT(AL,NN,T,ANA,ANB,NR)
      INTEGER AL(120),ALAB(120),AN(120),ANA(120)
      DIMENSION NNYL(120),L(120),J(120),M(120),K(120),ST(120),
     1 NN(120),JJ(120),KK(120),T(120),KOUNT(120),ANB(120)
C          FOR TRACE METAL DATA ANALYSIS...UNKNOWN CARD COUNT.
C          PLACE 9'S CARD AFTER EACH INDIVIDUAL DATA DECK.
      IPUT=2
      IOUT=5
C          INPUT DATA
      I=0
      NR=0
19    I=I+1
      NG=I-1
```

```
      READ(IPUT,1) ALAB(I),NNYL(I),L(I),J(I),M(I),K(I),AN(I),ST(I),
     1 KOUNT(I)
      IF(KOUNT(I)) 10,10,99
10    IF(L(I)-16448) 19,11,19
11    IF(M(I)-16448) 21,19,21
21    IF(AN(I)-16448) 19,20,19
20    NR=NR+1
      AL(NR) = ALAB(I)
      NN(NR) = NNYL(I)
      JJ(NR) = J(I)
      KK(NR) = K(I)
      ANA(NR) = AN(I)
      ANB(NR) = ST(I)
      GO TO 19
C
99    WRITE(IOUT,71)
      DO 40 I=1,NR
      CALL CONV2(JJ,KK,T,NR)
      WRITE(IOUT,31) AL(I),NN(I),T(I),ANA(I)
40    CONTINUE
      WRITE(IOUT,32) NG,NR
C         FORMAT STATEMENTS
1     FORMAT(I3,A1,1X,I4,A1,I2,A1,62X,A2,I2)
31    FORMAT(1H ,I3,A1,5X,F10.2,A1)
32    FORMAT(1H0,5X,'INPUT DATA COUNT = ',I4,' WITH NULL VALUES'/1H ,
     1 5X,'OUTPUT DATA COUNT = ',I4,' CONSOLIDATED REAL DATA'///)
71    FORMAT(1H )
      RETURN
      END
```

SUBROUTINE CONV2

The purpose of this subroutine is to convert a validated input number, entered as an integer variable followed by a literal character (the decimal point) and followed by a second integer number. The data were entered by this format, I4,A1,I2, for the purpose of screening the data. Censored data and missing data were removed from the gross input data vector. This subroutine takes the two integers and converts these to the decimal number.

INPUT REQUIREMENTS

Variable	Purpose
J(I)	Integer to the left of the decimal point
K(I)	Integer to the right of the decimal point

OUTPUT REQUIREMENTS

Variable	Purpose
T(I)	Output valid data vector
N	Number of data elements to be converted

```
      SUBROUTINE CONV2(J,K,T,N)
      DIMENSION J(120),K(120),T(120)
      DO 10 I=1,N
      A = J(I)
      B = (FLOAT(K(I)))/100.
      T(I) = A + B
10    CONTINUE
      RETURN
      END
```

SUBROUTINE COLS1

This subroutine calculates the sample statistics on a set of data points. Up to and including 120 data points may be accommodated.

The following computations are made:

Sample Mean = Sum/N where Sample Mean = mean of the data points
Sum = sum of the data points
N = number of data points
Total = sum of (A(I)-Sample Mean)**2

and

Sample Variance = Total/(N-1)
Sample Standard Deviation = Square root of the Sample Variance

INPUT REQUIREMENTS

Variable	Purpose
A(I)	Data element
N	Number of data elements

OUTPUT REQUIREMENTS

Variable	Purpose
XBAR	Sample mean
SS	Sample variance
S	Sample standard deviation

```
      SUBROUTINE COLS1(A,N,XBAR,SS,S)
      DIMENSION A(120)
      TOTAL = 0.0
      DO 10 I=1,N
      TOTAL = TOTAL + A(I)
10    CONTINUE
      AN = N
      BN = N-1
      XBAR = TOTAL/AN
      T = 0.0
      DO 20 I=1,N
      T = T + (A(I)-XBAR)**2
20    CONTINUE
      SS = T/BN
      S = SQRT(SS)
      RETURN
      END
```

SUBROUTINE COLT2

This subroutine performs the four sigma screening test. Data are arbitrarily considered to be unacceptable if their difference from the mean is greater than four standard deviations from the mean. The test is performed on each data element. An unacceptable data list is printed, the acceptable data vector is stored and returned to the main program.

INPUT REQUIREMENTS

Variable	Purpose
G(I)	Raw data element
XBAR	Mean on raw data
FSD	Value of four standard deviations of raw data vector
M	Number of raw data elements
KOR(I)	Numerical identification of laboratory
KDER(I)	Numerical identification of analyst
ANSA(I)	Symbol: D = Different method Blank = Official method of test
ANSB(I)	Spare field, unused at this time

OUTPUT REQUIREMENTS

Variable	Purpose
X(I)	Data element, acceptable data vector
NA	Number of acceptable data elements
IPUT	Input device number
IOUT	Output device number
KUR(I)	Numerical identification of laboratory
KDUR(I)	Numerical identification of analyst
ANA(I)	Symbol: D = Different method Blank = Official method of test
ANB(I)	Spare field, unused at this time

```
      SUBROUTINE COLT2(G,FSD,M,KOR,KDER,X,ANSA,ANSB,NA,IPUT,IOUT,KUR,
     1 KDUR,ANA,ANB,XBAR)
      INTEGER ANSA(120),ANA(120)
      DIMENSION G(120),KOR(120),KDER(120),X(120),KUR(120),KDUR(120),
     1 ANSB(120),ANB(120)
      N=M
      NA=0
      DO 10 I=1,N
      AMAA = ABS(G(I)-XBAR)
      IF(AMAA-FSD) 20,20,30
30    WRITE(IOUT,2) KOR(I),KDER(I),G(I),ANSA(I)
      GO TO 10
20    NA=NA+1
```

```
      X(NA) = G(I)
      KUR(NA) = KOR(I)
      KDUR(NA) = KDER(I)
      ANA(NA) = ANSA(I)
      ANB(NA) = ANSB(I)
10    CONTINUE
2     FORMAT(1H ,I3,3X,A1,F10.2,2X,A1)
      RETURN
      END
```

SUBROUTINE COLS3

This subroutine calculates sample statistics and population statistics on a set of data points. The population standard deviation is used in the calculation of skewness. The following computations are made:

Mean = Sum/N where Mean = mean of the data points;
Sum = sum of data points; N = number of data points
Total = sum of (A(I)-Mean)**2

and

Sample variance = Total/(N-1)
Sample standardard deviation = Square root of the sample variance
Population variance = Total/N
Population standard deviation = Square root of the population variance

INPUT REQUIREMENTS

Variable	Purpose
A(I)	Data element
N	Number of data elements

OUTPUT REQUIREMENTS

Variable	Purpose
XBAR	Mean of data elements
VAR	Population variance
VR	Sample variance
SD	Population standard deviation
SD1	Sample standard deviation
S196	Sample standard deviation X 1.96

```
      SUBROUTINE COLS3(A,N,XBAR,VAR,VR,SD,SD1,S196)
      DIMENSION A(120)
      TOTAL = 0.0
      DO 10 I=1,N
      TOTAL = TOTAL + A(I)
10    CONTINUE
      AN = N
      BN = N-1
      XBAR = TOTAL/AN
      T = 0.0
      DO 20 I=1,N
      T = T + (A(I)-XBAR)**2
20    CONTINUE
      VAR = T/AN
      VR  = T/BN
      SD  = SQRT(VAR)
      SD1 = SQRT(VR)
      S196 = SD1*1.96
      RETURN
      END
```

SUBROUTINE COLS4

This subroutine calculates the coefficient of skewness which is a measure of lack of symmetry of the data. The expression for this coefficient is:

Skewness = Sum of ((A(I)-XBAR)**3/N)*SD**3
A(I) = data element
XBAR = Smple Mean of data elements
N = number of data elements
SD = population standard deviation

INPUT REQUIREMENTS

Variable	Purpose
X(I)	Data element
N	Number of data elements
XBAR	Sample Mean of data elements
SD	Population standard deviation

OUTPUT REQUIREMENTS

Variable	Purpose
SKEW	Coefficient of skewness

```
      SUBROUTINE COLS4(X,N,XBAR,SD,SKEW)
      DIMENSION X(120)
      SKW1 = 0.0
      DO 10 I=1,N
      SKW1 = SKW1 + (X(I) - XBAR)**3
10    CONTINUE
      SKW2 = N * SD**3
      SKEW = SKW1/SKW2
      RETURN
      END
```

SUBROUTINE COLS5

This subroutine calculates the median in a set of data. The median is calculated by the following expression:

X = data element
Median = (X(J) + X(K))/2
J = (N+1)/2
K = (N+2)/2
N = Number of data points

INPUT REQUIREMENTS

Variable	Purpose
X(I)	Data element
N	Number of data elements

OUTPUT REQUIREMENTS

Variable	Purpose
XMED	Median of data elements

```
      SUBROUTINE COLS5(X,N,MED)
      DIMENSION X(120)
      J = (N+1)/2
      K = (N+2)/2
      XMED = (X(J) + X(K))/2.0
      RETURN
      END
```

SUBROUTINE COLS6

This subroutine calculates the coefficient of variation of a set of data elements. The expression for this calculation follows:

Coefficient of variation = Sample standard deviation/Mean

INPUT REQUIREMENTS

Variable	Purpose
SD	Sample standard deviation
XBAR	Sample mean

OUTPUT REQUIREMENTS

Variable	Purpose
COEFV	Coefficient of variation

```
      SUBROUTINE COLS6(SD,XBAR,COEFV)
      COEFV = SD/XBAR
      RETURN
      END
```

SUBROUTINE COLS7

This subroutine calculates the range of a set of data elements. The range is the difference between the largest element and the smallest element. The set of data elements have previously been sorted and placed in ascending order.

INPUT REQUIREMENTS

Variable	Purpose
X(I)	Data element
N	Number of data elements

OUTPUT REQUIREMENTS

Variable	Purpose
RANGE	Range

```
      SUBROUTINE COLS7(X,RANGE,N)
      DIMENSION X(120)
      RANGE = X(N) - X(1)
      RETURN
      END
```

SUBROUTINE COLS8

This subroutine calculates the accuracy of the mean of a set of data elements. For the purpose of this method study, the accuracy is based upon the known value or "true value" of the material sought in the sample. The accuracy is expressed as percent of true value.

INPUT REQUIREMENTS

Variable	Purpose
TV	True value
XBAR	Sample Mean of data set

OUTPUT REQUIREMENTS

Variable	Purpose
ACC	Accuracy

```
      SUBROUTINE COLS8(TV,XBAR,ACC)
C
      ACC = (XBAR - TV)/TV
      ACC = ACC*100.0
C
      RETURN
      END
```

SUBROUTINES COL1, COL2, COL3, COL4

These closely related subroutines provide for the printing of data elements in columns 1, 2, 3 or 4 by subroutines COL1, COL2, COL3 or COL4, respectively. The proper format for printing the data is selected according to the value of the input variable, IJKL.

INPUT AND OUTPUT REQUIREMENTS

Variable	Purpose
X(I)	Data element
W(I)	Symbol of t-test result: 'R' = Rejected ' ' = Retained
LL	Data element counter
IJKL	Integer equal to the number of digits to the right of the decimal point
IOUT	Output device number

```
      SUBROUTINE COL1(IJKL,X,W,LL,IOUT)
      DIMENSION X(120),W(120)
790   FORMAT(1H ,F8.0,A1)
791   FORMAT(1H ,F8.1,A1)
792   FORMAT(1H ,F8.2,A1)
793   FORMAT(1H ,F8.3,A1)
794   FORMAT(1H ,F8.4,A1)
      MAA = IJKL+1
      GO TO (1,2,3,4,5),MAA
1     WRITE(IOUT,790) X(LL),W(LL)
      GO TO 50
2     WRITE(IOUT,791) X(LL),W(LL)
      GO TO 50
3     WRITE(IOUT,792) X(LL),W(LL)
      GO TO 50
4     WRITE(IOUT,793) X(LL),W(LL)
      GO TO 50
5     WRITE(IOUT,794) X(LL),W(LL)
50    RETURN
      END

      SUBROUTINE COL2(IJKL,X,W,LL,IOUT)
      DIMENSION X(120),W(120)
790   FORMAT(1H+,11X,F8.0,A1)
791   FORMAT(1H+,11X,F8.1,A1)
792   FORMAT(1H+,11X,F8.2,A1)
793   FORMAT(1H+,11X,F8.3,A1)
794   FORMAT(1H+,11X,F8.4,A1)
      MAA = IJKL+1
      GO TO (1,2,3,4,5),MAA
1     WRITE(IOUT,790) X(LL),W(LL)
      GO TO 50
```

```
2       WRITE(IOUT,791) X(LL),W(LL)
        GO TO 50
3       WRITE(IOUT,792) X(LL),W(LL)
        GO TO 50
4       WRITE(IOUT,793) X(LL),W(LL)
        GO TO 50
5       WRITE(IOUT,794) X(LL),W(LL)
50      RETURN
        END

        SUBROUTINE COL3(IJKL,X,W,LL,IOUT)
        DIMENSION X(120),W(120)
790     FORMAT(1H+,21X,F8.0,A1)
791     FORMAT(1H+,21X,F8.1,A1)
792     FORMAT(1H+,21X,F8.2,A1)
793     FORMAT(1H+,21X,F8.3,A1)
794     FORMAT(1H+,21X,F8.4,A1)
        MAA = IJKL+1
        GO TO (1,2,3,4,5),MAA
1       WRITE(IOUT,790) X(LL),W(LL)
        GO TO 50
2       WRITE(IOUT,791) X(LL),W(LL)
        GO TO 50
3       WRITE(IOUT,792) X(LL),W(LL)
        GO TO 50
4       WRITE(IOUT,793) X(LL),W(LL)
        GO TO 50
5       WRITE(IOUT,794) X(LL),W(LL)
50      RETURN
        END

        SUBROUTINE COL4(IJKL,X,W,LL,IOUT)
        DIMENSION X(120),W(120)
790     FORMAT(1H+,31X,F8.0,A1)
791     FORMAT(1H+,31X,F8.1,A1)
792     FORMAT(1H+,31X,F8.2,A1)
793     FORMAT(1H+,31X,F8.3,A1)
794     FORMAT(1H+,31X,F8.4,A1)
        MAA = IJKL+1
        GO TO (1,2,3,4,5),MAA
1       WRITE(IOUT,790) X(LL),W(LL)
        GO TO 50
2       WRITE(IOUT791) X(LL),W(LL)
        GO TO 50
3       WRITE(IOUT,792) X(LL),W(LL)
        GO TO 50
4       WRITE(IOUT,793) X(LL),W(LL)
        GO TO 50
5       WRITE(IOUT,794) X(LL),W(LL)
50      RETURN
        END
```

SUBROUTINE DLIST

This subroutine prints a data list in accordance with the number of digits to the right of the decimal point. The following range of decimals are allowed: xx., xx.x, x.xx, x.xxx, and x.xxxx.

INPUT REQUIREMENTS

Variable	Purpose
IJKL	Integer representing number of digits to the right of the decimal point
I	Count of data element in the vector
IOUT	Output device number

OUTPUT REQUIREMENTS

Variable	Purpose	Format
KUR(I)	Laboratory identification number	I3
KDUR(I)	Analyst identification number	A1
XH(I)	Unsorted vector data element	F7.2
V(I)	Symbol of t-test results: "R" = Rejected " " = Retained	A1
ANA(I)	Method used: "D" = Different method " " = Official method	A1
ANB(I)	Spare field, unused at this time	A2

```
      SUBROUTINE DLIST(IJKL,KUR,KDUR,XH,V,ANA,ANB,I,IOUT)
      INTEGER ANA(120)
      DIMENSION KUR(120),KDUR(120),XH(120),V(120),ANB(120)
430   FORMAT(1H ,23X,I3,4X,A1,8X,F7.0,1X,A1,A1,A2)
431   FORMAT(1H ,23X,I3,4X,A1,8X,F7.1,1X,A1,A1,A2)
432   FORMAT(1H ,23X,I3,4X,A1,8X,F7.2,1X,A1,A1,A2)
433   FORMAT(1H ,23X,I3,4X,A1,8X,F7.3,1X,A1,A1,A2)
434   FORMAT(1H ,23X,I3,4X,A1,8X,F7.4,1X,A1,A1,A2)
      MAA = IJKL+1
      GO TO (1,2,3,4,5),MAA
1     WRITE(IOUT,430) KUR(I),KDUR(I),XH(I),V(I),ANA(I),ANB(I)
      GO TO 50
2     WRITE(IOUT,431) KUR(I),KDUR(I),XH(I),V(I),ANA(I),ANB(I)
      GO TO 50
3     WRITE(IOUT,432) KUR(I),KDUR(I),XH(I),V(I),ANA(I),ANB(I)
      GO TO 50
4     WRITE(IOUT,433) KUR(I),KDUR(I),XH(I),V(I),ANA(I),ANB(I)
      GO TO 50
5     WRITE(IOUT,434) KUR(I),KDUR(I),XH(I),V(I),ANA(I),ANB(I)
50    RETURN
      END
```

HEADER & DATA DECK CONFIGURATION

HEADER DECK FOR n SETS OF DATA

Card	Contents	Remarks
1	0001	For n sets of data; n=1
2	T-Table Deck	120 cards
3	R	Symbol card; blank,' ', 'R'
4	X	Symbol card; 'X'
5	nn/nn/nn	Date card
6	QUALITY ASSURANCE & LABORATORY EVALUATION BRANCH	
7	EPA METHOD STUDY 7, TRACE METALS	
8	ANALYSES FOR ARSENIC IN WATER	
9	ALL DATA, EPA & NON-EPA LABORATORIES	
10	UNACCEPTABLE DATA, EPA & NON-EPA LABORATORIES	
11	ACCEPTABLE DATA, EPA & NON-EPA LABORATORIES	
12	STATISTICS ON DATA, EPA & NON-EPA LABORATORIES	
13	RECOVERY OF INCREMENT FROM DISTILLED WATER	
14	(blank card)	
15	(blank card)	
16	0001	NR-card
17	FOOTNOTE 1	
18	FOOTNOTE 2	

HEADER & DATA DECK CONFIGURATION

DATA DECK (first of n data decks)

Card	Contents	Remarks
1	2	Digit in CC-33
2	bbbbb292.0	'True' Value
3	AMPUL 1 INCREMENT = 292 UG/LITER	
4	1011 405. AS01D (AS01D is arbitrary ID not read by program)	Data card: example
.	. . .	
.	. . .	
.	. . .	
m	55	last card two digits; CC-79,80

QUALITY ASSURANCE & LABORATORY EVALUATION BRANCH, MDQARL
EPA METHOD STUDY 7, TRACE METALS

EVALUATION DATE = 10/30/74

ANALYSES FOR ARSENIC IN WATER
ALL DATA, EPA & NON-EPA LABORATORIES
RECOVERY OF INCREMENT FROM DISTILLED WATER

AMPUL 1 INCREMENT = 292 UG/LITER ARSENIC

1011	405.00
1031	215.00
1061	308.00
1092	257.00
1102	620.00
1131	311.00
1241	285.00
1371	11.40
1481	306.00
1521	250.00
1571	220.00
1681	280.00
1691	280.00
1901	274.00
1951	253.00
2041	325.00
2591	246.00
2911	1900.00
3291	199.00
3381	246.00
3521	270.00
3931	250.00
4021	369.00
4431	315.00
4441	156.00
4461	290.00
4472	250.00
4481	240.00
4531	220.00
4551	314.00
4561	190.00
4581	206.00
4641	25.00
4681	210.00
4702	140.00
4751	398.00
4861	336.00
4881	170.80
4921	109.00
4941	234.00
4961	145.00
5041	271.00

INPUT DATA COUNT = 113 WITH NULL VALUES
OUTPUT DATA COUNT = 42 CONSOLIDATED REAL DATA

QUALITY ASSURANCE & LABORATORY EVALUATION BRANCH, MDQARL
EPA METHOD STUDY 7, TRACE METALS

EVALUATION DATE = 10/30/74

ANALYSES FOR ARSENIC IN WATER
UNACCEPTABLE DATA, EPA & NON-EPA LABORATORIES
RECOVERY OF INCREMENT FROM DISTILLED WATER

AMPUL 1 INCREMENT = 292 UG/LITER ARSENIC

UNACCEPTABLE DATA LIST

291 1 1900.00

QUALITY ASSURANCE & LABORATORY EVALUATION BRANCH, MDQARL
EPA METHOD STUDY 7, TRACE METALS

EVALUATION DATE = 10/30/74

ANALYSES FOR ARSENIC IN WATER
ACCEPTABLE DATA, EPA & NON-EPA LABORATORIES
RECOVERY OF INCREMENT FROM DISTILLED WATER

AMPUL 1 INCREMENT = 292 UG/LITER ARSENIC

	NUMBER OF LAB/ANALYST	SAMPLE RECOVERY BY LAB.	
101	1	405.00	
103	1	215.00	
106	1	308.00	
109	2	257.00	
110	2	620.00	R
113	1	311.00	
124	1	285.00	
137	1	11.40	R
148	1	306.00	
152	1	250.00	
157	1	220.00	
168	1	280.00	
169	1	280.00	
190	1	274.00	
195	1	253.00	
204	1	325.00	
259	1	246.00	
329	1	199.00	
338	1	246.00	
352	1	270.00	
393	1	250.00	
402	1	369.00	
443	1	315.00	
444	1	156.00	
446	1	290.00	
447	2	250.00	
448	1	240.00	
453	1	220.00	
455	1	314.00	
456	1	190.00	
458	1	206.00	
464	1	25.00	
468	1	210.00	
470	2	140.00	
475	1	398.00	

R = REJECTED DATA

QUALITY ASSURANCE & LABORATORY EVALUATION BRANCH, MDQARL
EPA METHOD STUDY 7, TRACE METALS

EVALUATION DATE = 10/

ANALYSES FOR ARSENIC IN WATER
ACCEPTABLE DATA, EPA & NON-EPA LABORATORIES
RECOVERY OF INCREMENT FROM DISTILLED WATER

AMPUL 1 INCREMENT = 292 UG/LITER ARSENIC

LAB	NUMBER OF ANALYST	SAMPLE RECOVERY BY LAB.
486	1	336.00
488	1	170.80
492	1	109.00
494	1	234.00
496	1	145.00
504	1	271.00

R = REJECTED DATA

QUALITY ASSURANCE & LABORATORY EVALUATION BRANCH, MDQARL
EPA METHOD STUDY 7, TRACE METALS

EVALUATION DATE = 10/30/74

ANALYSES FOR ARSENIC IN WATER
STATISTICS ON DATA, EPA & NON-EPA LABORATORIES
RECOVERY OF INCREMENT FROM DISTILLED WATER

AMPUL 1 INCREMENT = 292 UG/LITER ARSENIC

N,ALL DATA	41	RANGE	380.00006	COEF. VAR.	0.30351
TRUE VAL.	292.0	VARIANCE	5779.82130	SKEWNESS	-0.47880
MEAN,ALL	253.66336	STD. DEV.	76.02513	NO. OF CELLS	6
MEAN,RET.	250.48202	CONF. LIM.	149.00921 (95 PCT)		
MEDIAN	250.00003				
ACCURACY	-14.21849	PCT RELATIVE ERROR, RETAINED DATA			

ACCEPTABLE DATA IN ASCENDING ORDER		MIDPOINT	FREQ. RETAINED DATA ONLY	HISTOGRAM
11.40R	325.00	25.0000	1	X
25.00	336.00	101.0000	1	X
109.00	369.00	177.0000	9	XXXXXXXXX
140.00	398.00	253.0000	18	XXXXXXXXXXXXXXX
145.00	405.00	329.0000	7	XXXXXXX
156.00	620.00R	405.0000	3	XXX
170.80				
190.00				
199.00				
206.00				
210.00				
215.00				
220.00				
220.00				
234.00				
240.00				
246.00				
246.00				
250.00				
250.00				
250.00				
253.00				
257.00				
270.00				
271.00				
274.00				
280.00				
280.00				
285.00				
290.00				
306.00				
308.00				
311.00				
314.00				
315.00				

APPENDIX I: Two-tailed t-Distribution at 0.99 Percentile

DF	T	DF	T	DF	T	DF	T
1	63.657	31	2.7441	61	2.6590	91	2.6310
2	9.9248	32	2.7385	62	2.6576	92	2.6303
3	5.8409	33	2.7333	63	2.6563	93	2.6298
4	4.6041	34	2.7284	64	2.6549	94	2.6292
5	4.0321	35	2.7239	65	2.6537	95	2.6286
6	3.7074	36	2.7195	66	2.6525	96	2.6280
7	3.3995	37	2.7155	67	2.6513	97	2.6275
8	3.3554	38	2.7116	68	2.6501	98	2.6270
9	3.2498	39	2.7079	69	2.6491	99	2.6265
10	3.1693	40	2.7045	70	2.6480	100	2.6260
11	3.1058	41	2.7012	71	2.6470	101	2.6255
12	3.0545	42	2.6981	72	2.6459	102	2.6249
13	3.0123	43	2.6952	73	2.6450	103	2.6245
14	2.9768	44	2.6923	74	2.6440	104	2.6240
15	2.9467	45	2.6896	75	2.6431	105	2.6236
16	2.9208	46	2.6870	76	2.6421	106	2.6231
17	2.8982	47	2.6846	77	2.6413	107	2.6227
18	2.8754	48	2.6822	78	2.6404	108	2.6222
19	2.8609	49	2.6800	79	2.6396	109	2.6218
20	2.8453	50	2.6778	80	2.6388	110	2.6214
21	2.8314	51	2.6758	81	2.6380	111	2.6209
22	2.8188	52	2.6738	82	2.6372	112	2.6205

APPENDIX I: Two-tailed t-Distribution at 0.99 Percentile (Continued)

DF	T	DF	T	DF	T	DF	T
23	2.8073	53	2.6719	83	2.6365	113	2.6201
24	2.7969	54	2.6700	84	2.6357	114	2.6197
25	2.7874	55	2.6683	85	2.6350	115	2.6193
26	2.7787	56	2.6666	86	2.6343	116	2.6190
27	2.7707	57	2.6650	87	2.6336	117	2.6186
28	2.7633	58	2.6633	88	2.6329	118	2.6182
29	2.7564	59	2.6618	89	2.6323	119	2.6179
30	2.7500	60	2.6603	90	2.6316	120	2.6175

TECHNICAL REPORT DATA
(Please read Instructions on the reverse before completing)

1. REPORT NO.	2.	3 RECIPIENT'S ACCESSION NO.
EPA-670/4-75-004a		

4. TITLE AND SUBTITLE	5. REPORT DATE
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	6. PERFORMING ORGANIZATION CODE
7. AUTHOR(S)	8. PERFORMING ORGANIZATION REPORT NO.
Elmo C. Julian	
9. PERFORMING ORGANIZATION NAME AND ADDRESS	10. PROGRAM ELEMENT NO. 1HA327
National Environmental Research Center Office of Research and Development U.S. Environmental Protection Agency Cincinnati, Ohio 45268	ROAP 24AEL; Task 006
	11. CONTRACT/GRANT NO.
12. SPONSORING AGENCY NAME AND ADDRESS	13. TYPE OF REPORT AND PERIOD COVERED
Same as above	14. SPONSORING AGENCY CODE

15. SUPPLEMENTARY NOTES

See Part II, EPA-670/4-75-004b

16. ABSTRACT

A FORTRAN program for IBM 1130 is described by which general statistics on inter-laboratory studies of chemical analytical methods may be obtained. Data screening followed by a statistical t-test for identifying outliers is included. A histogram of data in ascending order is provided.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
FORTRAN, Data, Statistics	Programs, Collaborative test	9B

18. DISTRIBUTION STATEMENT	19. SECURITY CLASS *(This Report)*	21. NO. OF PAGES
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