

EDUCATION/RESEARCH T2

062-5983-01

Data acquisition and statistical analyses are integral parts of research and education. Sixteen programs provide methods and algorithms to aid such endeavors. The individual abstracts describe each program.

Five of the programs must be transferred to their own dedicated tapes. The documentation contains complete instructions for accomplishing the transfers.

Title/ Previous Abstract

3D Function Plot
51/00-5506/0
Digitize and Modify Data
51/00-8033/0
Kaplan-Meier Survival Table Computer-
Plotter
51/00-5701/0

NMR Calculation for a Three Spin System
51/00-5202/0
Optical Ray-Trace
51/00-5404/0
CHROMPLOT
51/00-5204/0
Measurement of Absorption Spectra
51/00-5407/0
Cobalt-60 Calibration Chart
51/00-4001/0
Blood Pressure Evaluation and Patient Data With Statistical Analysis
51/00-4002/0
Timer Calculation For Cobalt-60 Treatment Plans
51/00-4003/0
One Factor Repeated Measures Analysis of Variance
51/00-5703/0
Two Factor Repeated Measures of Independent ANOVA
51/00-5702/0

Scheffe' Multiple Comparison Procedure
51/00-5721/0
Cubic Spline Interpolation
51/00-5504/0
On-Line Spectral Analysis (OLSA)
51/00-5205/0
On-Line Calorimetry Data Acquisition and Analysis (DCAL)
51/00-5206/0

Program 1

Title: **3D Function Plot**

Author: Dony Robert
Brussels, Belgium

Memory Requirement: 8K

Peripherals: Optional 4662 Plotter

Statements: 206

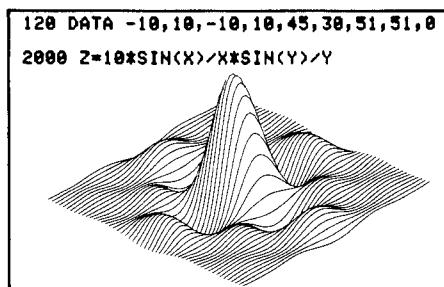
Files: 1 ASCII Program

This program draws a 3D plot of a two-variable mathematical function ($Z=F(X,Y)$), with the hidden lines removed from the plot. The user defines the function and enters real or representative data to obtain the plot. However, the program does not prompt for these inputs; the user simply enters them into the specified lines in the program.

The program provides the option of obtaining uniform scaling so that the plot surface fills the entire screen, which doesn't provide an accurate representation of the function, or obtaining true (rather than uniform) scaling. This option is set by changing a single program line.

The user may also set the following:

- interval on the X and Y axis
- azimuth angle in degrees
- dip angle in degrees
- number of lines on the surface
- number of points on each line
- file number to record the data on tape for later use or faster drawing



Program 2

Title: Digitize and Modify Data

Author: Barry T. Bates
Dept. of Physical Education
University of Oregon
Eugene, OR

Memory Requirement: 16K

Peripherals: Digitizer using GPIB

Statements: 505

Files: 1 ASCII Program

Data Files Required

The program inputs data from a digitizer and writes it to tape. Data may be stored in two forms: A) Two files per data point digitized, first file: IS,N,T1,X1,T2,X2, . . . ; second file: IS,N,T1,Y1,T2,Y2; or B) Single file: IS,N,P,X1,Y1,X2,Y2 . . . Xn,Yn,T1,T2, . . . TN; where T values are absolute time of occurrence or image number input as integer values and X and Y are the coordinates of the data points. Choice A is convenient if data is to be smoothed.

The user indicates the number of data points to be digitized per frame/image and the total number of frames/images is determined by

memory. The data for each frame/image may be digitized once or several times and averaged for storage. In addition the user can input a reference point as the last data point and all values can be shifted so they are identified relative to this point. This references all frames/images to a common coordinate system without reorientation of the coordinate system with each new frame/image. Program is terminated by a time or counter value greater than 99. The data may be corrected during or following digitizing. User-Definable Keys scale, shift, print and graph the data.

Parts of the program may be overlaid to increase memory for data.

CHOOSE WHICH COMBINATION IS REQUIRED
NO OPTIONS ARE AVAILABLE OUTSIDE YOUR SELECTION
1 = DIGITIZE then TO TAPE 2 = FROM TAPE then CORRECT then TO TAPE 3 = FROM TAPE then SHIFT then TO TAPE 4 = FROM TAPE then SCALE then TO TAPE 5 = FROM TAPE then ADJUST FOR REF PT then TO TAPE 6 = FROM TAPE then PRINT/GRAPH
Which number is your choice:

MANIPULATION OF DATA IN COMPUTER

DATA FROM DIGITIZER	= KEY 2
STORE DATA ON TAPE	= KEY 3
CORRECTION OF DATA POINTS	= KEY 4
SHIFT ALL THE DATA POINTS	= KEY 5
SCALE ALL THE DATA POINTS	= KEY 6
ADJUST FOR REFERENCE POINT	= KEY 7
PRINT OR GRAPH THE DATA	= KEY 8
DATA FROM A TAPE FILE	= KEY 9
TO END THIS PROGRAM	= KEY 10
SOURCE OF PROGRAM TAPE: 4851(3D) OR 4924(1) 33	

This program occupies much of the unit's memory. If you will be manipulating a large data base you may elect to swap parts of the program in and out of memory to leave extra space for data. However you will trade off memory for time. Do you want to maximize memory (Y or N): N

Press the appropriate key when ready

If you run into problems in the middle of the program press the break key twice then press key 1 for menu.

1 = MAKE TEXT FROM KEYBOARD OR GET TEXT FROM FILE
2 = LIST LINES OF TEXT
3 = DELETE LINES OF TEXT
4 = INSERT LINES
5 = SHIFT LINES
6 = SEARCH AND REPLACE CHARACTERS
7 = RENUMBER LINES
8 = PRINT OR TAPE
9 = QUIT

WHICH ACTION?

Program 3

Title: Kaplan-Meier Survival Table

Compu-Plotter

Author: Paul W. Baim
Division of Biostatistics
University of Miami
School of Medicine
Miami, FL

Memory Requirement: 24K

Statements: 348

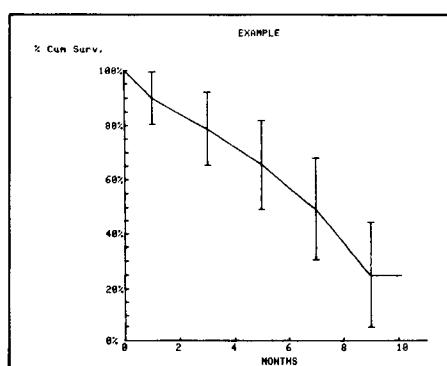
Files: 1 ASCII Program

The survival table is a means of measuring the response or nonresponse of subjects over time. This response may mean improvement of patients receiving a new drug, or failure of light bulbs using a new type of filament; both lend themselves equally well to this type of study.

The program accepts raw data from the keyboard in the form of dates and subject status (minimum of 2 cases, maximum of 85, with 24k). The dates correspond to the beginning and end of the interval during which a particular subject is under study. The subject status indicates whether the subject is still responding at the end of the interval, or has stopped responding; for instance, whether a battery is still producing current after six days time, or has gone dead. The program then converts the raw data into a table of three columns: the interval, the cumulative survival, and the standard error. The interval is the same as that mentioned earlier, the cumulative survival represents the percentage of subjects surviving (i.e. responding) for this particular interval or longer, and the standard error establishes the

reliability of the cumulative survival figure. Next, the program will, on demand, graph the calculated values, with the time intervals on the X axis and the cumulative survival percentages on the Y axis. The standard errors are shown by vertical lines. The purpose of the graph is to show clearly, how subjects are responding. Finally, the program will, on demand, list the data as it was entered.

Limitations: No provision to correct or store data.



Program 4

Title: NMR Calculation for a Three Spin System

Authors: Tom Price, Dr. Jack Reid
Lorillard Div. of Loews
Greensboro, NC

Memory Requirement: 16K

Peripherals: Optional-4641 Printer

Statements: 267

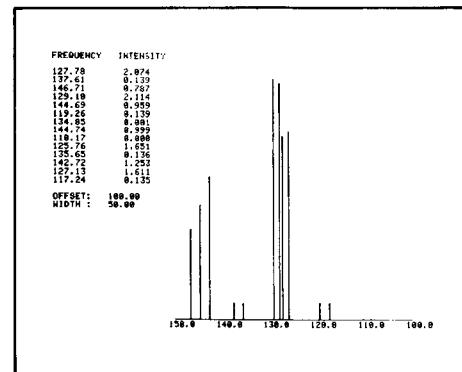
Files: 1 ASCII Program

This program calculates the spin-spin transition frequencies and relative intensities for a three spin Nuclear Magnetic Resonance (NMR) system. The energies of the eight possible energy states are calculated using the chemical shifts, in Hz, and coupling constants in Hz, entered from the keyboard.

In the three spin system there are four possible energy levels. The first and fourth each contain one spin state; however, the second and third each contain three spin states. The energies of these states are used as the diagonals of two 3×3 matrices. The off diagonal elements are calculated from the respective coupling constants. The two

matrices are diagonalized, by the method of Jacobi¹⁰, and the intensities calculated by identical diagonalization operations on an identity matrix. The final transition frequencies are calculated by the difference in the energies between adjacent energy levels.

The output is displayed as either a listing and an NMR line spectrum on the graphic terminal or a listing on the printer.



NMR PATTERN FOR THREE SPIN SYSTEM

CHEMICAL SHIFT FREQ: 125 Hz, 138 Hz, 144.6 Hz
COUPLING CONSTANTS: J1,2= 8.5 J2,3= 1.75 J1,3= 2.25

```
LINE( 1)= 127.78 Hz INT = 28.74
LINE( 2)= 137.61 Hz INT = 1.39
LINE( 3)= 146.71 Hz INT = 7.87
LINE( 4)= 129.18 Hz INT = 21.14
LINE( 5)= 144.61 Hz INT = 9.59
LINE( 6)= 125.76 Hz INT = 0.11
LINE( 7)= 119.26 Hz INT = 0.39
LINE( 8)= 134.85 Hz INT = 0.81
LINE( 9)= 144.74 Hz INT = 9.99
LINE(10)= 118.17 Hz INT = 0.88
LINE(11)= 125.76 Hz INT = 16.31
LINE(12)= 142.72 Hz INT = 12.53
LINE(13)= 142.72 Hz INT = 12.53
LINE(14)= 127.13 Hz INT = 16.11
LINE(15)= 117.24 Hz INT = 1.35
```

Program 5

Title: Optical Ray-Trace

Author: James L. Hutchinson
Dept. of Physics/Astronomy
Vassar College
Poughkeepsie, NY

Memory Requirement: 32K

Peripherals: 4662 Plotter

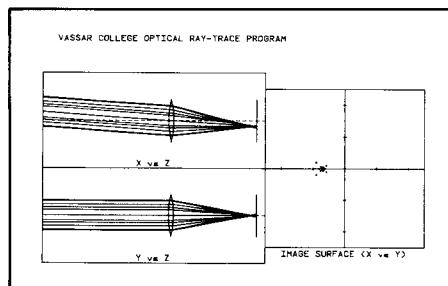
Statements: 555

Files: 1 ASCII Program

The program consists of two parts. The first part calculates the actual three-dimensional paths of light rays through a user-specified system of spherical or planar surfaces, lenses, mirrors or stops. A plot of the system is made in plane and elevation to show the paths of the rays along the Z-axis. Light rays proceed through the system normally from left to right and can be plotted in contrasting colors. The rays are followed until they intersect the image surface or a stop, or until they fail to intercept a subsequent optical surface. Distance units are arbitrary; the program plots the system to scale. A plot of the intersection of the rays with the chosen image surface is also given.

The rays traced through the system can be chosen manually or automatically. In the manual mode, you must separately specify the orientation of each incoming ray. In the automatic mode, rays are chosen from a standard set of 21 rays distributed over four zones of the first optical surface. The end results of the calculations can be saved internally in the program or on tape (manual mode only) to allow further investigation of the structure of the image.

In the second part of the program, you can select different locations of the image surface to see how the presence of aberrations affect the quality of focus of the image.



Program 6

Title: **Chromatographic Data Acquisition and Plotting (CHROMPLOT)**

Author: Leonard H. Ponder
American ENKA Company
Enka, NC

Memory Requirement: 24K/16K

Peripherals: Opt. 1 Data Communications Interface

Statements: 528

Files: 1 ASCII Program

Chromatographic data from an electronic integrator (or digitizer) is recorded on magnetic tape and subsequently plotted on the basis of the original time axis, relative time axis, or molecular size axis. Relative retentions and molecular sizes are calculated automatically. The program is useful in liquid chromatography, gel permeation chromatography, and gas chromatography, or with similar data.

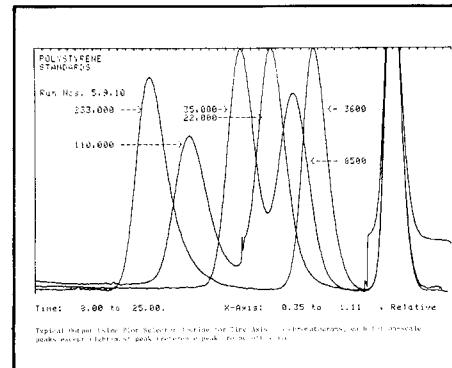
Each chromatogram or selection portion of the chromatogram is scaled to fit the allotted plotting area.

The program is easy to use. Pressing a User-Definable Key activates the desired routine; the routines are shown below. Documentation includes a variable table, flowcharts and detailed instructions.

UDK Function

- | | |
|----|---|
| 1 | Minimum and maximum for entire chromatogram |
| 2 | Scale and plot entire chromatogram |
| 3 | Data to tape |
| 4 | Plot entire chromatogram |
| 5 | Return to BASIC |
| 6 | Change ordinate and abscissa |
| 7 | Plot selector |
| 8 | Label under chromatogram |
| 9 | Read tape |
| 10 | Display-only (terminal mode) |
| 11 | Minimum and maximum, specific interval |
| 12 | Not used |

- | | |
|-------|--------------------------------|
| 13 | Data to tape (no instructions) |
| 14 | Molecular size label |
| 15 | Display molecular size |
| 16 | Print times and min-max |
| 17 | Continue over-plot |
| 18 | Label above chromatogram |
| 19&20 | Not used |



Program 7

Title: **Measurement of Absorption Spectra**

Author: John Rolfe
National Research Council
Ottawa, Canada

Memory Requirement: 16K

Peripherals: 4907 File Manager
GPIB Digital Voltmeter
Hewlett Packard 6940B
Multiprogrammer
300 Baud Printer
Optical Apparatus
Option 1 Data Communications Interface

Statements: 349

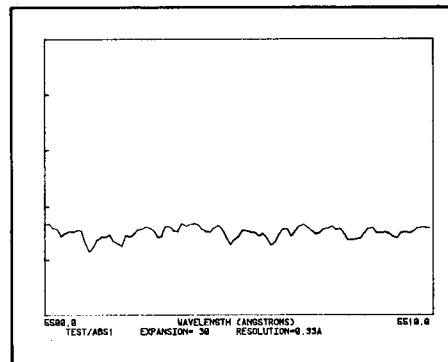
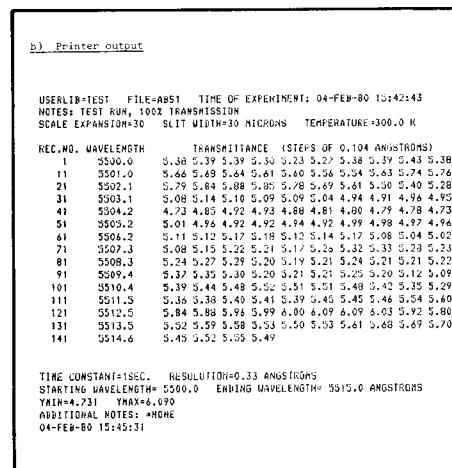
Files: 1 ASCII Program
Requires Data Files

The apparatus controlled by this program measures optical transmittance of a sample as a function of wavelength. Wavelength is varied by a stepping motor on a monochromator. An analog circuit with a voltage output of 0 to +10 volts monitors the transmittance.

The program controls the stepping motor through an HP 6940B with a 59500A GPIB Interface unit. The digital voltmeter used to read transmittance is a Systron-Donner 7344A. Program slews stepping motor to starting wavelength, scans through to ending wavelength in steps separated by time intervals. Step size and time intervals are calculated by the program for optimum information collection based on the monochromator band width (calculated from the slit width) and the time constant of the analog circuit.

The data is printed in tabular form, plotted on the 4050 screen and recorded on the 4907 disc as the run progresses. The main data file is random access binary, each record containing the transmittance. The wavelength is easily calculated from the record number since readings are taken at equal wavelength intervals. At the end of the experiment all parameters are written on a separate header file, a short sequential file which is useful for subsequent data processing.

User-Definable Keys allow for interruption or stopping the run, manual stepping of the monochromator, and some housekeeping functions.



Program 8

Title: Cobalt-60 Calibration Chart

Author: C.S. Narayanan
Lutheran Hospital
Ft. Wayne, IN

Memory Requirement: 8K
Statements: 48
Files: 1 ASCII Program

The program calibrates treatment time for CO-60 Teletherapy units, which are used to treat cancer patients. The CO-60 radioactive source decays (loses its strength) according to its half life. The output of the therapy unit must be calibrated and changed accordingly. This program will give you the output calibration. Enter the present output for various field sizes, and the calibrated output will be displayed. The display can be copied with the 4631 Hard Copy Unit.

ACCL COBALT UNIT, LUTHERAN HOSP., FT. WAYNE, IND.	
CAL PERIOD FROM	TRIMMERS EXTENDED
10-1-78 TO 12-1-78	
FIELD SIZE	OUTPUT
4X 4	98.91
5X 5	98.91
6X 6	98.91
7X 7	98.91
8X 8	98.91
9X 9	98.91
10X10	98.91
11X11	98.91
12X12	98.91
13X13	98.91
14X14	98.91
15X15	98.91
16X16	98.91
17X17	98.91
18X18	98.91
19X19	98.91
20X20	98.91
21X21	98.91
22X22	98.91
23X23	98.91
24X24	98.91
25X25	98.91

WARNING

The recipient of this program is solely responsible for checking the accuracy and appropriateness of this program and procedure.

Program 9

Title: Blood Pressure Evaluation and Patient Data With Statistical Analysis

Memory Requirement: 32K
Peripherals: Optional-4051R05 Binary Loader

Statements: 581
Files: 1 ASCII Program
Requires Data Tape & PLOT 50
Stat 4 Program

Although this program was custom designed for a particular hospital, it serves as a pattern for other medical users. The graphically-aided data entry for blood pressure readings and TcP02 readings is unique. It's user-oriented with all data entry initiated through User-Definable Keys.

The user keys in patient data:

Name
Record Number
Age
PVES #
Sex
Diabetic
Smoker
Standard Blood Pressure

Next a diagram of the lower torso guides blood pressure and TcP02 readings. These readings and the ratio of normal blood pressure to actual are displayed on the screen.

Then the patient's history is keyed in:

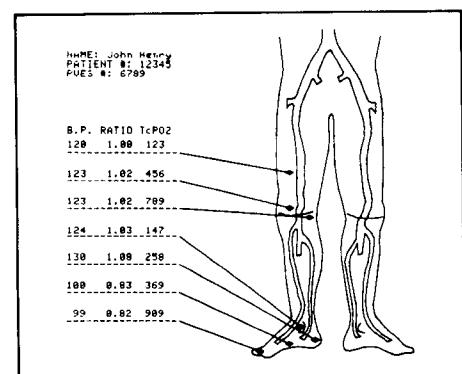
Influencing Drugs
Pertinent Laboratory Data

Operative Procedures
Outcome of Operative Procedures
Doppler Flow
Pre or Post

The program combines all of the data into one string and writes it to a patient data tape. Data for up to 240 patients may reside on one tape. A routine will select two data items from each patient file and write these items to another data tape in a format for use with Statistics Volume 4. In this case, the Linear Regression program analyzed sets of data.

The first file on the patient data tape contains the number of full data files on the tape, and an index into the files by patient record number.

Although no routines for data correction or special searching are provided, with the index already in place, it would be relatively simple to insert.



Program 10

Title: Timer Calculation For Cobalt-60 Treatment Plans

Author: David H. Robinson
St. Mary's Hospital
Waterbury, CT

Memory Requirements: 8K

Peripherals: 4662 Plotter

Statements: 154

Files: 1 ASCII Program

The program allows the user to specify the physical parameters necessary for implementing a completed treatment plan and performs the treatment time calculation for each beam. Data is entered via the keyboard and is then plotted on the treatment plan using the 4662 Plotter.

User Input:

Plan Description

number of beams
normalization number
total tumor dose

Individual Beam Parameters

field width
field length
output (RADS/ MIN at 80 SSD)
wedge angle
wedge factor

wedge orientation
gantry angles
beam weight
tray factor

Isocenter Location

The program calculates the treatment time for each beam. All plan parameters are then plotted on the plan. Space is allocated for the user to place an anatomical drawing and indicate the level(s) at which the patient contour was taken.

WARNING

The recipient of this program is solely responsible for verifying the accuracy and appropriateness of this program for his treatment planning system.

```
ENTER THE NUMBER OF FIELDS IN THIS PLAN: 3
ENTER THE NORMALIZATION NUMBER (I.E. 140): 150
ENTER THE TOTAL TUMOR DOSE AT NORMALIZATION LEVEL (RADS): 200

BEAM # 1:
FIELD WIDTH (CM): 8
FIELD LENGTH (CM): 18
EQUIVALENT SQUARE (CM): 8.9
OUTPUT (RADS/MIN AT 80 SSD): 88.8
WEDGE ANGLE (0=OPEN BEAM): 0
WEDGE FACTOR (0=OPEN BEAM): 0
WEDGE ORIENTATION (0=OPEN BEAM, 1=ANT, 2=POST, 3=LT,
4=RT, 5=SUP, 6=INF): 0
GANTRY ANGLE (START): 0
GANTRY ANGLE (STOP): 0
BEAM WEIGHT (I.E. 100): 100
TRAY FACTOR (I.E. 0.98): 1.00
TREATMENT TIME: 1.65 MINUTES

CHANGE DATA FOR BEAM # 1 ?(Y/N):
```

Program 11

Title: One Factor Repeated Measures Analysis of Variance

Author: Richard M. Engeman
U.S. Fish and Wildlife Service
Denver, CO

Memory Requirements: 16K

Peripherals: Optional—4641 Printer

Statements: 193

Files: 1 ASCII Program

The program calculates the univariate analysis of variance for data from a one factor repeated measures experimental design (see Winer, *Statistical Principles in Experimental Design*, pps 261-308).

Data is input from the keyboard and allows the user to make any necessary corrections. The program then outputs the following:

Analysis of variance table

Subject means

Means for treatment levels

All output, including the raw data, may be printed to the screen or to the 4641 Printer.

User Prompted Input:

Number of treatments

Number of subjects

Each subject's data
Output device (screen or printer)

THE DATA STRUCTURE AND NOTATION ARE AS FOLLOWS

TREATMENT	
SUBJECT	1 2....K
1	x11 x12....x1K
2	x21 x22....x2K
.	.
N	xN1 xN2 xNK

PRESS G & RETURN AND THE SCREEN WILL PAGE AND THE PROGRAM WILL CONTINUE

THIS IS YOUR RAW DATA

30 28 16 34
14 18 18 22
24 28 18 38
38 34 28 44
26 28 14 38

DO YOU WANT THE DATA PRINTED ON ANOTHER DEVICE? Y OR N

SOURCE	DF	SS	MS	F
WITHIN SUBJECT	4	688.898		
BETWEEN SUBJECT	15	811.088		
TREATMENTS	2	698.288	349.144	24.759
RESIDUAL	12	112.800	9.400	
TOTAL	19	1491.888		

PRESS G & RETURN AND THE SCREEN WILL PAGE AND THE PROGRAM WILL CONTINUE

SUBJECT MEANS

SUBJECT 1 27
SUBJECT 2 16
SUBJECT 3 23
SUBJECT 4 34
SUBJECT 5 24.5

PRESS G & RETURN AND THE SCREEN WILL PAGE AND THE MEANS FOR TREATMENT LEVELS WILL PRINT OUT

Program 12

Title: **Two Factor Repeated Measures and Independent ANOVA**

Author: Barry T. Bates
 Dept. of Physical Education
 University of Oregon
 Eugene, OR
 Memory Requirement: 16K
 Peripherals: 4051R05 Binary ROM Pack
 TransEra Auxiliary Memory Manager
 Statements: 744
 Files: 1 ASCII Auto Load
 8 Binary Program
 Requires dedicated tape

This statistical package analyzes two factor repeated measure designs (AxBxS). Data may be input from the keyboard or from tape, and stored on tape. In addition to the summary table, the marginal means of each of the three matrices can be evaluated as well as any of the simple main effects. A final

feature collapses the data into a two-factor independent measures design (AxB) or simply analyzes two-factor independent measures data. All main effects and simple main effects can be evaluated.

The program is separated into eight sections. Although the sections are stored in the Auxiliary Memory Module, they could be called from tape or disc. User-Definable Keys drive the program:

Data from keyboard
 Data from tape
 Data to tape
 Compute
 Matrix Computations
 Summary Table (R)
 Matrix Analysis (R)
 Simple Main Effects (R)
 Main Effects (I)
 Summary Table (I)
 Simple Main Effects (I)

3. INTERNAL DATA STORAGE	
Simple Variables	Used to Store . . .
S	Number of subjects
C	Levels of one factor (conditions)
T	Levels of other factor (trials)
N, K1	Counters
N1	S
CS, CT, CR, R9	Variables used to identify different degrees of freedom
SR, ST, SR9, T9	F-ratio and file number for tape
F	Variables used to calculate partial values for F-ratio
X1, X2, X3, X4	Variables used to identify means for comparisons
Y1, Y2, Y3, Y4	Temporary variable for "S", "C", "T"
Z1, Z2, Z3, Z4	Title of tape file
W1, W2	Temporary string variables
P, Q, R, RS	
IS	
GS, 2S	
Array Variables	Used to Store . . .
A(N1+1,C+1)	New data plus row and column sums
A(1)	Sum of squares for G, S, T
A2(3)	Sum of Squares for CS, CT, ST
A4(1)	Sum of squared scores
B2(S)	Sum of scores for S factors
B3(T)	Sum of scores for T factors
A1(C+1)	Sum of scores for C factors
C1(CS)	Sum of scores for CS factors
C2(CT)	Sum of scores for CT factors
A(N1+1,1)	Sum of scores for ST factors
SI(T)	Sum of squared scores divided by number of scores for C, S, T
SZ(3)	Sum of squared scores divided by number of scores for CS, CT, ST
SG(1)	Sum of squared scores divided by number of scores for CST
SK(1)	Sum of squared scores
M1(S)	Mean for S
M1(C+1,C+1)	Data plus row and column sums for SC matrix
M2(T+1,C+1)	Data plus row and column sums for ST matrix
M3(S+1,T+1)	Data plus row and column sums for CT matrix
M4(P+1,Q+1)	Temporary array for simple main effects analysis

Program 13

Title: **Scheffe' Multiple Comparison Procedure**

Author: Glenn Galfond
 Patuxent Wildlife Research
 Laurel MD
 Memory Requirement: 16K
 Statements: 329
 Files: 2 ASCII Program
 Requires dedicated tape

This performs the Scheffe' multiple comparison procedure to separate linear model parameters in an analysis of variance (see Scheffe', *The Analysis of Variance*, pages 68-72).

File one allows the user to enter from the keyboard and conveniently edit the covariance matrix. The matrix is then stored on tape.

EXAMPLE				
Interval	Cum. Surv.	# Ppl. rem.	Std. Error	
0	1.00	10	0.095	
1	0.769	9	0.134	
2	0.675	5	0.164	
3	0.6563	3	0.188	
4	0.632	1	0.198	
5	0.2461	0	0.198	
6	0.2461	0	0.198	

File two contains the multiple comparison procedure. The user enters the coefficient vector, the desired confidence level, and the file number on which the covariance matrix is stored. The analysis returns the half-length of the confidence interval.

Program 14

Title: **Cubic Spline Interpolation**

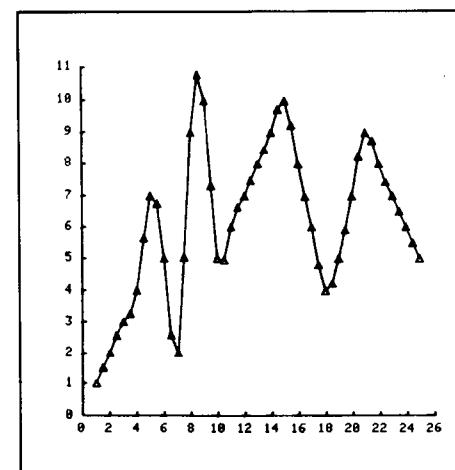
Authors: Monty McGraw
 Jim Yadon
 Memory Requirement: 8K
 Statements: 135
 Files: 2 ASCII Program
 1 Binary Data (example)
 Requires dedicated tape

This program will fit a smooth curve to up to 25 ordered X-Y data pairs (more if more memory) by generating piecewise cubic equations of the form:

$$Y_0 = A_3 X_0^3 + A_2 X_0^2 + A_1 X_0 + A_0$$

The cubic equations allow up to 290 interpolations of Y values and derivatives of the curve between data points. The program allows keyboard or tape entry of the data points and records the interpolated values on tape. The data file structure is compatible with the 4050 System Software X-Y Plot Program.

Limitations: No provision for data correction.



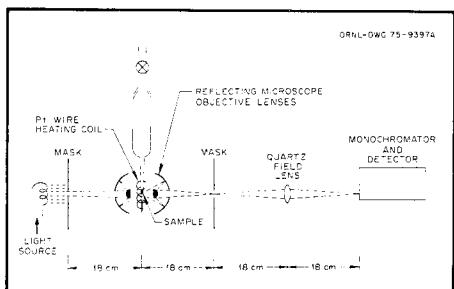
X(1)= 1	Y(1)= 1
X(2)= 1.5	Y(2)= 1.47795950612
X(3)= 2	Y(3)= 2
X(4)= 2.5	Y(4)= 2.56612148164
X(5)= 3	Y(5)= 3
X(6)= 3.5	Y(6)= 3.25755456731
X(7)= 4	Y(7)= 4
X(8)= 4.5	Y(8)= 5.63366024913
X(9)= 5	Y(9)= 7
X(10)= 5.5	Y(10)= 6.75288443614
X(11)= 6	Y(11)= 5
X(12)= 6.5	Y(12)= 5.28512200625
X(13)= 7	Y(13)= 1.99999999996
X(14)= 7.5	Y(14)= 5.83178753864
X(15)= 8	Y(15)= 9.99999999997
X(16)= 8.5	Y(16)= 18
X(17)= 9	Y(17)= 10.00000000001
X(18)= 9.5	Y(18)= 7.316181180548
X(19)= 10	Y(19)= 4.99999999999
X(20)= 10.5	Y(20)= 4.9475477398
X(21)= 11	Y(21)= 5.99999999998
X(22)= 11.5	Y(22)= 6.22663243416
X(23)= 12	Y(23)= 6.5
X(24)= 12.5	Y(24)= 7.4776285886
X(25)= 13	Y(25)= 8.00000000002
X(26)= 13.5	Y(26)= 8.4458180263
X(27)= 14	Y(27)= 8.99999999999
X(28)= 14.5	Y(28)= 9.73913938468
X(29)= 15	Y(29)= 9.99999999997
X(30)= 15.5	Y(30)= 9.22623243416
X(31)= 16	Y(31)= 8.00000000003
X(32)= 16.5	Y(32)= 7.316181180548
X(33)= 17	Y(33)= 6.00000000001
X(34)= 17.5	Y(34)= 4.75684405264
X(35)= 18	Y(35)= 4.00000000002
X(36)= 18.5	Y(36)= 4.49999999999
X(37)= 19	Y(37)= 5.000000000012
X(38)= 19.5	Y(38)= 5.92158438245
X(39)= 20	Y(39)= 7.000000000002
X(40)= 20.5	Y(40)= 6.241569880845
X(41)= 21	Y(41)= 8.95376299997
X(42)= 21.5	Y(42)= 9.36774626113
X(43)= 22	Y(43)= 9.999999999983
X(44)= 22.5	Y(44)= 7.43648541629
X(45)= 23	Y(45)= 6.999999999996
X(46)= 23.5	Y(46)= 6.51732215918
X(47)= 24	Y(47)= 6.0000000000084
X(48)= 24.5	Y(48)= 5.45422394624
X(49)= 25	Y(49)= 5.0000000000081

Program 15

Title: **On-Line Spectral Analysis (OLSA)**

Authors: R.J. Peterson
D.L. Raschella
J.R. Uchida
Dept. of Chemistry
University of Tennessee
Knoxville, TN
Memory Requirement: 32K
Peripherals: DVM
TransEra 641
4662 Plotter
Statements: 1327
Files: 5 ASCII Program
Requires dedicated tape

The program acquires spectrophotometric data from a digital voltmeter on a real-time basis. The data are recorded on magnetic tape and are subsequently analyzed and plotted. The resulting spectra may be displayed in several formats on either the 4050 Screen or the 4662 Plotter. Absorbance is plotted versus wave number and wavelength. Scale expansions and spectrum flattening routines are provided.



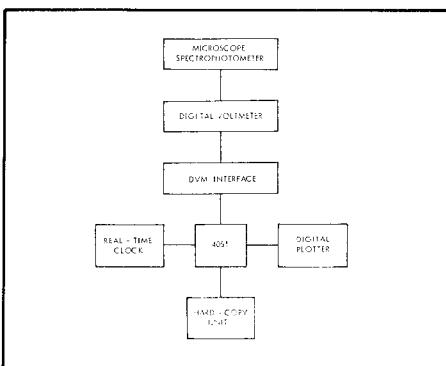
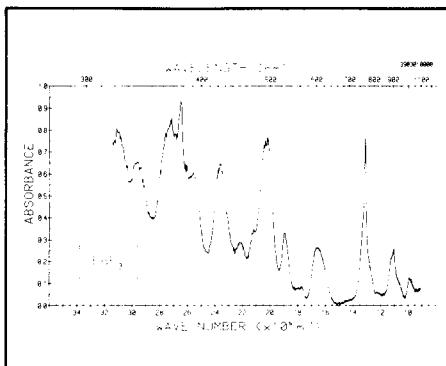
Program 16

Title: **On-Line Calorimetry Data Acquisition and Analysis (DCAL)**

Authors: J.R. Peterson
D.L. Raschella
J.R. Uchida
Dept of Chemistry
University of Tennessee
Knoxville, TN
Memory Requirement: 32K
Peripherals: Digital Voltmeter
Hewlett Packard 3495A
Scanner
TransEra 641
4924 Tape Drive
4662 Plotter
Statements: 1485
Files: 6 ASCII Program
Requires dedicated tape

The program acquires calorimetric data from a digital voltmeter and an HP 3495A Scanner on a real-time basis. Using a thermistor in the microcalorimeter, the changes in temperature are detected as changes in resistance. A Wheatstone bridge is used to measure this resistance change. The change

The program is divided into four segments: input, baseline fit, plotting and display edit routines. At the end of each segment, the operator can initiate the overlaying of the next segment or branching to another segment through the User-Definable Keys.



of resistance is monitored by the bridge detector. The output of the bridge detector and the voltages E_h and E_{std} are input to the 3495A Scanner. The 4050 System commands the scanner to connect the appropriate channel. It then directs the DVM to read the voltage and send it to the 4050 System, where it's stored on tape. The program operates on an interrupt mode, with the operator inputting bridge resistance values and initiating action by depressing appropriate User-Definable Keys. Reading rates may be altered. Experimental data that are collected consist of bridge calibrations, calibration heatings, and the dissolution reaction heat of the sample.

The data analysis/evaluation routine performs drift line extrapolations and all integrations; the results are stored on magnetic tape.

