NBS Technical Note 1238

An Interactive Nonlinear Least Squares Program

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July 1987

U.S. Department of Commerce
Malcolm Baldrige, Secretary

National Bureau of Standards
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Abstract

INVAR is an interactive computer code which uses the Stanford variable-separable nonlinear regression program VARPRO to solve nonlinear (and linear) least squares problems. The variable-separable feature of VARPRO makes it attractive to users with real-world fitting problems because it iterates only on the parameters which appear nonlinearly in the model. Not only does this simplify the iteration, but it also means that the user is not required to supply initial estimates for the parameters which appear linearly.

INVAR implements VARPRO within an environment providing the user with on-line feedback and the opportunity to make changes, transformations, and corrections in real-time. It provides extensive statistical diagnostics and plots of the results. It can provide publication-quality DISSPLA plots either at a graphics terminal during execution or at a hard copy device afterwards. The code is written mostly in standard Fortran with only a few instructions specific to the NBS Cyber 855. With minor changes it can easily be implemented on other computers.

This report is both a tutorial guide for beginners and a reference manual for experienced users who wish to make changes in the code. It contains three completely solved example problems. Three appendices contain information necessary for making changes in the programs.

Contents

Chapter 1

INTRODUCTION

INVAR is an interactive program which solves linear or nonlinear least squares problems. Its main advantage over other least squares programs is that it separates the linear and nonlinear parameters, iterating only on the nonlinear ones. This eliminates the need for initial guesses of the linear parameters, and usually improves the convergence properties for nonlinear problems. INVAR was built around the VARPRO subroutine package written originally by John Bolstad [1] at Stanford University, using an algorithm developed by Golub and Pereyra [7]. So far as we know, VARPRO is the only widely available, variable-separable nonlinear least squares code. Numerical analysts and statiticians have been slow to see the great practical advantages of a variable-separable algorithm, but scientists in other fields, with real world modelling problems, very quickly see the advantage and usually become enthusiatic VARPRO users after their first encounter with the code.

The original VARPRO was not widely used because it was difficult to implement. The user needed a detailed knowledge of FORTRAN in order to write a driver for the program and to alter the subroutine ADA which performed calculations specific to the individual problem. In addition, VARPRO was designed to be run in batch mode, involving much time and effort to change initial estimates of the nonlinear parameters and rerun the program.

J. E. Rall and R. E. Funderlic, who first implemented INVAR [12], greatly enhanced the utility of the original VARPRO routines. They wrote a driver for VARPRO which changed it from a batch to an interactive program. The driver provided greater flexibility to the program, allowing the user to try many different initial estimates all within one terminal session. Instead of altering the subroutine ADA to fit the particular problem, Rall and Funderlic rewrote ADA to call for three very simple subroutines. These subroutines are written by the user and provide all the necessary problem-specific calculations. These subroutines simplified the coding required by the user and allowed users with a minimal knowledge of FORTRAN to use the program with ease.

Other improvements found in the original INVAR include:

- an option allowing the use of numerical derivatives instead of calculating derivatives in closed form,
- extensive statistical diagnostics which can be applied to the results of the least squares fit,
- rudimentary graphics.

With excellent documentation on how to use the program [12], Rall and Funderlic developed VARPRO into a useful tool for solving linear and nonlinear least squares problems.

The present implementation of INVAR has been adapted from Rall and Funderlic's version. The least squares method used by Bolstad and the statistics added by Rall and Funderlic have been left virtually intact. One programming error found in the subroutine STAT has been corrected so that the variable (RMS) (residual mean square) is always assigned a value for later calculations regardless of which statistical tests the user chooses to run.

This version of INVAR has been developed to handle data more efficiently than the original. The program now allows the user many more options for manipulating the data. Among the more important of these options is the ability to transform both the independent and dependent variables before analysis. The user chooses the desired transformation by writing two simple subroutines which transform and back-transform the data.

Another major improvement is in the graphical output available to the user. The program can now be run on graphics terminals, or graphical output can be directed to other special plotting devices or to a conventional line printer. Graphs to be plotted on plotting terminals and hardcopy devices are created using the DISSPLA graphics package. The plots for CRTs and line printers are conventional line printer graphs, printed in a horizontal format or in a vertical format for time series data. The subroutines to create these plots have been adapted from those of the STATLIB library of P. V. Tryon and J. R. Donaldson [13].

This document is intended both as a tutorial guide for users not familiar with INVAR and as a reference manual for experienced users. New users should read the first 5 chapters before attempting to use the code.

Chapters 2 and 3 give the necessary information to write the user supplied subroutines. Chapter 2 deals with writing the model in variable separable form, while Chapter 3 describes the required FORTRAN subroutines in detail.

Chapter 4 gives a brief description of the logic of the INVAR driver program. It should be read by beginning users before trying to execute the program.

Chapters 5, 9 and 10 give examples of real world modelling problems solved with INVAR, including output from actual terminal sessions. The problem in Chapter 5 is simpler than the other two. Chapter 9 describes a time-series modelling problem and Chapter 10 describes a problem with two independent variables.

Chapter 6 describes some Cyber 855 Procedures that can be used to execute INVAR at the National Bureau of Standards and will probably be of interest only to NBS users.

Chapter 7 gives detailed explanations of the prompts and messages that the user will encounter during the execution of INVAR. Most users should be able to get started with INVAR after reading Chapter 5, but might want to refer to Chapter 7 for more details on specific points. Many users will probably also refer quite often to Table 7.1 which summarizes all of the INVAR command codes.

The statistical diagnostics generated by INVAR are described in Chapter 8, which is included for users who are not already familiar with the standard least squares diagnostic plots.

Users who want to change the INVAR programs to meet their own special needs should refer to Appendices A, B and C. Appendix A gives the subroutine hierarchy for the whole package, Appendix B tells how to make several changes that are particularly likely to be desired, and Appendix C defines the variables used in the various subroutines in the package.

The authors would like to acknowledge their indebtedness to the following people whose previous work formed the foundation for this version of INVAR:

- G. H. Golub and V. Pereyra, for their work on the variable separable nonlinear least squares algorithm;

- John Bolstad, for his work on the original batch version of VARPRO;
- J. E. Rall and R. E. Funderlic, for their implementation of the original interactive INVAR program;
- P. V. Tryon and J. R. Donaldson, for the STATLIB line printer plot routines.

Thanks also go to Ron Boisvert for his help and suggestions in writing the NOS Procedures for inplementing INVAR on the Cyber 855, and to David Tate for numerous suggestions to improve the program. Finally, we would like to thank Drs. Robert E. Funderlic, Takashi Kashwagi, and Larry Reed for their careful reviews of this manuscript.

Chapter 2

SOME LEAST SQUARES NOTATION

This chapter is reprinted with slight alterations from [12, pages 5-9].

2.1 An Introduction

It is assumed that the reader is familiar with the method of least squares. The purpose here is to familiarize the reader with the notation that will help with the use of INVAR. For motivation to understand this notation, some readers may immediately want to try to duplicate the simple example in Chapter 4.

2.2 Writing the Model for INVAR

The method of least squares seeks to minimize the sum of the squares of the difference between the observed value and the value predicted by the model equation at each observation point. (The difference is called the residual.) That is, one seeks to minimize the residual sum of squares

$$r_0 = \sum_{i=1}^{m} (y_i - \eta_i)^2 , \tag{2.1}$$

where the y_i are the observed values and the η_i are the predicted values for observations. Each η_i is a function of a vector $\boldsymbol{x}$ of unknown parameters and is evaluated at the observed value t_i of the independent variable t.

Least squares problems fall into the categories of linear or nonlinear depending on how the parameters enter into the model. A model such as

$$\eta(\boldsymbol{x}; t) = x_1 + x_2 t + x_3 t^3 + x_4 e^t \tag{2.2}$$

would be considered linear since the unknown parameters x_i can be written as coefficients of functions which depend only on the independent variable t. Geometrically, the model is linear in the sense that all first order partial derivatives with respect to the unknown parameters are independent of the parameter values, and consequently all higher order derivatives are zero. A model which cannot be written in this form would be considered nonlinear, e.g.,

$$\eta(\boldsymbol{x};t) = x_1 + x_2 e^{-x_3 t} + x_4 \sin(x_5 t) + e^{-x_6 t} . \tag{2.3}$$

In equation (2.3), x_1, x_2 and x_4 appear linearly whereas x_3, x_5 and x_6 appear nonlinearly.

Some recent techniques [7] for solving least squares problems take better advantage of the way the unknown parameters fit into the model. This is done not only by taking advantage of the sum of squares form of the problem but also by considering the models in separable form, i.e., separating the unknown parameters into ones which are linear and ones which are nonlinear. Thus for INVAR, we must write our models in the form

$$\eta(\boldsymbol{c},\boldsymbol{\alpha};t) = c_1\Phi_1(\boldsymbol{\alpha};t) + \cdots + c_n\Phi_n(\boldsymbol{\alpha};t) + \Phi_{n+1}(\boldsymbol{\alpha};t) , \tag{2.4}$$

where the linear parameters c_i are coefficients multiplying the functions Φ_i of the nonlinear parameters $\boldsymbol{\alpha}$ and the independent variables t. The separable form can be used for considering linear problems (no unknown $\boldsymbol{\alpha}$) and strictly nonlinear problems (no unknown $\boldsymbol{c}$) as well as a combination of the two. To emphasize the difference between the unknown linear and nonlinear parameters, example (2.3) would be rewritten as

$$\begin{aligned}\eta(\boldsymbol{c},\boldsymbol{\alpha};t) &= c_1 + c_2 e^{-\alpha_1 t} + c_3 \sin(\alpha_2 t) + e^{-\alpha_3 t} \\ &= c_1\Phi_1(\boldsymbol{\alpha};t) + c_2\Phi_2(\boldsymbol{\alpha};t) + c_3\Phi_3(\boldsymbol{\alpha};t) + \Phi_4(\boldsymbol{\alpha};t) ,\end{aligned}$$

where

$$\begin{aligned}&n = 3 ,\\ &\Phi_1 = 1 ,\\ &\Phi_2 = e^{-\alpha_1 t} ,\\ &\Phi_3 = \sin(\alpha_2 t) ,\\ &\Phi_4 = e^{-\alpha_3 t} .\end{aligned}$$

For this example: To the INVAR question of how many linear parameters are there, the user would respond 3; to how many nonlinear, 3; to which terms depend on nonlinear parameter 1, 2; i.e., Φ_2 depends on α_1. Similarly term 3 depends on nonlinear parameter 2, and 4 on 3. Of course, the user may want to crudely assume $n = 0$ in (2.4) so that

$$\eta = \Phi_1(\boldsymbol{\alpha};t) ,$$

where

$$\Phi_1 = \alpha_1 + \alpha_2 e^{-\alpha_3 t} + \alpha_4 \sin(\alpha_5 t) + e^{-\alpha_6 t} ,$$

and treat all the parameters nonlinearly. In this case INVAR will not be as efficient and the user will have to supply estimates for all the parameters. When the linear and nonlinear parameters are separated, only the latter require estimates.

2.3 Weighted Least Squares

It is often useful to modify the least squares problem by taking into consideration the "goodness" of the observations. Thus instead of (2.1) we will consider

$$r_0 = \sum_{i=1}^{m} W_i^2 (y_i - \eta_i)^2 \ , \tag{2.5}$$

where W_i is a positive weight assigned to the ith observation (e.g., $W_i = 1/\sigma_i$, where σ_i is the standard deviation of the uncertainty in y_i). According to the notation here the FORTRAN array $WEIGHT(I)$ is W_i^2. The user should note that in the output table that gives the weighted residual, the quantity

$$W_i(y_i - \eta_i) = (WEIGHT(I) **1/2) * (Y(I) - ETA(I))$$

is printed (cf. the sample problems in Chapters 4 and 7).

It has been the authors' experience that there is considerable confusion as to what a weight is. It is our hope that distinguishing between W and $WEIGHT$ will decrease this confusion. (We changed the name of W to $WEIGHT$ in several places in the coding to accomplish this consistency.)

Linear least squares problems are often written in the following form: Find $\boldsymbol{x}$ such that

$$r_0 = \min_{\boldsymbol{x} \in \mathcal{R}^n} \{ \| \boldsymbol{A}\boldsymbol{x} - \boldsymbol{y} \| \} \ , \tag{2.6}$$

where $\boldsymbol{A}$ is the $m \times n$ matrix of the functions of the independent variables (i.e., the coefficients of the unknown parameters) at each point, $\boldsymbol{x}$ is the n-vector of unknown parameters, $\boldsymbol{y}$ is the m-vector of observed values, and $\| \cdots \|$ is the Euclidean norm. Thus to put (2.5) in the notation of (2.6) the problem is to minimize $\| \boldsymbol{W}(\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b}) \|$ over all $\boldsymbol{x}$ in $\mathcal{R}^n$, where

$$\boldsymbol{W} = \boldsymbol{diag}(W_1, W_2, \ldots, W_m) \ .$$

Chapter 3

THE USER SUPPLIED SUBROUTINES

3.1 General Information

In order to use INVAR the user must supply at least one very simple Fortran subroutine, called CALC, which computes the functions Φ and η:

CALC a subroutine which, for a given data point (t_i, y_i) and the current values of the nonlinear parameters α, computes the functions Φ and η.

Four additional optional subroutines can also be supplied. These four subroutines are:

DERIV a subroutine for calculating the partial derivatives of the Φ with respect to the nonlinear paramenters α,

WT a subroutine for calculating or otherwise specifying the weights W_i used to define the weighted sum of squared residuals [cf., Equation (2.5)],

TRANS a subroutine for making mathematical transformations on the data before making the fit,

BAKTRN a subroutine used in conjuction with TRANS to back-transform the fit obtained.

These four can be dummy routines if the user so chooses, but it is necessary to create one file containing all five subroutines. After the subroutines are written, they must be compiled, and loaded with the rest of the INVAR program.

All of the subroutines except for CALC are optional. However, any subroutine not used in the problem must be present in the user's element as a dummy subroutine. A dummy subroutine consists of the statement SUBROUTINE (along with the required name and argument list), followed by the statements RETURN and END. For examples of the subroutines see Chapters 5, 9 and 10.

3.2 Subroutine CALC

The subroutine CALC calculates the predicted value of the dependent variable for each observation. To write CALC the user must first write the model of the problem in separable form (cf. Chapter 2). The vectors ALF and C contain the values for the nonlinear parameters and linear parameters, respectively. The array T contains the values of the independent variables, where T(K,J) is the Jth independent variable at the Kth observation. The variable K is passed into CALC as a parameter, while J must be specified in the subroutine. The arguments NL, N, MMAX and IV are all used to dimension the arrays in the subroutine. NL is the number of nonlinear parameters, N is the number of linear parameters, MMAX is the leading dimension of the T array and IV is the number of independent variables.

The first four statements in CALC must be written as follows:

```
SUBROUTINE CALC (K,NL,N,MMAX,IV,C,ALF,T,ETA)

PARAMETER (MAXN1=11)

DIMENSION C(N), ALF(NL), T(MMAX,IV)

COMMON /BLKPH/ PH(MAXN1)  .
```

Next, the separate functions Φ of the model are assigned to the vector PH. All PH(I) which are independent of the nonlinear parameters ALF must appear first, followed by the remaining PH(I). If the moded contains a function Φ_{n+1} which does not have a linear coefficient, then the corresponding value PHI(N+1) should be be final element in the array. Following the calculation of the separate functions, their linear combination, ETA, should be assigned a value. The general format of this statement is

```
ETA = C(1)*PH(1) + C(2)*PH(2) + ... + C(N)*PH(N) + PH(N+1)
```

See Chapter 2 for instructions on how to construct this equation.

3.3 Subroutine DERIV

The subroutine DERIV need be written only when some or all of the partial derivatives of the PH functions are to be calculated in closed form. If all derivatives are to be calculated numerically, a dummy subroutine is sufficient. DERIV assigns the partial derivatives to the array DPH, where DPH(I,J) is the partial derivative of the Ith function PH(I) with respect to the Jth nonlinear parameter ALF(J).

The first eight statements must be written as follows:

```
      SUBROUTINE DERIV (K,T,MMAX,IV,ALF,NL,NP1)

      PARAMETER (MAXN1=11, MAXKG=8)

      DIMENSION T(MMAX,IV), ALF(NL)

      COMMON /BLKDPH/ DPH(MAXN1,MAXKG)

      DO 10 J=1,NL

         DO 10 I=1,NP1

            DPH(I,J) = 0.0

10    CONTINUE .
```

The DO loop serves to initialize all the partial derivatives to zero, and is not necessary when using a dummy routine. Parameters K, MMAX, IV, and

NL are the same as in subroutine CALC, and NP1 = N + 1. The remaining statements depend upon the specific problem, but each derivative the user wishes to calculate in closed form must be assigned a value here.

3.4 Subroutine WT

The subroutine WT, also optional, calculates the weights for the problem. If the user does not wish to calculate weights, a dummy subroutine must still be provided. In this case, weights can still be entered with the data points, or an equal weighting (WEIGHT(I) = 1) will be assumed. In WT, the vector Y contains all the observed values of the dependent variable. WT should assign the weighting values to the vector WEIGHT.

The first two statements of WT must be written as follows:

```
SUBROUTINE WT (M,WEIGHT,Y)

DIMENSION WEIGHT(M), Y(M) .
```

The remaining statements may be written by the user to suit the individual problem, but a weight must be assigned for each of the M observations of Y.

3.5 Subroutine TRANS

If the user wants to transform the independent and/or the dependent variables before the fit, the subroutine TRANS must be written. Otherwise, a dummy subroutine will suffice. The T array and the Y vector contain the independent and the dependent variables, respectively. On entering TRANS, these arrays contain the original data, and on exiting TRANS, they contain the transformed data.

The first two statements must be written as follows:

```
SUBROUTINE TRANS (T,BT,Y,BY,IV,M,MMAX)

DIMENSION T(MMAX,IV), BT(MMAX,IV), Y(M), BY(M) .
```

TRANS should not only transform variables but should also retain their original values (the "back-transformed" values) in array BT for the independent variable and vector BY for the dependent variable. Therefore, the user must include DO loops containing the statements

```
BT(I,J) = T(I,J)

BY(I) = Y(I)
```

before the values are transformed. Even if only one of the variables is to be transformed, the user must always assign these "back-transformed" values to both variables. The user then transforms the variables as desired, assigning the transformed values to the original T array and Y vector.

3.6 Subroutine BAKTRN

The subroutine BAKTRN must also be written if transformed values are desired. Otherwise, BAKTRN need only be a dummy subroutine. If data has been transformed, the predicted values in vector ETA are calculated in CALC using the transformed data. INVAR plots the observed and predicted values twice, once as transformed data, and once as back-transformed data. Therefore, ETA must be back-transformed in order to be plotted with the original values of the dependent variable. BAKTRN performs this back-transformation of ETA, placing the new values in the vector BETA.

The first two statements must be written as follows:

```
SUBROUTINE BAKTRN (ETA,BETA,M)

DIMENSION ETA(M), BETA(M) .
```

The remainder of the subroutine is written by the user to do the required back-transformation of ETA. ETA must be backtransformed by exactly the inverse method used to transform the vector Y in the subroutine TRANS.

Chapter 4

THE LOGIC OF THE INVAR DRIVER PROGRAM

No attempt is made here to describe the program package in detail. Anyone interested in these details is referred to Rall and Funderlic's documentation on INVAR [12]. However, a general understanding of how the program works is desirable to ensure efficient use of INVAR.

The program's driver is divided into two sections. The first of these sections is the Initialization Segment which asks for the data and initial values needed to run the least squares program. These values include the number of data points, linear and nonlinear parameters and independent variables, along with the data itself (independent and dependent variables and weights) and initial estimates for the nonlinear parameters. Also the program must be told which terms in the model depend on each of the nonlinear parameters, and it must be given increments for the numerical derivatives if the latter are used.

The second section of the driver is the Command Segment which contains the bulk of the program. The user enters into this segment at the Command Point when the program cues "**NEXT STEP?**". There are four types of steps which can be taken: (1) print current values of the data or turn on/off printing flags; (2) change the current parameter estimates, transform the data, or add/delete data points; (3) run the least squares program or the statistical analysis; and (4) save the current data in a file and/or exit the program.

All of these steps terminate by returning to the Command Point, except for those steps which exit the program. It is this looping in the Command Segment that makes INVAR such a flexible program. The user can run the least squares program as many times as desired in one execution of INVAR, each time changing various values and running statistical analyses, in order to find the best fit.

An extremely abbreviated flowchart depicting INVAR's driver is given in Figure 4.1. Except for the data initialization, all actions of INVAR are initiated by typing in a command code at the Command Point. Table 7.1 gives a list of all the command codes which may be chosen by the user at the Command Point. The same table is available interactively during execution of the program by typing "H" at the Command Point and, after the program's response, entering "A".

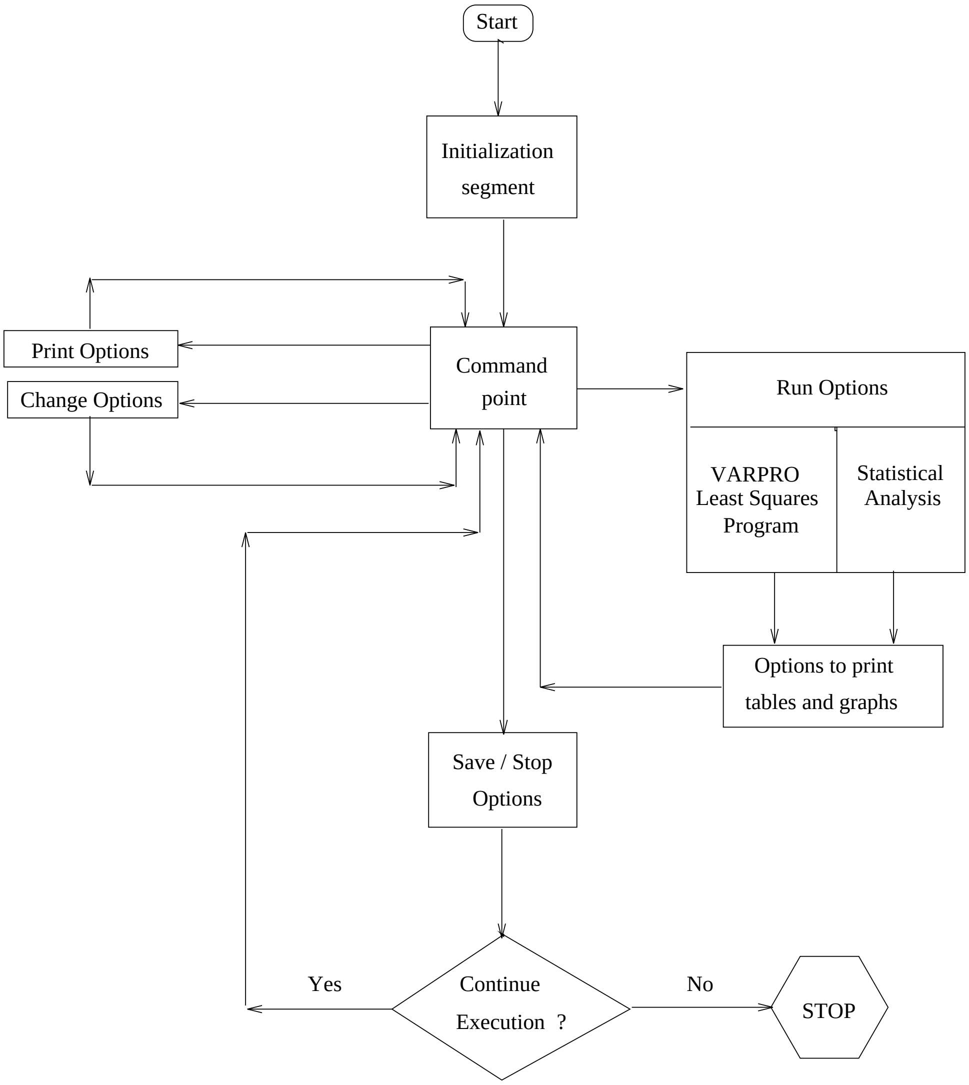


Figure 4.1: Abbreviated flowchart of the INVAR driver program

Chapter 5

EXAMPLE 1 – LIGHT CURVE OF A SUPERNOVA

5.1 The Model and the Data

Type I supernovae have been found to follow a specific pattern of luminosity. The latter part of this pattern may be described by the model

$$y(t) = C_1 \exp(-\frac{t}{\alpha_1}) + C_2 \exp(-\frac{t}{\alpha_2}) ,$$

where t is the time (in days) after maximum luminosity and y is the relative luminosity (relative to max. luminosity). In terms of the notation discussed in Chapter 2, this model is written as

$$\eta(C_1, C_2, \alpha_1, \alpha_2; t) = C_1 \Phi_1(\alpha_1; t) + C_2 \Phi_2(\alpha_2; t) ,$$

where

$$\Phi_1(\alpha_1; t) = \exp(-\tfrac{t}{\alpha_1}) ,$$

$$\Phi_2(\alpha_2; t) = \exp(-\tfrac{t}{\alpha_2}) .$$

The model above will be fitted to data collected in 1939 for the type I supernova SN1939A. The data are given in Table 5.1. The peak luminosity occurred at day 0.0, but all measurements taken before day 7.0 will not be used here since the above model cannot account for the luminosity before and immediately after the peak. These data were written, as two columns

Table 5.1: Luminosity of SN1939A (Relative to Peak Luminosity)

Day	Luminosity	Day	Luminosity	Day	Luminosity
7.0	0.6310	19.0	0.1318	57.0	0.05754
7.0	0.8318	20.9	0.1585	85.0	0.03631
14.8	0.2754	25.8	0.1096	109.0	0.02291
16.0	0.1445	26.8	0.1445	110.0	0.02291
16.9	0.2089	28.0	0.09120	141.0	0.01738
17.0	0.1585	53.0	0.06310	142.0	0.01585
18.8	0.1585	54.0	0.06918	168.0	0.009120

of numbers, into a file named SNDATA which will be used in the following as an input file for the INVAR program.

5.2 The User-Supplied Subroutines

The user-supplied subroutines reqired to make the fit are given in the following paragraph. These subroutines were all written into a single file, called SNCALC, in accordance with the directions given in Chapter 3. Subroutine CALC uses the values of PH and ETA obtained from writing the model in separable form. In this example, there is only one independent variable, t = time (days). DERIV calculates the derivatives from the closed form expressions

$$\begin{aligned} \frac{\partial\Phi_1}{\partial\alpha_1} &= \left(\frac{t}{\alpha_1^2}\right)\exp(-\frac{t}{\alpha_1}) \quad , \quad \frac{\partial\Phi_1}{\partial\alpha_2} = 0 \; , \\ \frac{\partial\Phi_2}{\partial\alpha_1} &= 0 \quad , \quad \frac{\partial\Phi_2}{\partial\alpha_2} = \left(\frac{t}{\alpha_2^2}\right)\exp(-\frac{t}{\alpha_2}) \; , \end{aligned}$$

assigning non-zero values only to DPH(1,1) and DPH(2,2) since PH(1) depends only on ALF(1) and PH(2) depends only on ALF(2). Subroutine WT assigns a weighting of $1/y_i^2$ to each data point (t_i, y_i) in order to assure that the observations make roughly equal contributions to the determination of the fitting parameters. This is a very common procedure when the y-values span several orders of magnitude.

The subroutines for this example are:

```
C
```

```
C
      SUBROUTINE CALC ( K, NL, N, MMAX, IV, C, ALF, T, ETA )
C
C
      PARAMETER ( MAXN1 = 11 )
C
      DIMENSION C(N), ALF(NL), T(MMAX,IV)
C
      COMMON /BLKPH/ PH(MAXN1)
C
      PH(1) = EXP(-T(K,1) / ALF(1))
      PH(2) = EXP(-T(K,1) / ALF(2))
C
      ETA = C(1)*PH(1) + C(2)*PH(2)
C
      RETURN
      END
C
C
C--------------------------------------------------------------
C
C
      SUBROUTINE DERIV ( K, T, MMAX, IV, ALF, NL, NP1 )
C
C
      PARAMETER ( MAXN1 = 11 , MAXKG = 8 )
C
      DIMENSION ALF(NL),T(MMAX,IV)
C
      COMMON /BLKDPH/ DPH(MAXN1,MAXKG)
C
      DO 10 J=1,NL
        DO 10 I=1,NP1
          DPH(I,J) = 0.0
   10 CONTINUE
C
C           DPH(I,J) SHOULD BE SET TO THE PARTIAL DERIVATIVE
C                    OF PH(I) WITH RESPECT TO ALF(J)
C
```

```
      DPH(1,1) = T(K,1) / (ALF(1)**2) * EXP(-T(K,1)/ALF(1))
      DPH(2,2) = T(K,1) / (ALF(2)**2) * EXP(-T(K,1)/ALF(2))
C
      RETURN
      END
C
C
C---------------------------------------------------------------
C
C
      SUBROUTINE WT ( M, WEIGHT, Y )
C
C
      DIMENSION Y(M),WEIGHT(M)
C
       DO 10 I=1,M
         WEIGHT(I) = 1.0/Y(I)**2
   10  CONTINUE
C
      RETURN
      END
C
C
C---------------------------------------------------------------
C
C
      SUBROUTINE TRANS ( T, BT, Y, BY, IV, M, MMAX )
C
C
      DIMENSION T(MMAX,IV), BT(MMAX,IV), Y(M), BY(M)
C
C--------- DUMMY SUBROUTINE
C
      RETURN
      END
C
C
C---------------------------------------------------------------
C
```

```
      SUBROUTINE BAKTRN ( ETA, BETA, M )
C
      DIMENSION ETA(M), BETA(M)
C
C--------- DUMMY SUBROUTINE
C
      RETURN
      END        .
```

No transformations of the data are required so the subroutines TRANS and BAKTRN are dummy subroutines.

The above subroutines were written into a file named SNCALC which was compiled and loaded with the INVAR programs and then executed in a terminal session to be described in the following sections.

5.3 Input-Output Options

There are basically three options for inputting data to INVAR:

1. Type all of the data, including the observations (t_i, y_i), into the program during execution,
2. Type in only the specifications for the Φ functions and their derivatives with respect to the α parameters, but read the observations (t_i, y_i) from a data file,
3. Read all of the specifications and the observations from a file that was previously written by the INVAR program.

Initially, one of the first two options must be used, but once this has been done, INVAR allows the user to save the resulting data set in a special "VARPRO defined" file so that the final option can be used in subsequent runs with the same data set. This third option reduces the amount of typing for the user. The second option was used in the terminal session described in the next section.

Because INVAR is an interactive program the basic output file is the user's terminal, but the program also provides the option of writing all the results to a file (unit 10) which is saved for later processing. If the user exercises this option he can obtain a hard copy of his results on the printer of his choice.

There are actually two versions of INVAR: INVAR2 which uses the DISSPLA plotting package and INVAR1 which provides only line-printer graphs of the results. INVAR2 also provides line printer graphs in case the program crashes and the DISSPLA plots are lost. If INVAR2 is chosen, the user has two ways to get the graphs. If he is running on a Tektronics graphical terminal he can receive the graphs interactively during execution of the program. In this case the program uses `CALL PTEKAL` to initialize the DISSPLA plotting package. The other option is to write the plots to a file which will be plotted on a QMS laser printer after the terminal session has been completed. In this case the program uses `CALL TK4014` and `CALL HWSPEC` to initialize DISSPLA. Users can easily change the program to accomodate other plotting devices. Instructions for making the required changes are given in Appendix B.

5.4 The Terminal Session

The sample terminal session output that follows was obtained by executing INVAR2 on the NBS CYBER 855. It illustrates only some of the options available in INVAR. (For a more comprehensive example, see Chapter 9.) The program was run from a Tektronics plotting terminal, using the option of interactive DISSPLA plots and requesting line printer output as well as the normal terminal output. Before reading this example, the following points should be noted:

1. The first 17 non-blank lines have nothing to do with the INVAR program. They were generated by the NOS procedures used to initialize execution on the NBS Cyber 855. The first line generated by INVAR is the command "`ENTER TITLE (MAXIMUM OF 40 CHARACTERS):`".

2. The question mark at the beginning of each line immediately following an INVAR request for information is the Cyber 855 prompt to remind the user to type in something.

3. Prompts requiring a yes or no response were answered with a "Y" for yes and a "N" for no, although any character other than "Y" will be interpreted as no.

4. The four queries immediately following the choice of "`PLOTS SHOWN INTERACTIVELY ON A PLOTTING SCREEN`" were issued by the Tectronics software called by the DISSPLA initialization "`CALL PTEKAL`".

5. The 21 observations (t_i, y_i) were read from the file SNDATA.

6. The program requires initial estimates for all of the nonlinear parameters. The initial estimates used for α_1 and α_2 were 5 and 60 days, respectively.

7. When the model and the data have been specified, INVAR prints the prompt "`NEXT STEP? (TYPE "H" FOR HELP)`" and waits for the user to type in a command code for one of several possible tasks. When such a task has been completed, INVAR will again print the above prompt for the next task. A complete list of the possible tasks and their command codes is given in Table 7.1. The present example used the command codes "RV", for running the VARPRO least squares programs, "RS", for running a statistical analysis of the results, and "S0", to stop without saving the input data in a VARPRO defined file.

8. The Tektronics software clears the screen before making each plot and then the program stops awaiting a response from the user. The Cyber 855 prints a question mark in the upper left corner of the screen to indicate that some response is expected. In the present example, we responded with a "C" followed by a carriage return because a carriage return by itself is interpreted by the 855 as an end of file, causing the program to crash.

9. When using interactive Tektronics plotting, it is a good idea for the user to clear the screen after each plot since otherwise new INVAR prompts or results may be written over the preceding plot.

Chapters 6 and 7 give more detailed explanations of the prompts and responses. The reader may find it useful to refer to them while reading the following sample terminal session.

```
/INVOKE,INVAR


 INTERACTIVE NONLINEAR LEAST SQUARES PROGRAM


        PROC,INVARX,CALCF[,QMSADDR][,DATAF][,INV102].

  Executes one of two versions, INVAR1 or INVAR2, of INVAR, an
  interactive, variable separable, nonlinear least squares program.
```

```
   Local file CALCF contains FORTRAN coded, user-supplied subroutines.

   Hardcopy output and plots can be sent to QMS laser printer with
   address QMSADDR.

   Permanent file DATAF contains data to be fit (not needed if data
   already in a local file, or is to be typed in during exection).

   Version to be executed specified by parameter INV1O2.  Default is
   INVAR2 which does DISSPLA plots.  INVAR1 does not use DISSPLA.

 PARAMETERS FOR INVARX ARE  CALCF, QMSADDR, DATAF, INV1O2
 Enter CALCF  FORTRAN file of user-supplied subroutines? SNCALC

 Enter QMSADDR  QMS Address for output (Default = NONE)? B225

 Enter DATAF  Data file (Default = NONE)? SNDATA

 Enter INV1O2  INVAR1 or INVAR2 (Default = INVAR2)?

 ENTER TITLE (MAXIMUM OF 40 CHARACTERS):
? LIGHT CURVE FOR SN1939A

 DO YOU WANT DISSPLA PLOTS? (TYPE "Y" FOR YES)
? Y

 DO YOU WANT THESE PLOTS SHOWN INTERACTIVELY ON
 A PLOTTING SCREEN (TYPE "1");
 OR SAVED IN A FILE TO BE PRINTED OUT LATER (TYPE "2")?
? 1

 ENTER DESIRED MODEL
? 4014

 ENTER LINESPEED (CHARACTERS PER SECOND)
? 960

 ENTER RESOLUTION MODE (0=LOW)
? 1

 ENTER OPTION (0=DEF,31=8 PENS ON 4662,36=PAPER FEED ON 4663)
? 0

 ENTER LABEL FOR INDEPENDENT VARIABLE 1 (MAX. OF 47 CHARACTERS):
? DAY

 ENTER LABEL FOR DEPENDENT VARIABLE (MAX. OF 47 CHARACTERS):
```

```
? RELATIVE LUMINOSITY

 DO YOU WANT LINE PRINTER OUTPUT?
? Y

 ARE YOUR DATA, WEIGHTS, INITIAL VALUES, ETC.
                ALREADY IN A VARPRO-DEFINED FILE ?
? N

 NO. OF DATA POINTS:
? 21

 NO. OF LINEAR PARAMETERS:
? 2

 NO. OF NONLINEAR PARAMETERS:
? 2

 NO. OF INDEPENDENT VARIABLES:
? 1

 ARE DATA IN A FILE?
? Y

 WHAT IS THE FILENAME?--NO MORE THAN 26 CHARS

      (TYPE "QUIT" TO EXIT)
? SNDATA

 ARE WEIGHTS TO BE CALCULATED IN SUBROUTINE WT?
? Y


 DO DEPENDENT OR INDEPENDENT VARIABLES
 NEED TO BE TRANSFORMED BEFORE ANALYSIS?
? N


 INITIAL VALUES OF NONLINEAR PARAMETERS
   1
? 5.0

   2
? 60.0

 HOW MANY TERMS OF THE MODEL DEPEND ON NONLINEAR PARAMETER  1:
? 1
```

```
 WHICH TERMS ARE THEY?
? 1

 HOW MANY TERMS OF THE MODEL DEPEND ON NONLINEAR PARAMETER  2:
? 1

 WHICH TERMS ARE THEY?
? 2

 ALL DERIVATIVES IN CLOSED FORM?
? Y


 WOULD YOU LIKE TO SAVE THE DATA JUST INPUT?
? N


 DOES DATA FOLLOW AN EVENLY SPACED TIME SERIES?
? N



   NOTE:   THE COMMAND "SC" WILL SAVE YOUR DATA FILE AT ANY TIME

 NEXT STEP? (TYPE "H" FOR HELP)
? RV


 DO YOU WISH TO CHANGE ANY DEFAULTS IN THE LEAST SQUARES PROGRAM?
        (50: MAX. NO. OF ITERATIONS)
        (1.0E-5: CONVERG. TOLERANCE)
        (1: OUTPUT PRINTING INDEX)
? N

1                    LIGHT CURVE FOR SUPERNOVA 1939A



    0  WEIGHTED NORM OF RESIDUAL =   6.7995272E-01
     NU =   .1000000E+01


   ITERATION   1    NONLINEAR PARAMETERS

    4.5931719E+00         6.0532666E+01
```

```
 1  WEIGHTED NORM OF RESIDUAL =   6.4835577E-01
  NU =   .5000000E+00
  NORM(DELTA-ALF) / NORM(ALF) =   1.104E-02


ITERATION   2    NONLINEAR PARAMETERS

 4.2715541E+00          6.0017367E+01

 1  WEIGHTED NORM OF RESIDUAL =   6.3826557E-01
  NU =   .2500000E+00
  NORM(DELTA-ALF) / NORM(ALF) =   1.010E-02


ITERATION   3    NONLINEAR PARAMETERS

 4.1469268E+00          5.9472842E+01

 1  WEIGHTED NORM OF RESIDUAL =   6.3711532E-01
  NU =   .1250000E+00
  NORM(DELTA-ALF) / NORM(ALF) =   9.370E-03


ITERATION   4    NONLINEAR PARAMETERS

 4.1228519E+00          5.9353197E+01

 1  WEIGHTED NORM OF RESIDUAL =   6.3707619E-01
  NU =   .6250000E-01
  NORM(DELTA-ALF) / NORM(ALF) =   2.051E-03


ITERATION   5    NONLINEAR PARAMETERS

 4.1202209E+00          5.9339858E+01

 1  WEIGHTED NORM OF RESIDUAL =   6.3707574E-01
  NU =   .3125000E-01
  NORM(DELTA-ALF) / NORM(ALF) =   2.286E-04


ITERATION   6    NONLINEAR PARAMETERS

 4.1199966E+00          5.9338726E+01

 1  WEIGHTED NORM OF RESIDUAL =   6.3707573E-01
  NU =   .1562500E-01
```

```
    NORM(DELTA-ALF) / NORM(ALF) =   1.941E-05


  ITERATION   7    NONLINEAR PARAMETERS

   4.1199788E+00          5.9338638E+01

   1  WEIGHTED NORM OF RESIDUAL =   6.3707573E-01
    NU =   .7812500E-02
    NORM(DELTA-ALF) / NORM(ALF) =   1.517E-06

 ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,

  LINEAR PARAMETERS

  .3069174E+01   .1586064E+00

  NONLINEAR PARAMETERS

  .4119979E+01   .5933864E+02

  WEIGHTED NORM OF RESIDUAL =   .6370757E+00

  WEIGHTED ESTIMATED VARIANCE =   .2387444E-01

 ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,
 INDICATE WHICH OF THE FOLLOWING SHOULD BE PRINTED
 BY TYPING "Y":
  TABLE OF OBSERVED & PREDICTED VALUES, WTD RESIDUAL:
? Y

  COVARIANCE MATRIX:
? Y

  CORRELATION MATRIX:
? Y


1                COVARIANCE MATRIX


 ROW      COLUMN    1     COLUMN    2     COLUMN    3     COLUMN    4

   1      9.156764E-01   7.485032E-03  -5.032086E-01  -1.393200E+00
   2      7.485032E-03   2.775185E-04  -6.579036E-03  -5.516856E-02
   3     -5.032086E-01  -6.579036E-03   3.362799E-01   1.235154E+00
   4     -1.393200E+00  -5.516856E-02   1.235154E+00   1.371202E+01
```

1

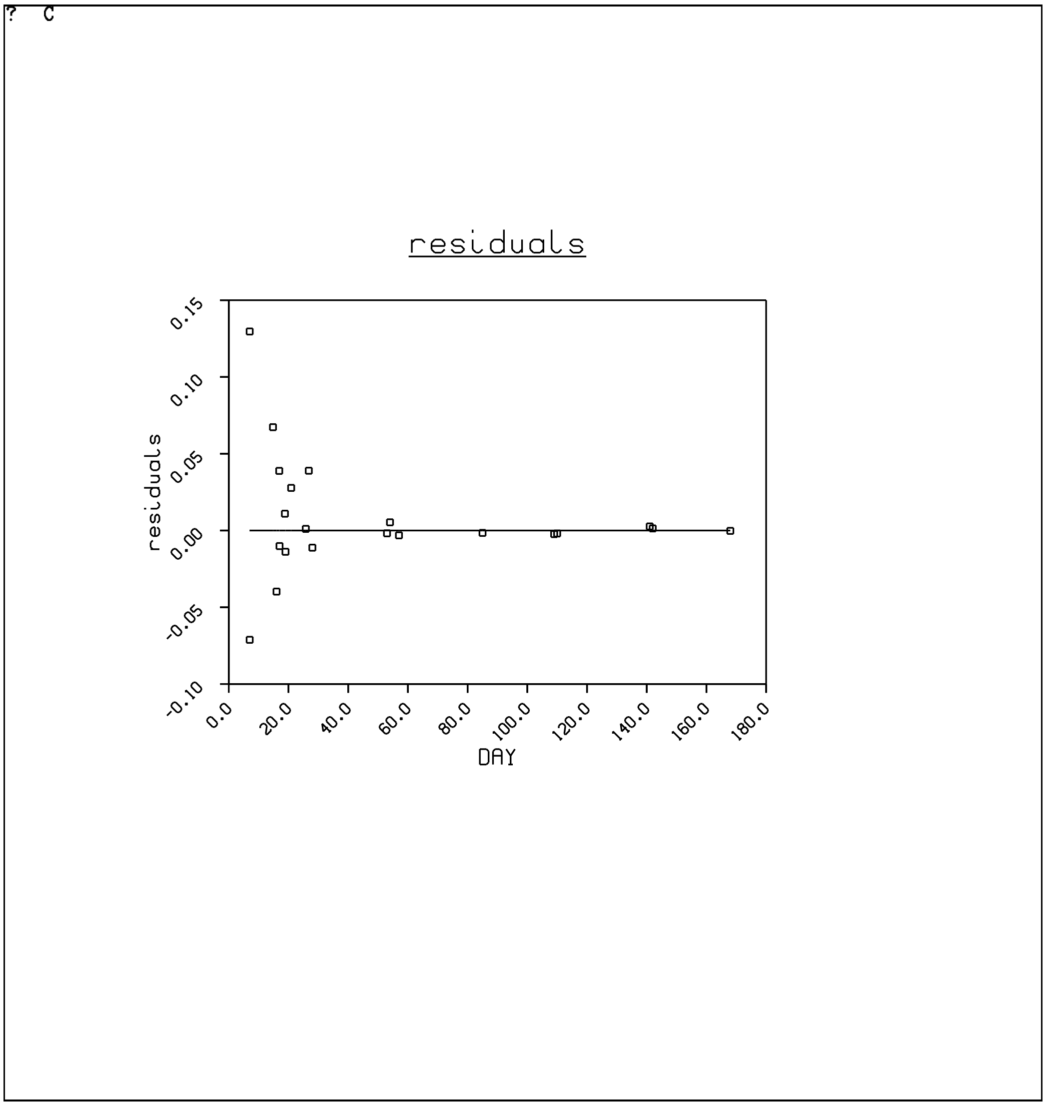
INDEX	IND VAR 1	OBS VAL	PRED VAL	WTD RESID	WEIGHTS
1	7.00000E+00	6.31000E-01	7.02185E-01	-1.12813E-01	2.51155E+00
2	7.00000E+00	8.31800E-01	7.02185E-01	1.55825E-01	1.44531E+00
3	1.48000E+01	2.75400E-01	2.08109E-01	2.44341E-01	1.31848E+01
4	1.60000E+01	1.44500E-01	1.84279E-01	-2.75288E-01	4.78921E+01
5	1.69000E+01	2.08900E-01	1.70062E-01	1.85916E-01	2.29152E+01
6	1.70000E+01	1.58500E-01	1.68644E-01	-6.39993E-02	3.98054E+01
7	1.88000E+01	1.58500E-01	1.47548E-01	6.91004E-02	3.98054E+01
8	1.90000E+01	1.31800E-01	1.45642E-01	-1.05023E-01	5.75664E+01
9	2.09000E+01	1.58500E-01	1.30748E-01	1.75093E-01	3.98054E+01
10	2.58000E+01	1.09600E-01	1.08535E-01	9.71850E-03	8.32490E+01
11	2.68000E+01	1.44500E-01	1.05557E-01	2.69498E-01	4.78921E+01
12	2.80000E+01	9.12000E-02	1.02376E-01	-1.22543E-01	1.20229E+02
13	5.30000E+01	6.31000E-02	6.49339E-02	-2.90630E-02	2.51155E+02
14	5.40000E+01	6.91800E-02	6.38472E-02	7.70863E-02	2.08948E+02
15	5.70000E+01	5.75400E-02	6.06966E-02	-5.48584E-02	3.02037E+02
16	8.50000E+01	3.63100E-02	3.78628E-02	-4.27655E-02	7.58486E+02
17	1.09000E+02	2.29100E-02	2.52673E-02	-1.02894E-01	1.90524E+03
18	1.10000E+02	2.29100E-02	2.48451E-02	-8.44634E-02	1.90524E+03
19	1.41000E+02	1.73800E-02	1.47351E-02	1.52180E-01	3.31055E+03
20	1.42000E+02	1.58500E-02	1.44889E-02	8.58754E-02	3.98054E+03
21	1.68000E+02	9.12000E-03	9.34852E-03	-2.50570E-02	1.20229E+04

1

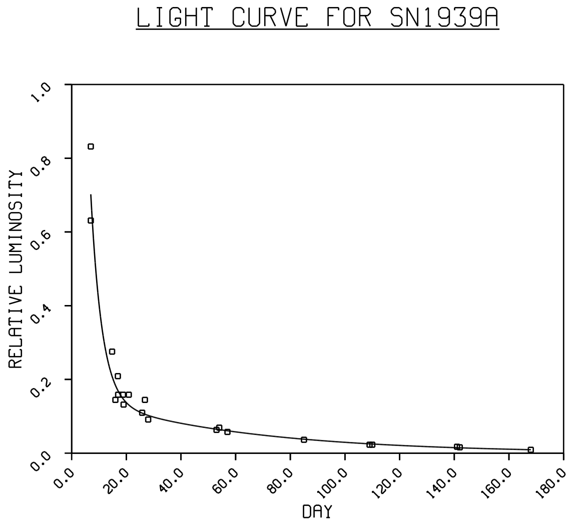
CORRELATION MATRIX

ROW	COLUMN 1	COLUMN 2	COLUMN 3	COLUMN 4
1	1.000000E+00	4.695444E-01	-9.068314E-01	-3.931802E-01
2	4.695444E-01	1.000000E+00	-6.810293E-01	-8.943241E-01
3	-9.068314E-01	-6.810293E-01	1.000000E+00	5.752013E-01
4	-3.931802E-01	-8.943241E-01	5.752013E-01	1.000000E+00

```
 PLOT ROUTINE CURRENTLY SET NOT TO DO ANY PLOTS.
 DO YOU WANT TO START PLOTTING?
? Y

 IF YOU WANT TO PLOT RESIDUALS, TYPE "1"
 IF YOU WANT TO PLOT OBSERVED & PREDICTED VALUES, TYPE "2"
 IF YOU WANT TO PLOT BOTH, TYPE "3":
? 3
```


? C
residuals
residuals
DAY
0.15
0.10
0.05
0.00
-0.05
-0.10
0.0
20.0
40.0
60.0
80.0
100.0
120.0
140.0
160.0
180.0

? C


LIGHT CURVE FOR SN1939A
RELATIVE LUMINOSITY
0.0
0.2
0.4
0.6
0.8
1.0
0.0
20.0
40.0
60.0
80.0
100.0
120.0
140.0
160.0
180.0
DAY

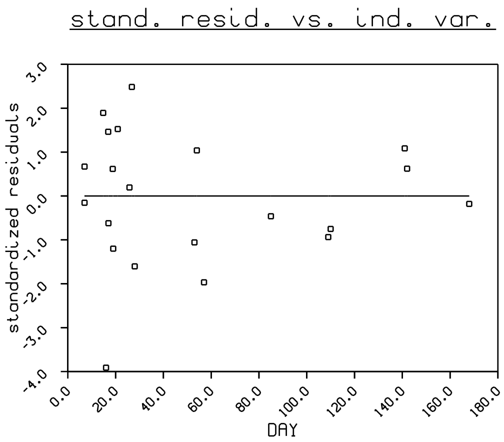
```
 NEXT STEP? (TYPE "H" FOR HELP)
? RS

 INDICATE WHICH OF THE FOLLOWING SHOULD BE PRINTED:
   PARAMETERS, THEIR STD DEV & T-RATIO:
? Y

   RES SUM OF SQS, RES MEAN SQ, RES STD DEV &
       COEFF OF DETERMINATION:
? Y

   TABLE OF OBS, PRED VAL, RESID & STD RESID:
? Y

   PLOT OF STD RES VS IND VAR:
? Y

   PLOT OF STD RES VS PRED VAL:
? Y

   NORMAL PROBABILITY PLOT:
? Y

1
    PARAMETER      S.D. OF PARM.     T-RATIO

     3.069174E+00    9.569098E-01    3.207380E+00
     1.586064E-01    1.665889E-02    9.520828E+00
     4.119979E+00    5.798965E-01    7.104680E+00
     5.933864E+01    3.702975E+00    1.602459E+01


 WTD RESIDUAL SUM OF SQUARES:      4.058655E-01

 WTD RESIDUAL MEAN SQUARE:         2.387444E-02

 WTD RESIDUAL STANDARD ERROR:      1.545136E-01


 COEFFICIENT OF DETERMINATION (R-SQUARE):     9.673397E-01


1
```

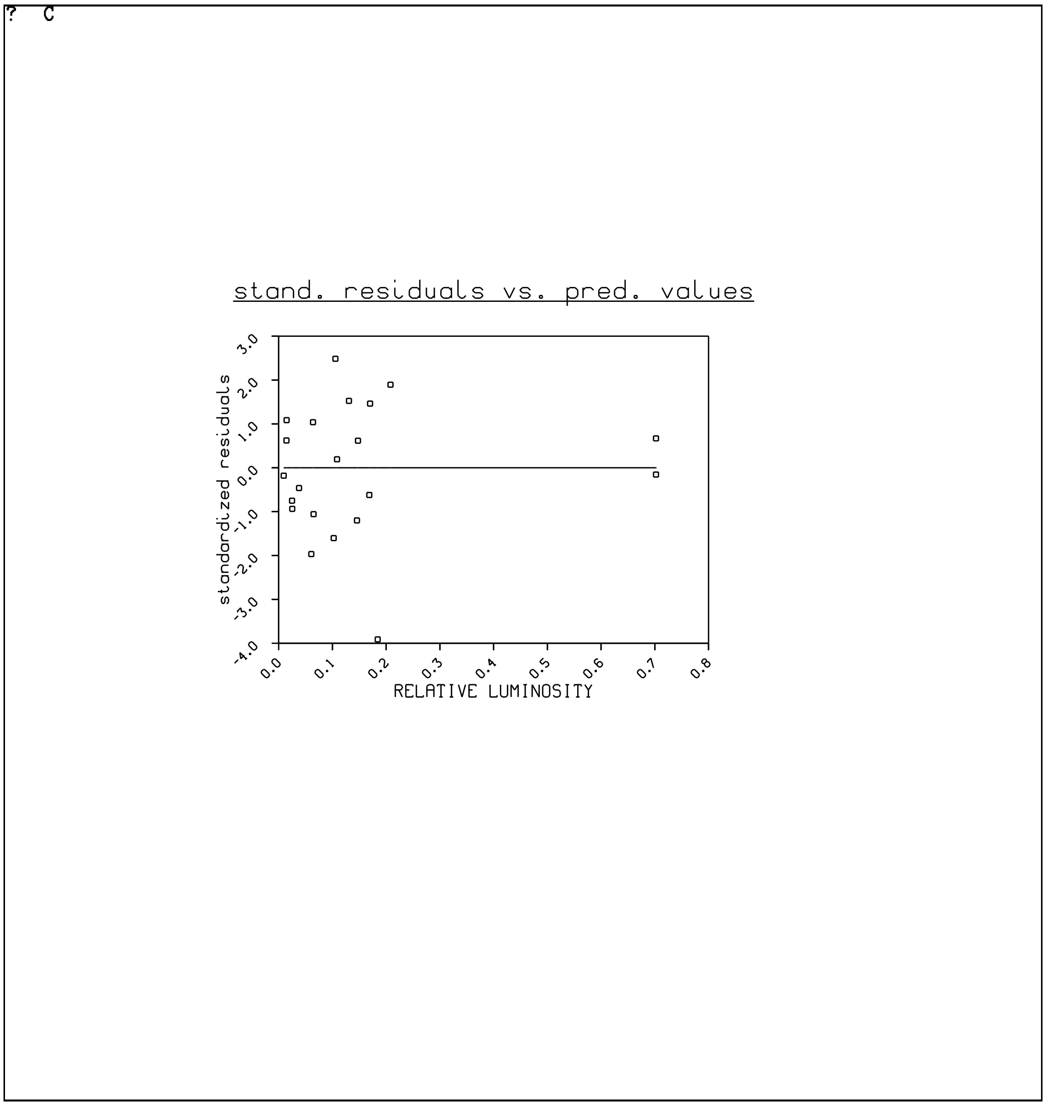
INDEX	IND VAR 1	OBS VAL	PRED VAL	RESID	STD RES
1	7.00000E+00	6.31000E-01	7.02185E-01	-7.11847E-02	-1.54296E-01
2	7.00000E+00	8.31800E-01	7.02185E-01	1.29615E-01	6.69810E-01
3	1.48000E+01	2.75400E-01	2.08109E-01	6.72915E-02	1.89306E+00
4	1.60000E+01	1.44500E-01	1.84279E-01	-3.97792E-02	-3.91233E+00
5	1.69000E+01	2.08900E-01	1.70062E-01	3.88379E-02	1.46276E+00
6	1.70000E+01	1.58500E-01	1.68644E-01	-1.01439E-02	-6.20178E-01
7	1.88000E+01	1.58500E-01	1.47548E-01	1.09524E-02	6.16663E-01
8	1.90000E+01	1.31800E-01	1.45642E-01	-1.38421E-02	-1.20026E+00
9	2.09000E+01	1.58500E-01	1.30748E-01	2.77522E-02	1.52520E+00
10	2.58000E+01	1.09600E-01	1.08535E-01	1.06515E-03	1.94168E-01
11	2.68000E+01	1.44500E-01	1.05557E-01	3.89425E-02	2.48441E+00
12	2.80000E+01	9.12000E-02	1.02376E-01	-1.11759E-02	-1.60334E+00
13	5.30000E+01	6.31000E-02	6.49339E-02	-1.83388E-03	-1.05740E+00
14	5.40000E+01	6.91800E-02	6.38472E-02	5.33283E-03	1.03859E+00
15	5.70000E+01	5.75400E-02	6.06966E-02	-3.15655E-03	-1.96701E+00
16	8.50000E+01	3.63100E-02	3.78628E-02	-1.55282E-03	-4.61768E-01
17	1.09000E+02	2.29100E-02	2.52673E-02	-2.35730E-03	-9.36326E-01
18	1.10000E+02	2.29100E-02	2.48451E-02	-1.93506E-03	-7.51009E-01
19	1.41000E+02	1.73800E-02	1.47351E-02	2.64488E-03	1.08520E+00
20	1.42000E+02	1.58500E-02	1.44889E-02	1.36112E-03	6.22178E-01
21	1.68000E+02	9.12000E-03	9.34852E-03	-2.28520E-04	-1.80473E-01

ENTER ANY INTEGER TO CONTINUE

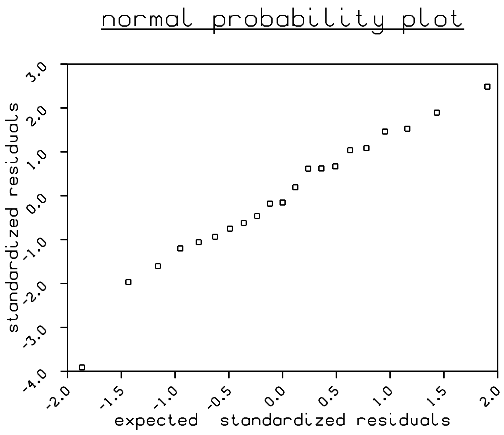
? 1

? C


stand. resid. vs. ind. var.
standardized residuals
3.0
2.0
1.0
0.0
-1.0
-2.0
-3.0
-4.0
0.0
20.0
40.0
60.0
80.0
100.0
120.0
140.0
160.0
180.0
DAY


? C
stand. residuals vs. pred. values
standardized residuals
3.0
2.0
1.0
0.0
-1.0
-2.0
-3.0
-4.0
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
RELATIVE LUMINOSITY

? C


normal probability plot
standardized residuals
expected standardized residuals
3.0
2.0
1.0
0.0
-1.0
-2.0
-3.0
-4.0
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1.0
1.5
2.0

```
 NEXT STEP? (TYPE "H" FOR HELP)
? S0

END OF DISSPLA 9.0 -- 5447 VECTORS IN 5 PLOTS.
RUN ON 4/13/87 USING SERIAL NUMBER 0 AT NBS/CS**2 -
GAITHERSBURG, MD.
PROPRIETARY SOFTWARE PRODUCT OF ISSCO, SAN DIEGO, CA.
2870 VIRTUAL STORAGE REFERENCES; 4 READS; 0 WRITES.


  PROCESSING FILE - ZZLPOUT  PLEASE WAIT . .


EXIT.
/
```

Note that after the user typed in the command code "S0" the INVAR program was terminated. The next five line were written by the DISSPLA programs and the line beginning with "PROCESSING FILE" was written by the QMS procedure for printing the user's hard copy output.

Chapter 6

RUNNING INVAR AT THE NATIONAL BUREAU OF STANDARDS

6.1 The INVOKE,INVAR Procedure on the Cyber 855

Users at the National Bureau of Standards can run INVAR on the Cyber 855 simply by typing in the command

```
INVOKE,INVAR.
```

This initiates an interactive NOS procedure called INVARX which asks the user to provide one required and three optional pieces of information.

The required information is the name of the file containing the user-supplied subroutines CALC, DERIV, WT, TRANS, and BAKTRN (see Chapter 3). If this is not already a local file, INVARX assumes that it is a permanent file and attempts to GET it for the user. When loading the INVAR object code with the user-supplied subroutines, the INVOKE procedure attaches the CMLIB, IMSL and NAG libraries. Thus the user is free to call any routine in these libraries from his own subroutines.

The three optional pieces of information requested by INVARX are:

1. <u>The address of a QMS laser printer</u> for printing the optional hardcopy (line-printer) output and the optional DISSPLA plots. If an address is

specified, the user will always receive cross-referenced Fortran compilation listings of the user-supplied subroutines. The INVAR program will also ask if he wants hardcopy output, and, if the reply is affirmative, the INVAR output will follow the compilation listings. Some users may wish to delay the decision about whether to get hardcopy output until after the terminal session has been completed. Others may wish to receive hardcopy on some printer other than a QMS printer. Such users should not specify a QMS address to the INVARX procedure, but should answer the INVAR query in the affirmative. When the program execution is completed, they will receive the message

```
YOUR HARDCOPY OUTPUT IS IN FILE  ZZLPOUT  .
```

They can then either discard the local file ZZLPOUT or send it to the printer of their choice. Note, however, if the user exercises the DISSPLA plotting option (see below) for QMS plots, he must specify a QMS address.

2. <u>The name of the file containing the observational data</u>. If the data file is already a local file, there is no need to specify anything here. When the INVAR program asks for the name of the data file the user simply types it in. If the data are in a permanent file but not in a local file, the user should type the permanent file name so that the INVARX procedure can GET it for him. The INVAR program will still ask for the data file name, and the user must type it in again. Recall that there are two kinds of data files that might be used (see Chapter 5).

3. <u>The version of INVAR to use</u>. There are two versions of INVAR available to the user. INVAR1 does not have the option of producing DISSPLA graphics while INVAR2 does have that option. If neither version is specified, INVAR2 is taken as the default. If INVAR2 is used, there are two ways to receive the DISSPLA plots: on a Tektronics graphical terminal, or as QMS laser printer plots. If the latter option is chosen a QMS printer address must be specified as described above.

For an example of the use of the INVOKE,INVAR procedure while in line mode (eg., on a Tektronics terminal) see the sample terminal session given in Chapter 5. For a example of its use in screen mode see the sample terminal session in Chapter 9.

6.2 Other Ways to Run INVAR

Many NBS users may not be satisfied with the options provided by the INVOKE procedure or by the INVAR program, and others may not want to run on the Cyber 855.

The INVAR source code can be obtained by any 855 user by typing

$$\texttt{GET,SOURCE/UN} = \texttt{INVAR} .$$

The file SOURCE contains two records: INVAR1 and INVAR2. Instructions for altering these codes are given in Appendix B. Possible alterations include:

1. Changing the DISSPLA plotting device nominations,
2. Changing the maximum number of observations,
3. Changing the maximum number of independent variables,
4. Changing the maximum number of linear and/or nonlinear parameters,
5. Changing the iteration specification parameters.

Users who are satisfied with the INVAR codes and are content to run on the 855, but do not like the INVOKE procedure, can write their own procedures to use one of the object code files

$$\texttt{OBJECT1/UN} = \texttt{INVAR} \quad \textit{or} \quad \texttt{OBJECT2/UN} = \texttt{INVAR} \;,$$

which contain INVAR1 and INVAR2.

Users who want develop their own procedures by altering the ones used by INVOKE,INVAR can get the latter from

$$\texttt{INVARX/UN} = \texttt{INVAR} \quad \textit{and} \quad \texttt{IOPROCS/UN} = \texttt{INVAR} \;.$$

Chapter 7

PROMPTS, OPTIONS AND DIAGNOSTIC MESSAGES

7.1 General Information

The following list, which will continue through several sections, contains prompts that INVAR may give during a terminal session. Following each prompt (which is written in upper case letters) is an explanation of the option and the various ways in which the user can respond. The prompts are listed in roughly the same order in which they will be encountered, but INVAR follows many possible paths of logic and the route taken depends on how the user answers these prompts. Not all prompts will always be given in one terminal session.

7.2 Data Initialization Prompts

1) **ENTER TITLE: (MAXIMUM OF 40 CHARACTERS)** The user enters a title for the problem (up to 40 characters long). This title becomes the heading for each run of the least squares program and the title for the DISSPLA graph of observed and predicted values (if the DISSPLA plotting option is chosen). If INVAR1 is being run, the program advances to prompt **6**). INVAR2 advances to prompt **2**). (Chapter 6 explains the difference between INVAR1 and INVAR2.)

2) **DO YOU WANT DISSPLA PLOTS? (TYPE "Y" FOR YES)** If the answer is not "Y", the program advances to prompt **6**).

3) **DO YOU WANT THESE PLOTS SHOWN INTERACTIVELY ON A PLOTTING SCREEN (TYPE "1"); OR SAVED IN A FILE TO BE PRINTED OUT LATER (TYPE "2")?** If the answer is "1", DISSPLA queries the user about terminal model number, linespeed, resolution mode, etc. (The user should refer to the DISSPLA documentation [3] for the correct answers to these questions.) DISSPLA plots will now appear on the terminal instead of line printer plots. If the answer is "2", line printer plots (the default) will be displayed on the terminal, and DISSPLA plots will be saved in the local file ZZZPLOT for later access.

4) **ENTER LABEL FOR INDEPENDENT VARIABLE 1 (MAX. OF 47 CHARACTERS):** If the model has only one independent variable, the user enters a label for that variable to be used in DISSPLA plots (up to 47 characters). If the problem has more than one independent variable, the user enters the label for the first one, and an opportunity to enter labels for the others will occur later (see prompt **26**)).

5) **ENTER LABEL FOR DEPENDENT VARIABLE (MAX. OF 47 CHARACTERS):** The user enters a label for the dependent variable to be used in DISSPLA plots (up to 47 characters).

6) **DO YOU WANT LINE PRINTER OUTPUT?** If the answer is "Y", the program writes hardcopy output to a local file named LPOUT which is assigned to unit 10. This output includes line printer graphs of the plots requested, as well as iteration details, tables of results and all other information requested by the user.

7) **ARE YOUR DATA, WEIGHTS, INITIAL VALUES, ETC. ALREADY IN A VARPRO-DEFINED FILE?** In any session the user may save the data, weights and initial values in a file (see prompt **21**)). If such a file has been written during a previous session, the user may enter "Y" and that file will provide the data, weights and initial values for this session. The user is asked to enter the name of the file (maximum of 26 characters) and is given the option to have these initial values printed. The program then advances to prompt

21). If no such file exists, the user should respond with a "N" and the subroutine will continue with prompt **8**).

8) **NO. OF DATA POINTS:** The user enters the number of observations (maximum of 300).

9) **NO. OF LINEAR PARAMETERS:** The user enters the number of linear parameters (maximum of 10).

10) **NO. OF NONLINEAR PARAMETERS:** The user enters the number of nonlinear parameters (maximum of 8).

11) **NO. OF INDEPENDENT VARIABLES:** The user enters the number of independent variables per observation (maximum of 6).

12) **ARE DATA IN A FILE?** The data can be read in from a file containing one line per observation. Each line should contain the values of the independent variables (max. of 6) followed by the corresponding value of the dependent variable. If the user answers "Y" to this prompt, the program asks for the name of the file (max. of 26 characters), and, upon receiving it, reads the data into the program. The program then skips to prompt **14**).

13a) **ARE WEIGHTS TO BE ENTERED WITH DATA?** This prompt is issued only in the user responded negatively to the one in prompt **12**). Such a response means that he must type in the data from the terminal. For each observation he must type in the values of the independent and dependent variables. He is also given the option of typing in the weight to be associated with each observation. If the answer to this prompt is "Y", weights will be entered by the user.

13b) **DATA POINTS: LIST INDEPENDENT VARIABLES AND DEPENDENT VARIABLE (AND WEIGHTS), SEPARATED BY BLANKS OR COMMAS** An index number is printed for each point. The user types in all the necessary values for each observation. Values are accepted in free format with or without decimal points or exponents (e.g., 100, 100.1 or 1.001E+02 are all valid).

14) **ARE WEIGHTS TO BE CALCULATED IN SUBROUTINE WT?** If the answer is "Y", the user must have previously written the subroutine WT to calculate the weights. If the answer is not "Y", all weights are set to 1.0 (equal weighting).

15) **DO DEPENDENT OR INDEPENDENT VARIABLES NEED TO BE TRANSFORMED BEFORE ANALYSIS?** If the answer is "Y", the user must have previously written the subroutines TRANS and BAKTRN to do the desired transformation and back-transformation (cf. Chapter 3). (Please note: If data is transformed, all subsequent tables and graphs will contain the transformed values, unless specifically stated otherwise.)

16) **INITIAL VALUES OF NONLINEAR PARAMETERS** An index number appears for each nonlinear parameter. The user enters the initial estimate of that parameter.

17) **HOW MANY TERMS OF THE MODEL DEPEND ON NONLINEAR PARAMETER j:** This prompt is repeated for each of the nonlinear parameters α_j. A term depends on a nonlinear parameter if that parameter is contained in the formula that defines the term. The user enters the number of dependent terms. The program then queries "**WHICH TERMS ARE THEY?**". The user enters the index numbers of all the dependent terms for that parameter, separated by blanks or commas.

18) **ALL DERIVATIVES IN CLOSED FORM?** If the answer is "Y", the user must have previously written the subroutine DERIV to calculate the derivatives. The program then advances to prompt **21)**. If the answer is not "Y", numerical derivatives must be specified (prompts **19)** and **20)**).

19) **ALL NUMERICAL DERIVATIVE INCREMENTS THE SAME?** IF the answer is "Y", the user is asked to enter the increment value and the program advances to prompt **21)**.

20) **NUMERICAL DERIVATIVE INCREMENTS** An index number appears for each increment value. The increments are ordered by nonlinear parameter and then by term of the model. For example, if terms 1 and 2 depend on nolinear parameter 1, and terms 2 and 3 depend on nonlinear parameter 2, then the increments would be ordered DPH(1,1), DPH(2,1), DPH(2,2) and finally DPH(3,2). (The first subscript corresponds to term and the second to parameter.) Any single derivative may still be calculated in closed form in subroutine DERIV by setting that increment value equal to zero.

21) WOULD YOU LIKE TO SAVE THE DATA JUST INPUT? If the answer is "Y", the user enters a file name (maximum of 26 characters) for a local file into which the data just specified are read. After the INVAR session is completed, the user can store this file as a permanent file which can then be used in any subsequent session to automatically read in the data, weights and initial values (cf. prompt **7**)). If the user chose to transform the data (prompt **15**)), then this file will contain transformed, not original, values.

22) DOES DATA FOLLOW AN EVENLY SPACED TIMES SERIES? If the answer is "Y", all line printer graphs containing the independent variable as the X axis will be printed as vertical plots. DISSPLA graphs containing the independent variable as the X axis will have a longer X axis than the other DISSPLA graphs in this case.

7.3 The Command Point

23) NEXT STEP (TYPE "H" FOR HELP) This is the command point where the user must decide what is to be done next. A list of all the options is given in Table 7.1. Entering an "H" at the command point will produce the following message:

```
THE COMMAND CODES FALL INTO FOUR MAIN CATEGORIES

    PRINT-  TO EXAMINE CURRENT VALUES OF INITIALIZED DATA
    CHANGE- TO CORRECT ANY INITIALIZED VALUE, TRANSFORM
            DATA, AND EITHER ADD OR DELETE DATA POINTS
    RUN-    TO RUN THE LEAST SQUARES PROGRAM TO FIND THE
            OPTIMAL PARAMETERS, OR TO RUN A STATISTICAL
            ANALYSIS OF THE DATA RETURNED
    SAVE/   TO SAVE CURRENT DATA OR
    STOP-   TO STOP THE PROGRAM, WITH OR WITHOUT
            SAVING THE INITIALIZED DATA.

TYPE "P","C","R", OR "S" FOR THE SPECIFIC COMMANDS IN
THE ABOVE CATEGORIES.   TYPE "A" TO OBTAIN A LISTING OF
ALL COMMAND CODES.
```

Bascially the options fall into four categories:

Table 7.1: The INVAR command codes

```
COMMAND CODES FOR PRINTING
    PM    PRINT THE NO. OF DATA POINTS
    PN    PRINT THE NO. OF LINEAR PARAMETERS
    PKG   PRINT THE NO. OF NONLINEAR PARAMETERS
    PIV   PRINT THE NO. OF INDEPENDENT VARIABLES
    PTW   PRINT THE DATA POINTS & WEIGHTS
    PALF  PRINT THE VALUES OF THE NONLINEAR PARAMETERS
    PNDI  PRINT THE NUMERICAL DERIVATIVE INCREMENTS
    PINC  PRINT WHICH TERMS DEPEND ON NONLIN PARAMETERS
    LP    TURN ON THE LINE PRINTER FLAG
    NP    TURN OFF THE LINE PRINTER FLAG
    TP    TURN ON THE FLAG TO PLOT ON CRT
    NTP   TURN OFF THE FLAG TO PLOT ON CRT

COMMAND CODES FOR CHANGING
    CM    CHANGE NO. OF DATA POINTS
    CN    CHANGE NO. OF LINEAR PARAMETERS
    CKG   CHANGE NO. OF NONLINEAR PARAMETERS
    CIV   CHANGE NO. OF INDEPENDENT VARIABLES
    CT    CHANGE ONE OR MORE DATA POINTS
    CW    CHANGE ONE OR MORE WEIGHTS
    CALF  CHANGE ONE OR MORE NONLINEAR PARAMETERS
    CNDI  CHANGE ONE OR MORE NUMER DERIV INCREMENTS
    CTRN  TRANSFORM THE DATA
    CINC  CHANGE WHICH TERMS DEPEND ON NONLIN PARAMETERS

COMMAND CODES FOR RUNNING
    RV    RUN THE LEAST SQUARES PROGRAM
    RS    RUN A STATISTICAL ANALYSIS OF RESULTS

COMMAND CODES TO SAVE DATA FILE AND/OR STOP
    SC    SAVE CURRENT VALUES OF DATA & CONTINUE
    SD    SAVE CURRENT VALUES OF DATA & STOP
    SR    SAVE CURRENT VALUES OF INDEP. VARIABLES AND
          RESIDUALS & CONTINUE
    SO    STOP WITHOUT SAVING
```

1. print any of the current values,
2. change any of the current values or transform the data;
3. run the least squares program or the statistical analysis; or
4. save the current values and/or end the terminal session.

Whichever command is chosen, the program cues the user to give all the necessary information to successfully execute that command. After execution is complete, the program returns to the command point (unless, of course, the user requests the commands S0 or SD, which result in program termination).

The print, change and save/stop commands are self explanatory and easy to follow, and will not be explained in detail here. The run commands take the user through one of two paths, both terminating back at the command point, prompt **23**).

7.4 Running The Least Squares Program

The code for running the least squares code VARPRO is "RV". It activates the following prompts:

24) DO YOU WANT TO CHANGE ANY DEFAULTS IN THE LEAST SQUARES PROGRAM? A list of default values appears. If the answer is "Y", a list of codes to change these defaults is printed. (For an explanation of the output printing index, see IPRINT in Appendix C.) The user enters the desired code and the program then specifies the limits to which that criterion can be changed and asks the user for a new value. The user enters the new value and is then given the option to change any of the other defaults. Finally, the least squares program begins.

25) INDICATE WHICH OF THE FOLLOWING SHOULD BE PRINTED BY TYPING "Y": After the least square calculations are completed, a list of 3 possible tables to be printed appears. After each table is listed, the user enters "Y" if that table is to be printed, or any other character if that table is to be skipped. All selected tables are then printed.

26) PLOT ROUTINE CURRENTLY SET NOT TO DO ANY PLOTS. DO YOU WANT TO START PLOTTING? This prompt will be repeated for each of the independent variables. If there are more than one independent variable, the user will be asked to type in a label for each one chosen except for the first whose label was typed in response to prompt **4**). When no more plots are desired, the user responds to this prompt with something other than "Y", and the program returns to the command point, prompt **23**). If the response to this prompt is "Y", a list of available plots appears, and the user enters the number of the plots to be printed. The plot of observed and predicted values is printed twice when the data has been transformed, once using the transformed data and once using the back-transformed data. The user also has the option of printing a table of the back-transformed values.

7.5 Running the Statistics Programs

When a VARPRO fit has been completed and the program has returned to the command point, the user can obtain a statistical analysis of the fit and the residuals by responding to the "**NEXT STEP?**" prompt with "RS" which activates the following prompt:

27) INDICATE WHICH OF THE FOLLOWING SHOULD BE PRINTED: A list of tables, data and plots to be printed appears. After each item is listed, the user enters "Y" to have that item printed, or some other character to skip it. All the selected items are then printed. A more detailed explanation of the various statistical quantities is given in Chapter 8. The plot of standardized residuals vs. independent variable is printed once for each independent variable. After all items are printed, the program returns to the command point, prompt **23**).

7.6 The VARPRO Error Diagnostic Messages

The actual least squares calculations are done in the VARPRO subroutine package which checks for various errors and indicates their occurence with one of the following diagnostic messages.

PROBLEM TERMINATED FOR EXCESSIVE ITERATIONS The maximum number of iterations was exceeded before the nonlinear parameters converged to the accuracy requested. The easiest thing to do about this message is simply to start the iteration again by typing in an "RV" command. The iteration will begin again using the nonlinear parameter values obtained in the previous run as the initial estimates. If the problem persists, the user may want to relax the convergence tolerance before running the problem again, or examine the residuals and fitted function for the unconverged parameter values.

PROBLEM TERMINATED BECAUSE OF ILL-CONDITIONING This message is usually obtained when the iteration has found an apparent minimum at a point where the parameters are highly correlated with one another. This situation can be verified by examining the correlation matrix. The occurence of this situation means that many other parameter combinations will give a fit that is essentially identical to the one obtained. The fit is usually good, but the user should be aware of the possibility that he has specified a model with more nonlinear parameters than the data can support. It is our impression that this message is overly pessimistic and can often be ignored.

INPUT ERROR IN PARAMETER N,KG,M,NPP2, OR MMAX. One or more of the indicated parameters is in error. The parameter values should be:

N The number of linear parameters,

KG The number of nonlinear parameters,

M The number of observations (data points),

NPP2 N + P + 2, where P is the number of nonvanishing partial derivatives $\partial\Phi/\partial\alpha$,

MMAX The maximum number of observations allowed by the code.

Note that MMAX is set by parameter statements in the program.

ERROR – INC MATRIX IMPROPERLY SPECIFIED OR DISAGREES WITH NPP2. The INC matrix is an "incidence matrix" that tells the program which of the Φ functions depends on which of the nonlinear parameters α. The user can print out this matrix by typing "PINC" and change it by typing "CINC".

ERROR – WEIGHT(nnn) NOT NONNEGATIVE. The weight W_{nnn} is negative.

CATASTROPHIC FAILURE – COLUMN nnn IS ZERO. SEE RALL AND FUNDERLIC'S DOCUMENTATION. VARPRO works with an M $\times$ N matrix $\mathbf{A}$ whose columns are set to the values of the Φ functions and their partial derivatives $\partial\Phi/\partial\alpha$ evaluated at the observation points. The ordering of the columns is:

1. The first N columns contain the Φ_k functions that have linear multipliers C_k, ordered in the same way as they are in user subroutine CALC. Recall that any Φ which do not depend on the nonlinear parameters should come first. Such function are called "constant functions" by the VARPRO comment cards.
2. The (N+1)st column contains the Φ_{N+1} which does not have a linear coefficient C. If the model does not have a Φ_{N+1} term, then the (N+1)st column is left blank.
3. The final P columns contain the nonvanishing partial derivatives $\partial\Phi_k/\partial\alpha_j$, ordered first on the α_k, i.e., all of the $\partial\Phi_k/\partial\alpha_1$ come first, then all of the $\partial\Phi_k/\partial\alpha_2$, and so on.

This error is usually caused either by a programming error in CALC or DERIV, or because the iteration has produced a set of nonlinear parameters α which yield vanishingly small values for one of the Φ functions or one of the partial derivatives. An example of the second situation might be an exponential $\Phi(t) = \exp(\alpha t)$ that gets out of hand because the iteration produces very negative values of α. In some cases this kind of error can be avoided by starting again with different initial estimates for the parameters, but if the iteration persists in converging to this error, the user should carefully examine his model and/or his CALC and DERIV subroutines.

ERROR – CONSTANT COLUMN MUST BE COMPUTED ONLY WHEN ISEL = 1. See the explanation of the preceding error stop for the definition of a constant column. We have never observed this error stop. It is caused when a constant column is computed more than once. Users who get this stop should check for an error in his subroutine CALC or in the incidence matrix INC.

Chapter 8

STATISTICAL CONSIDERATIONS

This chapter is reprinted with slight alterations from [12, pages 54-58].

A variety of statistics are available after the optimal parameter values have been calculated. These will be discussed in the order that they appear in the program. One should bear in mind that for nonlinear least squares many statistics can only be approximated, and their values should be treated accordingly.

The first statistical option is a table of the independent variables, observed and predicted values of the dependent variable, weighted residuals and weights. The weighted residual is the result of multiplying the residual by the appropriate weighting factor, i.e.,

$$W_i(y_i - \eta_i) = W_i r_i$$

Recall that WEIGHT(I) = W_i^2.

The variance-covariance matrix provides an estimate of the variance (or covariance) of the calculated parameters. Thus the diagonal elements are the variances of the parameters (i.e., the average of the squared deviations). The off-diagonal elements are the covariances of the parameters, where the covariance of two parameters x and y is defined as the average cross-product of the x and y deviations from their means $\bar{x}$ and $\bar{y}$ [5]. The covariance matrix is calculated as described by Lawson and Hanson [10], from the formula

$$\boldsymbol{V} = \sigma^2 \boldsymbol{T}^{-1} \boldsymbol{T}^{-T} = \sigma^2 (\boldsymbol{T}^T \boldsymbol{T})^{-1} ,$$

where the superscript T is transpose and σ^2 is a scalar factor such that

$$\sigma^2 = \frac{(norm\ of\ residual)^2}{(degrees\ of\ freedom)} .$$

[The quantity ($degrees\ of\ freedom$) is the number of observations minus the number of unknown parameters.] The matrix $\boldsymbol{T}$ is the final reduced form of the matrix of functions Φ and derivatives $\partial\Phi/\partial\alpha$ used in calculating the optimal parameters.

The correlation matrix is a scaled version of the covariance matrix. Its x, y element is $cov(x,y)/(\sigma(x)\sigma(y))$, where $\sigma(i)$ represents the standard deviation of the ith parameter. Thus the diagonal elements are all ones and the off-diagonal elements are the correlation coefficients and have absolute value between zero and one. The closer the values are to one, the stronger the relationship is between the two parameters. A negative coefficient indicates an inverse relationship, i.e., y decreases as x increases; a positive coefficient indicates that x and y tend to increase (or decrease) together. Plots of the residuals and of the observed and predicted values versus the independent variable give a pictorial view of the data in the table. One should note, however, that the plot is of the actual residuals, and not of the weighted residuals.

On execution of the RS command, several other statistical options are available. The first is a table of the parameters, their standard deviations and the t-ratio (the parameters divided by their standard deviations). The t-ratio follows the Student's t-distribution if the sample population is normal or near-normal [5]. It can be used to determine the level of significance of the hypothesis that the mean of the population takes on a particular value (e.g., the parameter takes on a particular value) or to construct a confidence interval for the mean of a normal population (e.g., the parameter) [2].

The weighted residual sum of squares (RSS) is the quantity which is minimized, i.e., the sum of the squares of the weighted residuals. The residual mean square (RMS), sometimes called the estimated variance, is the residual sum of squares divided by the degrees of freedom. The standard error is the square root of the residual mean square.

The coefficient of determination (also referred to as R^2 or the square of the multiple correlation coefficient) is another measure used to determine the goodness of fit. It is calculated from the formula

$$R^2 = 1 - \frac{(RSS)}{(CTSS)} \ ,$$

where the corrected total sum of squares is found by

$$(CTSS) = \sum_{i=1}^{m} W_i^2 (y_i - \bar{y})^2 \ ,$$

where $\bar{y}$ is the weighted mean of the observed values

$$\bar{y} = \frac{\sum_{i=1}^{m} W_i^2 y_i}{\sum_{i=1}^{m} W_i^2} \ .$$

The coefficient of determination is thus a normalized residual sum of squares and will always have a value between zero and one. The closer the value is to one, the better the fit. For example, a coefficient of .995 would indicate that 99.5 percent of the corrected total sum of squares is accounted for by the fitted equation [5].

One also has the option of printing a table of values of the independent variables, the observed and predicted values of the dependent variable, the residual and the standardized residual. The standardized residuals are the residuals divided by their standard deviations and are calculated from the formula

$$(SR)_i = \frac{r_i}{\sqrt{\frac{(RMS)}{W_i^2} - s_i^2}} ,$$

where s_i is the standard deviation of the predicted value of the ith parameter [8]. This latter quantity is given by

$$s_i = \sqrt{\boldsymbol{e}_i^T \boldsymbol{\Phi} \boldsymbol{V} \boldsymbol{\Phi}^T \boldsymbol{e}_i} ,$$

where $\boldsymbol{V}$ is the covariance matrix described above, $\boldsymbol{\Phi}$ is the matrix whose columns are the fitting functions Φ_j evaluated at the observation points, and $\boldsymbol{e}_i$ is the vector with a one in the ith element and zeroes everywhere else. Thus s_i^2 is the ith diagonal element of the matrix $\boldsymbol{\Phi} \boldsymbol{V} \boldsymbol{\Phi}^T$

Several plotting features are also available. The standardized residual is used to provide a common scale and to avoid distortion caused by differences in the standard deviations of the residuals.

The first is a plot of the standardized residuals versus the independent variable(s). If the values do not appear to lie in a vertical band about the axis, one of several things may be indicated. If the variance steadily increases (or decreases) over the range of values to form a wedge-shaped graph, the implication is that a suitable transformation or a weighted least squares analysis should have been performed. If the values lie in a linear band that is not vertical, a linear term should have been included in the model. If the band of values is curved, linear and quadratic terms should have been included in the model. One should realize that combinations of these defects can also occur [4].

The standardized residuals are also plotted against the predicted values. Here again the analysis is similar to that above. Nonrandomness might indicate the need to use weights or the omission of some important term from the model equation [8].

A probability plot of the standardized residuals versus the expected value of the standardized residuals is also provided [8]. In making this plot, it is assumed that the measurement errors are normally and independently distributed. If the model adequately represents the data, the points will lie roughly on a diagonal line extending approximately between the points $(-3, -3)$ and $(3, 3)$ and will tend to be clustered toward the center point $(0, 0)$.

Chapter 9

A TIME SERIES EXAMPLE – THE WILDLIFE CYCLE

9.1 The Model and the Data

The populations of many species of wildlife in the northern latitudes of the Northern Hemisphere exhibit a mysterious but very regular cycle of length approximately 10 years [6], [9]. Figure 9.1 is a plot of the annual total number of Canadian lynx pelts purchased from trappers in the MacKenzie River district by the Hudson's Bay Company in the years 1821-1934. The individual yearly totals are connected by straight line segments to emphasize the time-series nature of the data. The 10-year cycle is very pronounced, and there is a hint that it was modulated with a cycle of period approximately 40 years.

Since population processes tend to be exponential in nature, the usual procedure is to work with the natural logarithm of the population measure. Figure 9.2 was obtained by taking the natural logarithms of the numbers plotted in Figure 9.1 and then by subtracting a least squares trend line

$$y(t) = C_1 + C_2 t \ .$$

The purpose of the detrending was to facilitate a spectral analysis of the time series. Figure 9.3 is the periodogram of the data plotted in Figure 9.2. It is dominated by the "10-year" cycle which whose length appears to be

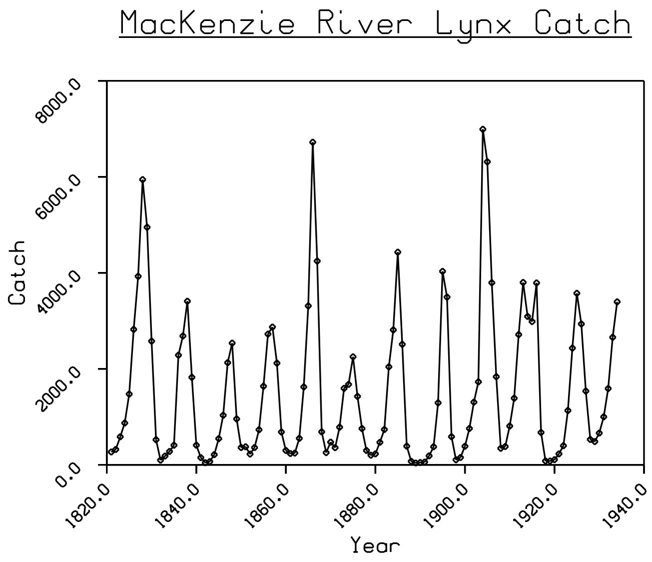


Figure 9.1: The MacKenzie River lynx catch in the years 1821-1934.

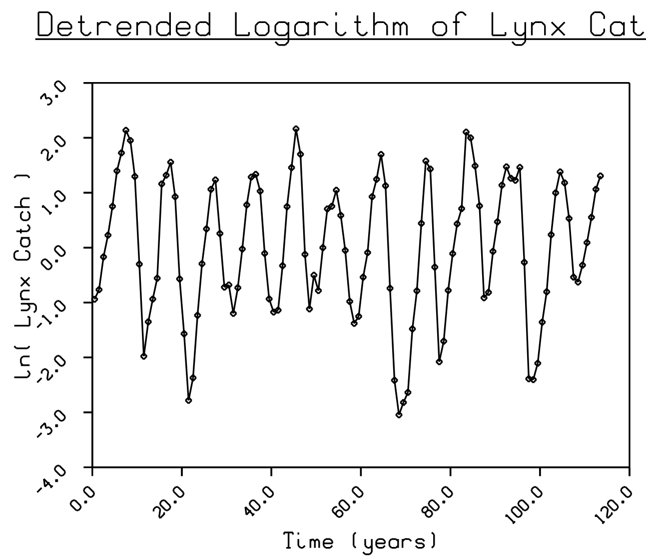


Figure 9.2: Natural logarithm of the MacKenzie River lynx catch with the least squares trend line removed.

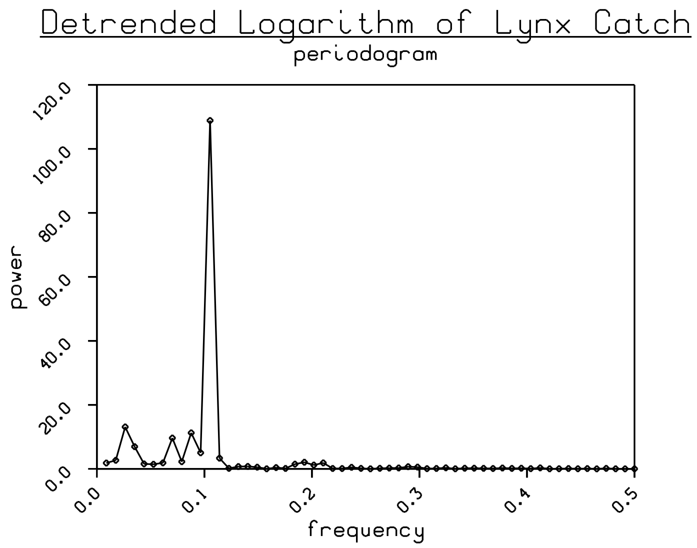


Figure 9.3: Periodogram of the detrended natural logarithm of the MacKenzie River lynx catch

closer to 9.5 years than to 10 years. There is also a hint of a cycle of length approximately 40 years.

Figures 9.2 and 9.3 suggest the following model for the MacKenzie River lynx catch:

$$y(t) = C_1 + C_2 t + C_3 \sin\left[\frac{2\pi}{T_{10}}(t + \theta_{10})\right] + C_4 \sin\left[\frac{2\pi}{T_{40}}(t + \theta_{40})\right] ,$$

where t is the year, $y(t)$ is the natural logarithm of the lynx catch in that year, T_{10} and T_{40} are the two periods (to be determined by the fit), and θ_{10} and θ_{40} are the corresponding phase constants. This model, as it is written, has four linear constants C_1, C_2, C_3, and C_4, and four nonlinear constants T_{10}, T_{40}, θ_{10}, and θ_{40}. It is possible to use the trigonometric identity for the sine of the sum of two angles to rewrite this model with 6 linear constants and only two nonlinear constants, but we will leave it in the form above for this example.

Taking

$$\begin{aligned} \alpha_1 &= T_{10} \quad , \quad \alpha_2 = T_{40} \ , \\ \alpha_3 &= \theta_{10} \quad , \quad \alpha_4 = \theta_{40} \ , \end{aligned}$$

we can write the model in the form

$$\eta(t) = C_1\Phi_1(t) + C_2\Phi_2(t) + C_3\Phi_3(t) + C_4\Phi_4(t) ,$$

where

$$\begin{aligned} \Phi_1(t) &= 1.0 \ , \\ \Phi_2(t) &= t \ , \\ \Phi_3(t) &= \sin\left[\tfrac{2\pi}{\alpha_1}(t + \alpha_3)\right] \ , \\ \Phi_4(t) &= \sin\left[\tfrac{2\pi}{\alpha_2}(t + \alpha_4)\right] \ . \end{aligned}$$

This is the model that was used for making the fits in this example. The initial estimates that were used are

$$\begin{aligned} \alpha_1^0 &= 9.0 \quad , \quad \alpha_2^0 = 38.0 \ , \\ \alpha_3^0 &= 5.0 \quad , \quad \alpha_4^0 = 15.0 \ . \end{aligned}$$

The data used in this example were the numbers plotted in Figure 9.1, i.e., the number of lynx caught as a function of year. These data were written as two columns of numbers in a file called LYNXCAT. Each line of the file contained a year number and the total lynx catch for that year. The model, however, applied to the natural logarithms of the catch numbers.

Therefore it was necessary to transform the data in the user-supplied suboutine TRANS before making the fit. When making this transformation, the independent variable t was also transfomed by moving the origin to the midpoint of the record (i.e., by subtracting 1878.0 from all of the year values). This is a standard practice which improves the conditioning of the fit.

9.2 The User-Supplied Subroutines

The user-supplied subroutines required to make the fit are given in the following paragraph. These subroutines were all written into a single file, called LYCALC, in accordance with the directions given in Chapter 3. Subroutine CALC is quite straightforward. We decided to let the program compute numerical approximations to the derivatives of the functions Φ_i with respect to the nonlinear parameters α_j, so subroutine DERIV is only a dummy subroutine. We used equal weighting in making the fit, so subroutine WT is also a dummy subroutine. Subroutine TRANS makes the transformations described at the end of the preceding section, and subroutine BAKTRN inverts the transformation on the dependent variable.

The subroutines used for this example are:

```
C
C
      SUBROUTINE CALC ( K, NL, N, MMAX, IV, C, ALF, T, ETA )
C
C
      PARAMETER ( MAXN1=11 )
C
      DIMENSION C(N), ALF(NL), T(MMAX,IV)
C
      COMMON /BLKPH/ PH(MAXN1)
C
      DATA PI /3.141592654/
C
      PH(1) = 1.
      PH(2) = T(K,1)
      PH(3) = SIN((2*PI/ALF(1))*(T(K,1)+ALF(3)))
      PH(4) = SIN((2*PI/ALF(2))*(T(K,1)+ALF(4)))
C
```

```
      ETA = C(1)*PH(1)+C(2)*PH(2)+C(3)*PH(3)+C(4)*PH(4)
C
      RETURN
      END
C
C
C--------------------------------------------------------------
C
C
      SUBROUTINE DERIV ( K, T, MMAX, IV, ALF, NL, NP1 )
C
C
C    ****** DUMMY SUBROUTINE ******
C
C
      PARAMETER ( MAXN1=11, MAXKG=8 )
C
      DIMENSION ALF(NL),T(MMAX,IV)
C
      COMMON /BLKDPH/ DPH(MAXN1,MAXKG)
C
      DO 10 J=1,NL
        DO 10 I=1,NP1
          DPH(I,J) = 0.0
   10 CONTINUE
C
C  AT THIS POINT INSERT THE STATEMENTS NEEDED TO SET THE
C    REQUIRED NON-ZERO DERIVATIVES IN THE ARRAY DPH(I,J).
C
C  DPH(I,J) = PARTIAL DERIVATIVE OF THE ITH FUNCTION PHI
C             WITH RESPECT TO THE JTH NON-LINEAR PARAMETER ALF
C              EVALUATED AT OBSERVATION NUMBER K,
C                 I.E. EVALUATED AT T(K,L), L=1,IV
C
      RETURN
      END
C
C
C--------------------------------------------------------------
```

```
C
C
      SUBROUTINE WT ( M, WEIGHT, Y )
C
C
      DIMENSION Y(M),WEIGHT(M)
C
C  ****** DUMMY SUBROUTINE ******
C
C  TO GET 1/Y**2 WEIGHTING, SIMPLY ACTIVATE THE NEXT 3 STATEMENTS
C
C       DO 10 I=1,M
C         WEIGHT(I) = 1.0/Y(I)**2
C  10   CONTINUE
C
C  OTHER WEIGHTINGS CAN BE GOTTEN BY CHANGING THE STATEMENT INSIDE
C          THE LOOP.
C
      RETURN
      END
C
C-------------------------------------------------------------
C
C
      SUBROUTINE TRANS ( T, BT, Y, BY, IV, M, MMAX )
C
C
      DIMENSION T(MMAX,IV), BT(MMAX,IV), Y(M), BY(M)
C
      DO 20 I=1,M
         DO 10 J=1,IV
            BT(I,J) = T(I,J)
C
            T(I,J) = T(I,J) - 1878.0
C
   10    CONTINUE
         BY(I) = Y(I)
C
         Y(I) = ALOG(Y(I))
```

```
C
   20 CONTINUE
C
      RETURN
      END
C
C
C--------------------------------------------------------------
C
C
      SUBROUTINE BAKTRN ( ETA, BETA, M )
C
C
      DIMENSION ETA(M), BETA(M)
C
      DO 10 I=1,M
C
         BETA(I) = EXP(ETA(I))
C
   10 CONTINUE
C
      RETURN
      END
```

These subroutines were written into a file named SNCALC which was compiled and loaded with the INVAR programs and then executed in a teminal session to be described in the following section.

9.3 The Terminal Session

The terminal session output that follows was obtained by executing INVAR2 on the NBS CYBER 855, running from a Qume QVT-201 terminal in screen mode. Since the terminal was not a plotting terminal, the DISSPLA plots were done after execution on the QMS laser printer with address B225. Before reading this example, the following points should be noted:

1. Since the terminal was running in screen mode, the INVOKE,INVAR command generated a new screen shown between the horizontal lines at the beginning of the session. This was done by the interactive

NOS Procedure to quiz the user for the location of the user-supplied subroutines, the address of the QMS printer for the plots and hardcopy output, and the name of the data file.

2. Since the derivatives were to be computed numerically, it was necessary to specify nonlinear parameter increment values to be used in the finite difference approximations. We chose to use the same increment value, 0.001, for all four parameters.

3. The VARPRO least squares iteration terminates with the warning, "PROBLEM TERMINATED BECAUSE OF ILL-CONDITIONING", but this does not indicate a fatal error. It occurs fairly often when using VARPRO, but the linear and nonlinear parameters calculated by the program are usually satisfactory.

4. Since this is a time-series problem, all the line-printer graphs with time as the independent variable are plotted in a vertical rather than a horizontal format.

5. After each line printer graph, the program stops with a question mark (?) prompt to which we replied with a "C" followed by a carriage return. The prompt was apparently issued by the TK4014 program used at NBS to generate the DISSPLA plots for the laser printer. Cyber users should always respond to this prompt with something more than just a carriage return in order to avoid an end-of-file error stop.

The terminal session follows:

```
/INVOKE,INVAR
```

```
                INTERACTIVE NONLINEAR LEAST SQUARES PROGRAM

 CALCF  FORTRAN file of user-supplied subroutines: LYCALC_
 QMSADDR  QMS Address for output (Default = NONE): B225___
              DATAF  Data file (Default = NONE): LYNXCAT
     INV102  INVAR1 or INVAR2 (Default = INVAR2): _______

                    Specify values and press NEXT when ready
 ----------------------------------- INVARX -----------------------------

        PROC,INVARX,CALCF[,QMSADDR][,DATAF][,INV102].

 Executes one of two versions, INVAR1 or INVAR2, of INVAR, an
 interactive, variable separable, nonlinear least squares program.

 Local file CALCF contains FORTRAN coded, user-supplied subroutines.

 Hardcopy output and plots can be sent to QMS laser printer with
 address QMSADDR.

 Permanent file DATAF contains data to be fit (not needed if data
 already in a local file, or is to be typed in during execution).
                         F3 HELP FWD                 F5   HELP    F6   QUIT
```

```
 ENTER TITLE (MAXIMUM OF 40 CHARACTERS):
? MACKENZIE RIVER LYNX CATCH

 DO YOU WANT DISSPLA PLOTS? (TYPE "Y" FOR YES)
? Y

 DO YOU WANT THESE PLOTS SHOWN INTERACTIVELY ON
 A PLOTTING SCREEN (TYPE "1");
 OR SAVED IN A FILE TO BE PRINTED OUT LATER (TYPE "2")?
? 2

 ENTER LABEL FOR INDEPENDENT VARIABLE (MAX. OF 47 CHARACTERS):
? YEAR

 ENTER LABEL FOR DEPENDENT VARIABLE (MAX. OF 47 CHARACTERS):
? CATCH

 DO YOU WANT LINE PRINTER OUTPUT?
? Y

 ARE YOUR DATA, WEIGHTS, INITIAL VALUES, ETC.
               ALREADY IN A VARPRO-DEFINED FILE ?
```

```
? N

 NO. OF DATA POINTS:
? 114

 NO. OF LINEAR PARAMETERS:
? 4

 NO. OF NONLINEAR PARAMETERS:
? 4

 NO. OF INDEPENDENT VARIABLES:
? 1

 ARE DATA IN A FILE?
? Y

 WHAT IS THE FILENAME?--NO MORE THAN 26 CHARS

      (TYPE "QUIT" TO EXIT)
? LYNXCAT

 ARE WEIGHTS TO BE CALCULATED IN SUBROUTINE WT?
? N

 WEIGHTS ARE SET TO 1


 DO DEPENDENT OR INDEPENDENT VARIABLES
 NEED TO BE TRANSFORMED BEFORE ANALYSIS?
? Y

 INITIAL VALUES OF NONLINEAR PARAMETERS
   1
? 9.0

   2
? 38.0

   3
? 5.0

   4
? 15.0

 HOW MANY TERMS OF THE MODEL DEPEND ON NONLINEAR PARAMETER  1:
? 1
```

```
 WHICH TERMS ARE THEY?
? 3

 HOW MANY TERMS OF THE MODEL DEPEND ON NONLINEAR PARAMETER  2:
? 1

 WHICH TERMS ARE THEY?
? 4

 HOW MANY TERMS OF THE MODEL DEPEND ON NONLINEAR PARAMETER  3:
? 1

 WHICH TERMS ARE THEY?
? 3

 HOW MANY TERMS OF THE MODEL DEPEND ON NONLINEAR PARAMETER  4:
? 1

 WHICH TERMS ARE THEY?
? 4

 ALL DERIVATIVES IN CLOSED FORM?
? N

 ALL NUMERICAL DERIVATIVE INCREMENTS THE SAME?
? Y

 INCREMENT VALUES:
? .001

 WOULD YOU LIKE TO SAVE THE DATA JUST INPUT?
? N


 DOES DATA FOLLOW AN EVENLY SPACED TIME SERIES?
? Y


   NOTE:   THE COMMAND "SC" WILL SAVE YOUR DATA FILE AT ANY TIME

 NEXT STEP? (TYPE "H" FOR HELP)
? RV


 DO YOU WISH TO CHANGE ANY DEFAULTS IN THE LEAST SQUARES PROGRAM?
        (50: MAX. NO. OF ITERATIONS)
```

```
        (1.0E-5: CONVERG. TOLERANCE)
        (1: OUTPUT PRINTING INDEX)
? N

1                    MACKENZIE RIVER LYNX CATCH



    0  WEIGHTED NORM OF RESIDUAL =   1.3034592E+01
     NU =   .1000000E+01


   ITERATION   1    NONLINEAR PARAMETERS

    9.4014515E+00          3.7990261E+01

    5.2013727E+00          1.9306338E+01

    1  WEIGHTED NORM OF RESIDUAL =   9.3597487E+00
     NU =   .5000000E+00
     NORM(DELTA-ALF) / NORM(ALF) =   9.852E-02


   ITERATION   2    NONLINEAR PARAMETERS

    9.5511209E+00          3.9674402E+01

    4.9024596E+00          2.1057477E+01

    1  WEIGHTED NORM OF RESIDUAL =   7.5367307E+00
     NU =   .2500000E+00
     NORM(DELTA-ALF) / NORM(ALF) =   5.310E-02


   ITERATION   3    NONLINEAR PARAMETERS

    9.6094909E+00          4.0501357E+01

    4.8074588E+00          2.1959035E+01

    1  WEIGHTED NORM OF RESIDUAL =   7.2985779E+00
     NU =   .1250000E+00
     NORM(DELTA-ALF) / NORM(ALF) =   2.597E-02


   ITERATION   4    NONLINEAR PARAMETERS
```

```
 9.6189932E+00          4.0536899E+01

 4.7925146E+00          2.1908877E+01

 1  WEIGHTED NORM OF RESIDUAL =   7.2930963E+00
  NU =   .6250000E-01
  NORM(DELTA-ALF) / NORM(ALF) =   1.352E-03


ITERATION   5    NONLINEAR PARAMETERS

 9.6198493E+00          4.0566491E+01

 4.7910923E+00          2.1917641E+01

 1  WEIGHTED NORM OF RESIDUAL =   7.2930368E+00
  NU =   .3125000E-01
  NORM(DELTA-ALF) / NORM(ALF) =   6.528E-04


                  .
                  .
                  .


ITERATION  38    NONLINEAR PARAMETERS

 9.6199005E+00          4.0579944E+01

 4.7910060E+00          2.1914852E+01

28  WEIGHTED NORM OF RESIDUAL =   7.2930340E+00
  NU =   .5548352E+02
  NORM(DELTA-ALF) / NORM(ALF) =   7.510E-10


ITERATION  39    NONLINEAR PARAMETERS

 9.6199005E+00          4.0579944E+01

 4.7910060E+00          2.1914852E+01

 1  WEIGHTED NORM OF RESIDUAL =   7.2930340E+00
  STEP RETRACTED, NU =  8.3225286E+01
```

```
ITERATION  40    NONLINEAR PARAMETERS

 9.6199005E+00          4.0579944E+01

 4.7910060E+00          2.1914852E+01

 2  WEIGHTED NORM OF RESIDUAL =    7.2930340E+00
  STEP RETRACTED, NU =  1.2483793E+02

PROBLEM TERMINATED BECAUSE OF ILL-CONDITIONING


,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,

 LINEAR PARAMETERS

 .6692901E+01   .3384831E-02   .1436036E+01   .4943990E+00

 NONLINEAR PARAMETERS

 .9619901E+01   .4057994E+02   .4791006E+01   .2191485E+02

 WEIGHTED NORM OF RESIDUAL =   .7293034E+01

 WEIGHTED ESTIMATED VARIANCE =   .5017768E+00

,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,
INDICATE WHICH OF THE FOLLOWING SHOULD BE PRINTED
BY TYPING "Y":
 TABLE OF OBSERVED & PREDICTED VALUES, WTD RESIDUAL:
? Y

 COVARIANCE MATRIX:
? N

 CORRELATION MATRIX:
? Y

1


INDEX  IND VAR 1    OBS VAL      PRED VAL     WTD RESID     WEIGHTS

  1 -5.70000E+01  5.59471E+00  6.23735E+00 -6.42634E-01  1.00000E+00
  2 -5.60000E+01  5.77144E+00  5.63420E+00  1.37242E-01  1.00000E+00
  3 -5.50000E+01  6.37161E+00  5.55072E+00  8.20896E-01  1.00000E+00
  4 -5.40000E+01  6.76964E+00  6.03655E+00  7.33093E-01  1.00000E+00
  5 -5.30000E+01  7.29641E+00  6.90279E+00  3.93622E-01  1.00000E+00
```

```
   6 -5.20000E+01  7.94485E+00  7.79950E+00  1.45343E-01  1.00000E+00
   7 -5.10000E+01  8.27589E+00  8.35964E+00 -8.37538E-02  1.00000E+00
   8 -5.00000E+01  8.68997E+00  8.35012E+00  3.39845E-01  1.00000E+00
   .       .            .            .            .            .
   .       .            .            .            .            .
   .       .            .            .            .            .

 107  4.90000E+01  7.33759E+00  5.58251E+00  1.75508E+00  1.00000E+00
 108  5.00000E+01  6.27099E+00  5.01960E+00  1.25139E+00  1.00000E+00
 109  5.10000E+01  6.18415E+00  5.02534E+00  1.15881E+00  1.00000E+00
 110  5.20000E+01  6.49527E+00  5.60513E+00  8.90135E-01  1.00000E+00
 111  5.30000E+01  6.90776E+00  6.53246E+00  3.75292E-01  1.00000E+00
 112  5.40000E+01  7.37149E+00  7.44190E+00 -7.04083E-02  1.00000E+00
 113  5.50000E+01  7.88495E+00  7.97913E+00 -9.41815E-02  1.00000E+00
 114  5.60000E+01  8.13035E+00  7.94642E+00  1.83936E-01  1.00000E+00
1


               CORRELATION MATRIX


 ROW      COLUMN    1     COLUMN    2     COLUMN    3     COLUMN    4

   1      1.000000E+00   6.913627E-03   9.202510E-03   1.585469E-02
   2      6.913627E-03   1.000000E+00  -7.093361E-02   2.470090E-01
   3      9.202510E-03  -7.093361E-02   1.000000E+00   1.993396E-03
   4      1.585469E-02   2.470090E-01   1.993396E-03   1.000000E+00
   5      2.159597E-02   4.740477E-02  -1.747922E-02  -1.875114E-02
   6      4.382337E-02  -2.098704E-01   9.025855E-02  -8.623688E-02
   7     -1.391344E-02  -2.037583E-02  -4.545045E-03  -5.482076E-03
   8      1.001278E-01  -1.543260E-01   5.609647E-02  -4.368950E-02


 ROW      COLUMN    5     COLUMN    6     COLUMN    7     COLUMN    8

   1      2.159597E-02   4.382337E-02  -1.391344E-02   1.001278E-01
   2      4.740477E-02  -2.098704E-01  -2.037583E-02  -1.543260E-01
   3     -1.747922E-02   9.025855E-02  -4.545045E-03   5.609647E-02
   4     -1.875114E-02  -8.623688E-02  -5.482076E-03  -4.368950E-02
   5      1.000000E+00  -4.964643E-02   1.177933E-01  -1.404177E-03
   6     -4.964643E-02   1.000000E+00   3.265023E-02   5.878888E-01
   7      1.177933E-01   3.265023E-02   1.000000E+00   9.272713E-03
   8     -1.404177E-03   5.878888E-01   9.272713E-03   1.000000E+00

 PLOT ROUTINE CURRENTLY SET NOT TO DO ANY PLOTS.
 DO YOU WANT TO START PLOTTING?
? Y
```

```
 IF YOU WANT TO PLOT RESIDUALS, TYPE "1"
 IF YOU WANT TO PLOT OBSERVED & PREDICTED VALUES, TYPE "2"
 IF YOU WANT TO PLOT BOTH, TYPE "3":
? 3

1               RESIDUALS
                IND VAR 1

 MEAN IS   .47144386E-10

 GRAPH INTERVAL IS   .67485643E-01
          -COMPUTED FROM MAXIMUM AND MINIMUM VALUES
     -1.62      -.94      -.27       .41      1.08      1.76
          -1.28      -.61       .07       .74      1.42
       I----I----I----I----I----I----I----I----I----I----I
      I                                                  I
   1  I              *         I                         I  -.64263E+00
   2  I                        I *                       I   .13724E+00
   3  I                        I          *              I   .82090E+00
   4  I                        I         *               I   .73309E+00
   5  I                        I    *                    I   .39362E+00
   6  I                        I *                       I   .14534E+00
   7  I                       *I                         I  -.83754E-01
   8  I                        I    *                    I   .33984E+00
   9  I                        I         *               I   .73925E+00
  10  I                        I             *           I   .10130E+01
  11  I                        I    *                    I   .32294E+00
  12  I            *           I                         I  -.82240E+00
  13  I                     *  I                         I  -.23451E+00
  14  I                  *     I                         I  -.38987E+00
  15  I           *            I                         I  -.84685E+00
  16  I                        I *                       I   .13947E+00
  17  I                        *                         I   .24994E-02
  18  I                        I       *                 I   .52962E+00
  19  I                        I         *               I   .68781E+00
  20  I                        I  *                      I   .17464E+00

      .                        .                         .        .
      .                        .                         .        .
      .                        .                         .        .

  95  I                      * I                         I  -.15581E+00
  96  I                        I           *             I   .88637E+00
  97  I                        I *                       I   .15373E+00
  98  I       *                I                         I  -.11610E+01
  99  I           *            I                         I  -.86253E+00
 100  I           *            I                         I  -.84513E+00
```

```
 101  I           *          I                          I  -.82754E+00
 102  I      *               I                          I  -.11315E+01
 103  I            *         I                          I  -.69832E+00
 104  I                      *                          I  -.24565E-01
 105  I                      I          *               I   .83975E+00
 106  I                      I                    *     I   .15053E+01
 107  I                      I                         *I   .17551E+01
 108  I                      I                 *        I   .12514E+01
 109  I                      I               *          I   .11588E+01
 110  I                      I           *              I   .89014E+00
 111  I                      I     *                    I   .37529E+00
 112  I                     *I                          I  -.70408E-01
 113  I                     *I                          I  -.94181E-01
 114  I                      I  *                       I   .18394E+00
       I----I----I----I----I----I----I----I----I----I----I
? C

1               OBSERVED (*) & PREDICTED (+) VALUES (TRANSFORMED DATA)
                IND VAR 1

 X1 VECTOR
 MEAN IS   6.6798163

 X2 VECTOR
 MEAN IS   6.6798163

 GRAPH INTERVAL IS   .10377634
          -COMPUTED FROM MAXIMUM AND MINIMUM VALUES
      3.66      4.70      5.74      6.78      7.81      8.85
           4.18      5.22      6.26      7.30      8.33
       I----I----I----I----I----I----I----I----I----I----I
      I                                                  I   X1 = *    X2 = +
   1  I                  *     +                         I  .559E+01  .624E+01
   2  I                  +*                              I  .577E+01  .563E+01
   3  I                 +       *                        I  .637E+01  .555E+01
   4  I                      +      *                    I  .677E+01  .604E+01
   5  I                              +   *               I  .730E+01  .690E+01
   6  I                                       +*         I  .794E+01  .780E+01
   7  I                                           *+     I  .828E+01  .836E+01
   8  I                                            +  *  I  .869E+01  .835E+01
   9  I                                       +      *   I  .851E+01  .777E+01
  10  I                              +        *          I  .785E+01  .684E+01
  11  I                     +  *                         I  .626E+01  .594E+01
  12  I          *       +                               I  .458E+01  .541E+01
  13  I                *  +                              I  .521E+01  .545E+01
  14  I                  *   +                           I  .563E+01  .602E+01
  15  I                      *       +                   I  .601E+01  .686E+01
  16  I                                     +*           I  .773E+01  .759E+01
```

```
  17  I                                        2         I  .790E+01  .789E+01
  18  I                                     +     *      I  .813E+01  .760E+01
  19  I                              +      *            I  .751E+01  .682E+01
  20  I                     + *                          I  .601E+01  .584E+01
  21  I             2                                    I  .502E+01  .504E+01
  22  I *        +                                       I  .381E+01  .473E+01
  23  I     *       +                                    I  .422E+01  .502E+01
  24  I                *   +                             I  .536E+01  .578E+01
  25  I                         *   +                    I  .630E+01  .668E+01
  26  I                               *   +              I  .694E+01  .736E+01
  27  I                                    + *           I  .766E+01  .752E+01

      .                                                  .      .         .
      .                                                  .      .         .
      .                                                  .      .         .

  93  I                                           2      I  .824E+01  .818E+01
  94  I                                         *   +    I  .804E+01  .847E+01
  95  I                                         *+       I  .800E+01  .816E+01
  96  I                                   +       *      I  .824E+01  .735E+01
  97  I                          +*                      I  .651E+01  .636E+01
  98  I       *          +                               I  .439E+01  .556E+01
  99  I       *      +                                   I  .438E+01  .524E+01
 100  I          *      +                                I  .468E+01  .553E+01
 101  I                *       +                         I  .543E+01  .626E+01
 102  I                     *       +                    I  .599E+01  .712E+01
 103  I                               *      +           I  .703E+01  .773E+01
 104  I                                       2          I  .780E+01  .782E+01
 105  I                                  +        *      I  .818E+01  .734E+01
 106  I                            +            *        I  .798E+01  .648E+01
 107  I                  +                +              I  .734E+01  .558E+01
 108  I             +          *                        I  .627E+01  .502E+01
 109  I             +         *                         I  .618E+01  .503E+01
 110  I                   +       *                      I  .650E+01  .561E+01
 111  I                             +  *                 I  .691E+01  .653E+01
 112  I                                   2              I  .737E+01  .744E+01
 113  I                                        *+        I  .788E+01  .798E+01
 114  I                                        + *       I  .813E+01  .795E+01
       I----I----I----I----I----I----I----I----I----I----I
? C

1               OBSERVED (*) & PREDICTED (+) VALUES (BACK-TRANSFORMED DATA)
               IND VAR 1

 X1 VECTOR
 MEAN IS   1522.7105
```

```
X2 VECTOR
MEAN IS   1346.4738

GRAPH INTERVAL IS   139.04000
         -COMPUTED FROM MAXIMUM AND MINIMUM VALUES
    39.00   1429.40   2819.80   4210.20   5600.60   6991.00
        734.20   2124.60   3515.00   4905.40   6295.80
      I----I----I----I----I----I----I----I----I----I----I
     I                                                  I   X1 = *    X2 = +
  1  I  *+                                              I  .269E+03  .511E+03
  2  I  2                                               I  .321E+03  .280E+03
  3  I  + *                                             I  .585E+03  .257E+03
  4  I   +  *                                           I  .871E+03  .418E+03
  5  I       +  *                                       I  .148E+04  .995E+03
  6  I                 +  *                             I  .282E+04  .244E+04
  7  I                            * +                   I  .393E+04  .427E+04
  8  I                              +           *       I  .594E+04  .423E+04
  9  I                 +                 *              I  .495E+04  .236E+04
 10  I      +           *                               I  .258E+04  .936E+03
 11  I  +*                                              I  .523E+03  .379E+03
 12  I*+                                                I  .980E+02  .223E+03
 13  I 2                                                I  .184E+03  .233E+03
 14  I  *+                                              I  .279E+03  .412E+03
 15  I   *   +                                          I  .409E+03  .954E+03
 16  I              + *                                 I  .229E+04  .199E+04
 17  I                   2                              I  .269E+04  .268E+04
 18  I              +          *                        I  .341E+04  .201E+04
 19  I      +      *                                    I  .182E+04  .917E+03
 20  I  +*                                              I  .409E+03  .343E+03
 21  I 2                                                I  .151E+03  .154E+03
 22  I*+                                                I  .450E+02  .113E+03
 23  I*+                                                I  .680E+02  .152E+03
 24  I *+                                               I  .213E+03  .324E+03
 25  I    *+                                            I  .546E+03  .800E+03
 26  I       *   +                                      I  .103E+04  .156E+04
 27  I             + *                                  I  .213E+04  .184E+04
 28  I          +        *                              I  .254E+04  .122E+04
 29  I    +  *                                          I  .957E+03  .547E+03
 30  I ++                                               I  .361E+03  .232E+03

     .                                                  .      .          .
     .                                                  .      .          .
     .                                                  .      .          .

 90  I  +   *                                           I  .808E+03  .386E+03
 91  I     +    *                                       I  .139E+04  .716E+03
 92  I            +      *                              I  .271E+04  .170E+04
 93  I                        + *                       I  .380E+04  .357E+04
```

```
 94  I                      *           +                I  .309E+04  .475E+04
 95  I                     *   +                         I  .299E+04  .349E+04
 96  I           +               *                       I  .379E+04  .156E+04
 97  I    +*                                             I  .674E+03  .578E+03
 98  I* +                                                I  .810E+02  .259E+03
 99  I*+                                                 I  .800E+02  .190E+03
100  I* +                                                I  .108E+03  .251E+03
101  I * +                                               I  .229E+03  .524E+03
102  I   *     +                                         I  .399E+03  .124E+04
103  I        *       +                                  I  .113E+04  .228E+04
104  I                 *+                                I  .243E+04  .249E+04
105  I           +             *                         I  .357E+04  .154E+04
106  I    +                *                             I  .294E+04  .651E+03
107  I  +        *                                       I  .154E+04  .266E+03
108  I +  *                                              I  .529E+03  .151E+03
109  I + *                                               I  .485E+03  .152E+03
110  I  + *                                              I  .662E+03  .272E+03
111  I     + *                                           I  .100E+04  .687E+03
112  I           *+                                      I  .159E+04  .171E+04
113  I                   * +                             I  .266E+04  .292E+04
114  I                    +   *                          I  .340E+04  .283E+04
      I----I----I----I----I----I----I----I----I----I----I
? C

 DO YOU WISH TO PRINT A TABLE OF THE BACK-TRANSFORMED VALUES?
? Y

1
 OBSERVED AND PREDICTED VALUES BACK-TRANSFORMED

 INDEX  IND VAR 1    OBS VAL      PRED VAL

   1  1.82100E+03  2.69000E+02  5.11499E+02
   2  1.82200E+03  3.21000E+02  2.79835E+02
   3  1.82300E+03  5.85000E+02  2.57422E+02
   4  1.82400E+03  8.71000E+02  4.18447E+02
   5  1.82500E+03  1.47500E+03  9.95049E+02
   6  1.82600E+03  2.82100E+03  2.43939E+03
   7  1.82700E+03  3.92800E+03  4.27115E+03
   8  1.82800E+03  5.94300E+03  4.23071E+03
   .       .            .            .
   .       .            .            .
   .       .            .            .

 107  1.92700E+03  1.53700E+03  2.65738E+02
 108  1.92800E+03  5.29000E+02  1.51351E+02
 109  1.92900E+03  4.85000E+02  1.52222E+02
 110  1.93000E+03  6.62000E+02  2.71817E+02
```

```
 111  1.93100E+03  1.00000E+03  6.87089E+02
 112  1.93200E+03  1.59000E+03  1.70598E+03
 113  1.93300E+03  2.65700E+03  2.91940E+03
 114  1.93400E+03  3.39600E+03  2.82543E+03

 NEXT STEP? (TYPE "H" FOR HELP)
? RS

 INDICATE WHICH OF THE FOLLOWING SHOULD BE PRINTED:
   PARAMETERS, THEIR STD DEV & T-RATIO:
? Y

   RES SUM OF SQS, RES MEAN SQ, RES STD DEV &
       COEFF OF DETERMINATION:
? Y

   TABLE OF OBS, PRED VAL, RESID & STD RESID:
? Y

   PLOT OF STD RES VS IND VAR:
? Y

   PLOT OF STD RES VS PRED VAL:
? Y

   NORMAL PROBABILITY PLOT:
? Y

1

    PARAMETER      S.D. OF PARM.     T-RATIO

     6.692901E+00    6.673607E-02    1.002891E+02
     3.384831E-03    2.129423E-03    1.589553E+00
     1.436036E+00    9.395270E-02    1.528467E+01
     4.943990E-01    9.466946E-02    5.222370E+00
     9.619901E+00    2.974943E-02    3.233642E+02
     4.057994E+01    1.679599E+00    2.416050E+01
     4.791006E+00    1.013214E-01    4.728523E+01
     2.191485E+01    1.563618E+00    1.401548E+01


 WTD RESIDUAL SUM OF SQUARES:      5.318834E+01

 WTD RESIDUAL MEAN SQUARE:         5.017768E-01

 WTD RESIDUAL STANDARD ERROR:      7.083621E-01
```

```
 COEFFICIENT OF DETERMINATION (R-SQUARE):     7.128861E-01


1
 INDEX  IND VAR 1    OBS VAL     PRED VAL      RESID        STD RES

   1 -5.70000E+01  5.59471E+00  6.23735E+00 -6.42634E-01 -9.35023E-01
   2 -5.60000E+01  5.77144E+00  5.63420E+00  1.37242E-01  2.04622E-01
   3 -5.50000E+01  6.37161E+00  5.55072E+00  8.20896E-01  1.19547E+00
   4 -5.40000E+01  6.76964E+00  6.03655E+00  7.33093E-01  1.06327E+00
   5 -5.30000E+01  7.29641E+00  6.90279E+00  3.93622E-01  5.88560E-01
   6 -5.20000E+01  7.94485E+00  7.79950E+00  1.45343E-01  2.15503E-01
   7 -5.10000E+01  8.27589E+00  8.35964E+00 -8.37538E-02 -1.22281E-01
   8 -5.00000E+01  8.68997E+00  8.35012E+00  3.39845E-01  4.95178E-01
   .       .            .            .            .            .
   .       .            .            .            .            .
   .       .            .            .            .            .

 107  4.90000E+01  7.33759E+00  5.58251E+00  1.75508E+00  2.61812E+00
 108  5.00000E+01  6.27099E+00  5.01960E+00  1.25139E+00  1.84149E+00
 109  5.10000E+01  6.18415E+00  5.02534E+00  1.15881E+00  1.70112E+00
 110  5.20000E+01  6.49527E+00  5.60513E+00  8.90135E-01  1.32354E+00
 111  5.30000E+01  6.90776E+00  6.53246E+00  3.75292E-01  5.63784E-01
 112  5.40000E+01  7.37149E+00  7.44190E+00 -7.04083E-02 -1.05332E-01
 113  5.50000E+01  7.88495E+00  7.97913E+00 -9.41815E-02 -1.40590E-01
 114  5.60000E+01  8.13035E+00  7.94642E+00  1.83936E-01  2.80809E-01

  ENTER ANY INTEGER TO CONTINUE
? 1

1               STANDARDIZED RESIDUAL VS INDEPENDENT VARIABLE 1

 MEAN IS   .16607042E-02


 GRAPH INTERVAL IS   .99228060E-01
          -COMPUTED FROM MAXIMUM AND MINIMUM VALUES
     -2.34     -1.35      -.36       .63      1.63      2.62
          -1.85      -.85       .14      1.13      2.12
       I----I----I----I----I----I----I----I----I----I----I
     I                                                  I
   1 I              *         I                         I  -.93502E+00
   2 I                        I *                       I   .20462E+00
   3 I                        I          *              I   .11955E+01
   4 I                        I        *                I   .10633E+01
   5 I                        I    *                    I   .58856E+00
```

```
  6  I                        I *                         I   .21550E+00
  7  I                      * I                           I  -.12228E+00
  8  I                        I    *                      I   .49518E+00
  9  I                        I          *                I   .10903E+01
 10  I                        I              *            I   .15080E+01
 11  I                        I   *                       I   .47927E+00
 12  I            *           I                           I  -.12156E+01
 13  I                     *  I                           I  -.34910E+00
 14  I                   *    I                           I  -.58755E+00
 15  I            *           I                           I  -.12772E+01
 16  I                        I *                         I   .20741E+00
 17  I                        *                           I   .36642E-02
 18  I                        I      *                    I   .77381E+00
 19  I                        I         *                 I   .10081E+01
 20  I                        I *                         I   .25590E+00

     .                        .                           .        .
     .                        .                           .        .
     .                        .                           .        .

 95  I                     *  I                           I  -.22937E+00
 96  I                        I           *               I   .13165E+01
 97  I                        I *                         I   .22844E+00
 98  I       *                I                           I  -.17096E+01
 99  I            *           I                           I  -.12623E+01
100  I            *           I                           I  -.12435E+01
101  I            *           I                           I  -.12278E+01
102  I        *               I                           I  -.16747E+01
103  I              *         I                           I  -.10225E+01
104  I                       *I                           I  -.35890E-01
105  I                        I          *                I   .12423E+01
106  I                        I                    *      I   .22550E+01
107  I                        I                          *I   .26181E+01
108  I                        I                *          I   .18415E+01
109  I                        I               *           I   .17011E+01
110  I                        I           *               I   .13235E+01
111  I                        I    *                      I   .56378E+00
112  I                       *I                           I  -.10533E+00
113  I                      * I                           I  -.14059E+00
114  I                        I *                         I   .28081E+00
      I----I----I----I----I----I----I----I----I----I----I
? C

1                STANDARDIZED RESIDUAL VS. PREDICTED VALUES

                   1 Y DIV=  .99228E-01 AND 1 X DIV=  .77613E-01
                 -I---------I---------I---------I---------I---------I-
         2.6181 -           *                                         -
```

```
        I
        I
        I
        I                        *
        I
        I
        I
        I     *
        I     *                 *
 1.6258 -     *                                               -
        I   *                        *
        I            *
        I            *                      *
        I            *                      *
        I                                       *
        I                 2*         *   **     *
        I                         * *
        I                     *
        I    *              *                * *
  .6336 -          *                  *          *            -
        I     *     **           *       *    *          *
        I            *  * *
        I                                            *      2
        I             * *      *             ***  ** *      *
        I               *        *      *             * *
        I                                          *
        I     *                              2    * *
        I            *             *          **    2    *
        I                *                            * *
 -.3587 -          *             *                            -
        I             * *
        I                  *       *                  *
        I               *     *             *             *
        I
        I             *                          *  *
        I                    *          *
        I                                        *
        I     *           *
        I        * **         *   *  2        *      *
-1.3510 - *                                                   -
        I   *                     *           *
        I                              *
        I       *                        *
        I            *
        I
        I
        I
```

```
                I      *
                I                    *
        -2.3433 -                *                                    -
                I
                 -I---------I---------I---------I---------I---------I-
                 4.7307    5.5069    6.2830    7.0591    7.8353    8.6114
? C

1               NORMAL PROBABILITY PLOT

                   1 Y DIV=  .99228E-01 AND 1 X DIV=  .10128
                 -I---------I---------I---------I---------I---------I-
         2.6181 -                                                   * -
                I
                I
                I
                I                                                *
                I
                I
                I
                I                                              *
                I                                           **
         1.6258 -                                          *          -
                I                                         2
                I                                        *
                I                                       2
                I                                      2
                I                                     *
                I                                   232
                I                                  **
                I                                  *
                I                                 3*
          .6336 -                                3                    -
                I                              24*
                I                             *2
                I                             3
                I                           54*
                I                          5
                I                         *
                I                        23
                I                       43
                I                      3
         -.3587 -                      2                              -
                I                     2
                I                    *2
                I                   22
                I
```

```
              I                *2
              I                2
              I               *
              I               2
              I            *232*
     -1.3510 -             *                                    -
              I           *2
              I          *
              I         2
              I       *
              I
              I
              I
              I      *
              I    *
     -2.3433 - *                                                -
              I
               -I---------I---------I---------I---------I---------I-
              -2.5166   -1.5038    -.4909     .5219    1.5348    2.5476
? C

 NEXT STEP? (TYPE "H" FOR HELP)
? SO

 END OF DISSPLA 9.0 -- 10773 VECTORS IN 6 PLOTS.
 RUN ON 4/30/87 USING SERIAL NUMBER 0 AT NBS/CS**2 -
 GAITHERSBERG, MD.
 PROPRIETARY SOFTWARE PRODUCT OF ISSCO, SAN DIEGO, CA.
 3544 VIRTUAL STORAGE REFERENCES; 4 READS; 0 WRITES.
```

9.4 The Graphical Output

The 6 DISSPLA plots generated by the run are shown in Figures 9.4-9.9. The last three of these were generated by the statistical analysis initiated by the "RS" command. They provide valuable diagnostic information for assessing the quality of the fit. The standardized residuals are the residuals divided by their standard deviations. The fact that no wedge-shaped patterns appear in Figures 9.7 and 9.8 indicates that we were probably right to use equal weighting in the VARPRO least squares procedure. The distribution of the points in Figure 9.9 along a straight line through the points (-3.0,-3.0) and (3.0,3.0) is also a good indicator, but it is obvious from inspecting the residual time series (Figure 9.4) that the residuals are significantly correlated. A really good model would give white-noise residuals.

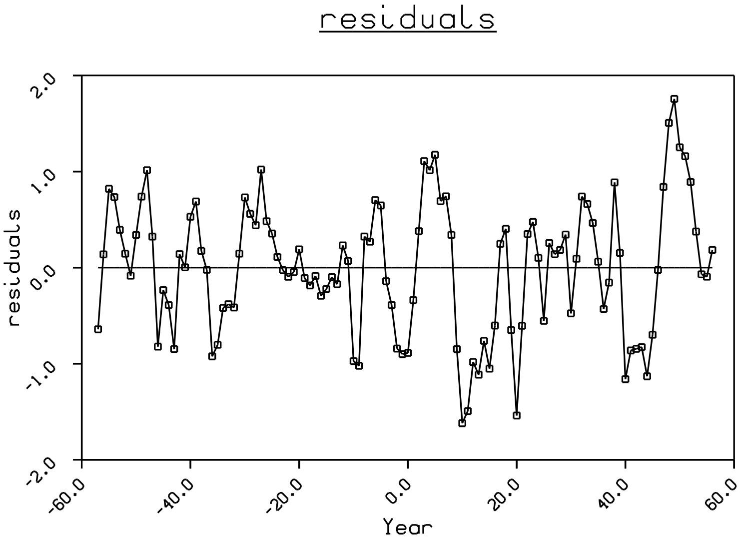


Figure 9.4: The residuals for the fit (transformed data - model)

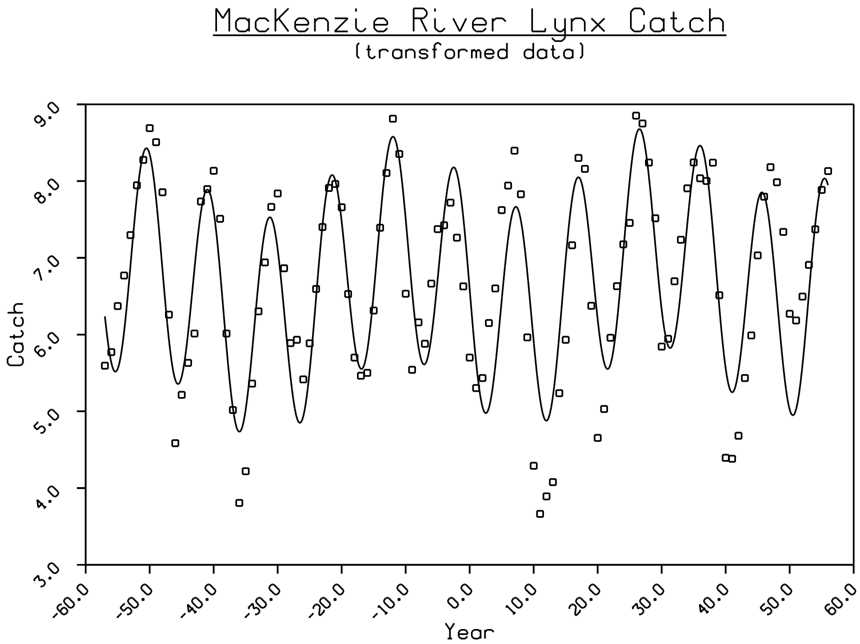


Figure 9.5: The transformed data (boxes) and the fitted model (continuous line)

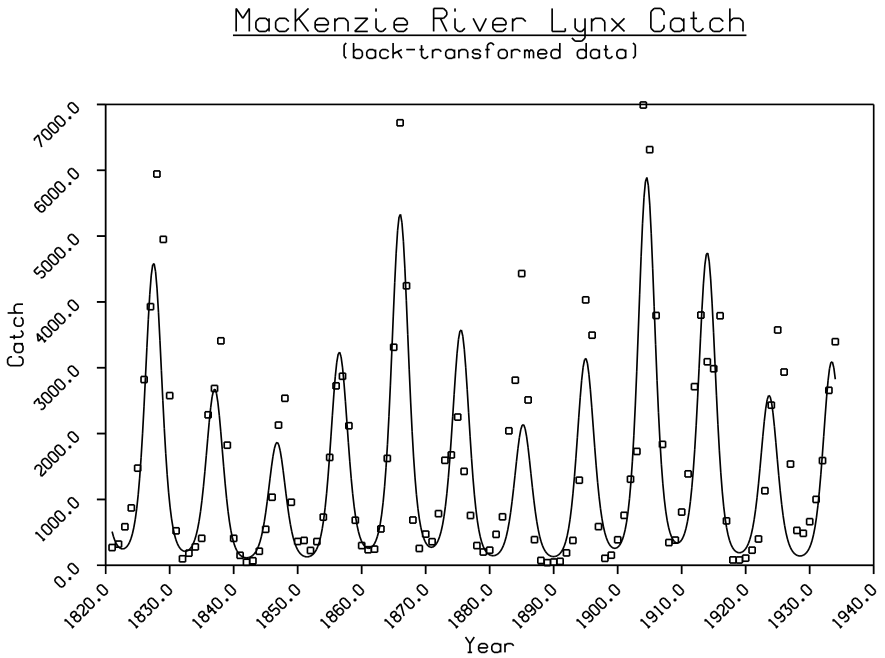


Figure 9.6: The original data and the back-transformed fit

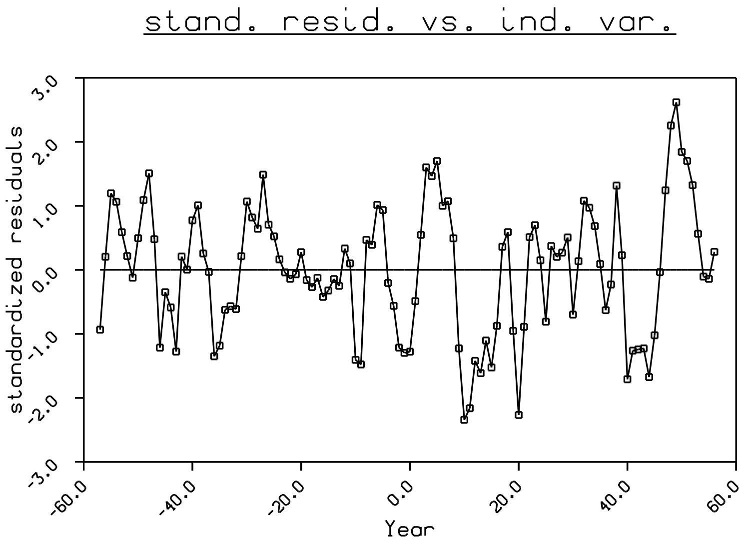


Figure 9.7: Standardized residuals versus the independent variable

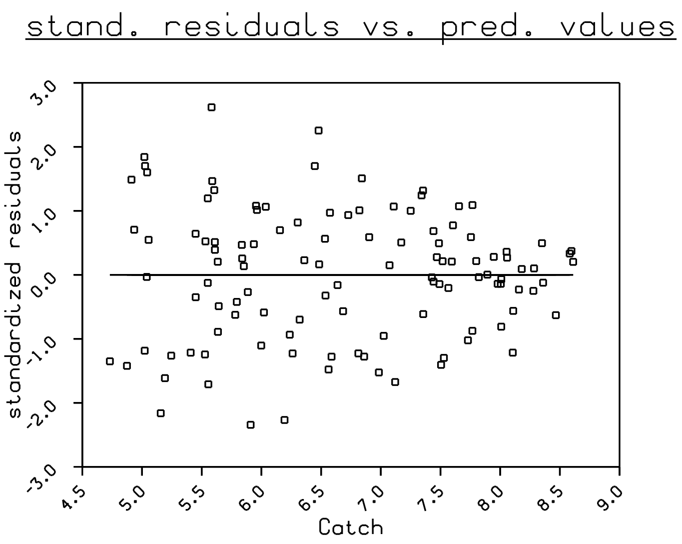


Figure 9.8: Standardized residuals versus the model prediction

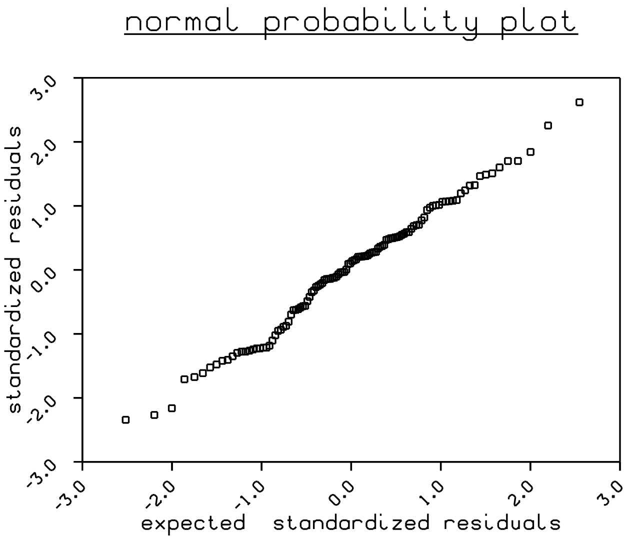


Figure 9.9: Standardized residuals versus the expected standardized residuals when it is assumed that the measurement errors are independently, normally distributed

Chapter 10

AN EXAMPLE WITH TWO INDEPENDENT VARIABLES – VISCOSITY OF ORGANIC COMPOUNDS

10.1 The Model and the Data

As a final example we present a fit of a bivariate model to measured viscosity data for cyclic polystyrene molecules [11]. The model is

$$V(T, M; a, b, \alpha, b_1, T_\infty) = (aM + bM^\alpha)10^{\frac{b_1}{T-T_\infty}} ,$$

where the measured temperature T (deg C) and the molecular weight M of the molecule are the indepedent variables of the fit, and the measured viscosity V is the dependent variable. The constants a, b, α, b_1, and T_∞ are the parameters to be determined by the fit. Since the viscosity data ranges over 12 orders of magnitude, the fitting is much easier is we take $\log_{10} V$ as the independent variable for the fit. Thus the model becomes

$$\eta(T, M) = \log_{10} V = b_1 \frac{1}{T - T_\infty} + \log_{10}(aM + bM^\alpha) ,$$

which can easily be written in the variable separable form described in Chapter 2. The model has a single linear parameter

$$C_1 = b_1 \ ,$$

and 4 nonlinear paramenters

$$\begin{array}{ll} \alpha_1 = T_\infty & , \quad \alpha_2 = a \ , \\ \alpha_3 = b & , \quad \alpha_4 = \alpha \ . \end{array}$$

Thus the model can be written in the form

$$\eta(T, M) = C_1 \Phi_1(T, M) + \Phi_2(T, M) \ ,$$

where

$$\begin{array}{l} \Phi_1(T, M) = \frac{1}{T - \alpha_1} = \frac{1}{T - T_\infty} \ , \\ \Phi_2(T, M) = \log_{10}(\alpha_2 M + \alpha_3 M^{\alpha_4}) = \log_{10}(aM + bM^{\alpha}) \ . \end{array}$$

The data consisted of 159 observed triplets (T_i, M_i, V_i), contained in a file named VISDAT. To make the desired fit, it was necessary to provide a subroutine TRANS to convert these observations to triplets of the form (T_i, M_i, η_i) and a subroutine BAKTRN to backtransform the fit once it had been obtained. These subroutines are given in the following section. On the first run of the program, the transformed data were saved, by using the SD command (see Table 7.1), in a file called VSTRDAT, and this file was used as input for subsequent runs, including the one in the terminal session to be given below. The input file contained the final estimates of the nonlinear parameters, saved from the previous run. These estimates, except for the one of $\alpha_3 = b$, were used as initial estimates in the current run. The statistical analysis from the previous run indicated a high degree of uncertainty for the value of α_3. The current run checks the stability of the fit by changing the estimate of α_3 and repeating the calculation.

10.2 The User-Supplied Subroutines

The user supplied subroutines required to make the fit are given in the following paragraph. These subroutines were all written into a single file, called VSCALC, in accordance with the instructions given in Chapter 3. Subroutine CALC is a straightforward coding of the model equations given in the preceding section. Subroutine DERIV calculates the derivatives with respect to the parameters from the exact, closed form expressions:

$$\frac{\partial\Phi_1}{\partial\alpha_1} = \frac{1}{(T-T_\infty)^2} ,$$
$$\frac{\partial\Phi_1}{\partial\alpha_2} = \frac{\partial\Phi_1}{\partial\alpha_3} = \frac{\partial\Phi_1}{\partial\alpha_4} = 0 ,$$

$$\frac{\partial\Phi_2}{\partial\alpha_1} = 0 ,$$
$$\frac{\partial\Phi_2}{\partial\alpha_2} = \log_{10}(e)\frac{M}{aM+bM^\alpha} ,$$
$$\frac{\partial\Phi_2}{\partial\alpha_3} = \log_{10}(e)\frac{M^\alpha}{aM+bM^\alpha} ,$$
$$\frac{\partial\Phi_2}{\partial\alpha_4} = \log_{10}(e)\frac{b\log_e(M)M^\alpha}{aM+bM^\alpha} .$$

Subroutine WT is designed to give $1/y_i^2$ weighting, but it was not used in the present calculations. The equal weighting default option was used instead. If the user is not sure beforehand about which weighting should be used, it is a good idea to include the WT subroutine given here in case it should be needed. The interactive driver program allows the user to choose which weighting scheme to use at execution time or even to change the weighting scheme if the first one chosen does not work satisfactorily. Subroutines TRANS and BAKTRN make the transformations described in the preceding section.

The subroutines used for this example are:

```
C
C
      SUBROUTINE CALC ( K, NL, N, MMAX, IV, C, ALF, T, ETA )
C
C
      PARAMETER ( MAXN1 = 11 )
C
      DIMENSION C(N), ALF(NL), T(MMAX,IV)
C
      COMMON /BLKPH/ PH(MAXN1)
C
C
      REAL MW
C
      TEMP = T(K,1)
```

```
      MW   = T(K,2)
C
      TMPINF = ALF(1)
      A      = ALF(2)
      B      = ALF(3)
      ALPHA  = ALF(4)
C
      PH(1) = 1.0 / ( TEMP - TMPINF )
      PH(2) = ALOG10 ( A*MW + B*MW**ALPHA )
C
      ETA = C(1)*PH(1) + PH(2)
C
      RETURN
      END
C
C
C-----------------------------------------------------------
C
C
      SUBROUTINE DERIV ( K, T, MMAX, IV, ALF, NL, NP1 )
C
C
      PARAMETER ( MAXN1 = 11 , MAXKG = 8 )
C
      DIMENSION ALF(NL),T(MMAX,IV)
C
      COMMON /BLKDPH/ DPH(MAXN1,MAXKG)
C
C
      REAL MW, LOG10E
C
      TEMP = T(K,1)
      MW   = T(K,2)
C
      TMPINF = ALF(1)
      A      = ALF(2)
      B      = ALF(3)
      ALPHA  = ALF(4)
C
```

```
      LOG10E = ALOG10 ( EXP(1.0) )
C
      DO 10 J=1,NL
        DO 10 I=1,NP1
          DPH(I,J) = 0.0
   10 CONTINUE
C
C
C           DPH(I,J) SHOULD BE SET TO THE PARTIAL DERIVATIVE
C                    OF PH(I) WITH RESPECT TO ALF(J)
C
      DPH(1,1) = 1.0 / ( TEMP - TMPINF )**2
C
      DENOM = A*MW + B*MW**ALPHA
C
      DPH(2,2) = LOG10E*MW / DENOM
      DPH(2,3) = LOG10E*MW**ALPHA / DENOM
      DPH(2,4) = LOG10E*B*ALOG(MW)*MW**ALPHA / DENOM
C
      RETURN
      END
C
C
C------------------------------------------------------------
C
C
      SUBROUTINE WT ( M, WEIGHT, Y )
C
C
      DIMENSION Y(M),WEIGHT(M)
C
       DO 10 I=1,M
         WEIGHT(I) = 1.0/Y(I)**2
   10  CONTINUE
C
      RETURN
      END
C
C------------------------------------------------------------
```

```
C
C
      SUBROUTINE TRANS ( T, BT, Y, BY, IV, M, MMAX )
C
C
      DIMENSION T(MMAX,IV), BT(MMAX,IV), Y(M), BY(M)
C
      DO 20 I=1,M
C
          BY(I) = Y(I)
C
          DO 10 J=1,IV
C
              BT(I,J) = T(I,J)
C
   10     CONTINUE
C
          Y(I) = ALOG10 ( Y(I) )
C
   20 CONTINUE
C
      RETURN
      END
C
C
C------------------------------------------------------------
C
C
      SUBROUTINE BAKTRN ( ETA, BETA, M )
C
C
      DIMENSION ETA(M), BETA(M)
C
      DO 10 I=1,M
C
         BETA(I) = 10.0**ETA(I)
C
   10 CONTINUE
C
```

```
      RETURN
      END
```

These subroutines were written into a file named VSCALC which was compiled and loaded with the INVAR programs and then executed in a terminal session to be described in the following section.

10.3 The Terminal Session

The terminal session output that follows was obtained by executing INVAR2 on the NBS CYBER 855, running from a Qume QVT-201 terminal in screen mode. Since the terminal was not a plotting terminal, the DISSPLA plots were done after execution on the QMS laser printer with address B225. Before reading this example, the following points should be noted:

1. Since the terminal was running in screen mode, the INVOKE,INVAR command generated a new screen shown between the horizontal lines at the beginning of the session. This was done by the interactive NOS Procedure INVARX in order to quiz the user for the location of the user-supplied subroutines, the address of the QMS printer for the plots and hardcopy output, and the name of the data file. Non-NBS users need not concern themselves with these responses.

2. The terminal session given here is not the first run of the problem. In a previous run the logarithmic transformation of the viscosity data was performed and the resulting transformed data was written into a file called VSTRDAT. This file is used as input for the current run so it is not necessary to perform the transformations again.

3. The file VSTRDAT also contained the final parameter estimates from the previous run. One of these was altered and the resulting set was used as initial estimates for the current run.

4. After each line printer graph, the program stops with a question mark prompt (?) generated by the TK4014 program used at NBS to generate DISSPLA plots for the laser printer. We replied to this prompt with a "C" followed by a carriage return since a carriage return alone would have caused an end-of-file error stop.

The terminal session follows:

```
/INVOKE,INVAR
```

```
                INTERACTIVE NONLINEAR LEAST SQUARES PROGRAM

 CALCF  FORTRAN file of user-supplied subroutines: VSCALC_
 QMSADDR  QMS Address for output (Default = NONE): B225___
               DATAF  Data file (Default = NONE): VSTRDAT
      INV102  INVAR1 or INVAR2 (Default = INVAR2): _______

                   Specify values and press NEXT when ready
 ------------------------------------ INVARX ------------------------------

        PROC,INVARX,CALCF[,QMSADDR][,DATAF][,INV102].

 Executes one of two versions, INVAR1 or INVAR2, of INVAR, an
 interactive, variable separable, nonlinear least squares program.

 Local file CALCF contains FORTRAN coded, user-supplied subroutines.

 Hardcopy output and plots can be sent to QMS laser printer with
 address QMSADDR.

 Permanent file DATAF contains data to be fit (not needed if data
 already in a local file, or is to be typed in during execution).
                          F3 HELP                   F5   HELP    F6   QUIT
```

```
 ENTER TITLE (MAXIMUM OF 40 CHARACTERS):
? VISCOSITY STUDY

 DO YOU WANT DISSPLA PLOTS? (TYPE "Y" FOR YES)
? Y

 DO YOU WANT THESE PLOTS SHOWN INTERACTIVELY ON
 A PLOTTING SCREEN (TYPE "1");
 OR SAVED IN A FILE TO BE PRINTED OUT LATER (TYPE "2")?
? 2

 ENTER LABEL FOR INDEPENDENT VARIABLE 1 (MAX. OF 47 CHARACTERS):
? TEMPERATURE

 ENTER LABEL FOR DEPENDENT VARIABLE (MAX. OF 47 CHARACTERS):
? LOG VISCOSITY

 DO YOU WANT LINE PRINTER OUTPUT?
? Y

 ARE YOUR DATA, WEIGHTS, INITIAL VALUES, ETC.
               ALREADY IN A VARPRO-DEFINED FILE ?
```

```
? Y

 TYPE NAME OF FILE (MAX. OF 26 CHARACTERS):
? VSTRDAT


 WOULD YOU LIKE YOUR INITIAL VALUES FILE PRINTED?
? Y

 NO. OF DATA POINTS:   159


 NO. OF LINEAR PARAMETERS:     1


 NO. OF NONLINEAR PARAMETERS:     4


 NO. OF INDEPENDENT VARIABLES:     2


 INDEX     WEIGHT         DEP VAR       IND VAR  1     IND VAR  2

   1      1.000000E+00   1.039110E+01   1.034000E+02   1.939992E+04
   2      1.000000E+00   1.042550E+01   1.034000E+02   1.939992E+04
   3      1.000000E+00   1.157900E+01   1.044000E+02   1.059986E+05
   4      1.000000E+00   1.111420E+01   1.055000E+02   1.059986E+05
   5      1.000000E+00   9.325700E+00   1.092000E+02   4.400480E+04
   6      1.000000E+00   9.458500E+00   1.092000E+02   4.400480E+04
   7      1.000000E+00   8.881800E+00   1.101000E+02   1.939992E+04
   8      1.000000E+00   9.621300E+00   1.137000E+02   1.060010E+05
   9      1.000000E+00   8.134600E+00   1.140000E+02   1.939992E+04
  10      1.000000E+00   1.133620E+01   1.144000E+02   1.815098E+05
  11      1.000000E+00   7.444100E+00   1.185000E+02   1.939992E+04
  12      1.000000E+00   7.449300E+00   1.185000E+02   1.939992E+04
  13      1.000000E+00   6.785000E+00   1.200000E+02   1.250259E+04
  14      1.000000E+00   7.829000E+00   1.201000E+02   5.046613E+04
  15      1.000000E+00   7.656400E+00   1.206000E+02   4.400480E+04

                .              .              .              .
                .              .              .              .
                .              .              .              .

 145      1.000000E+00   1.792000E+00   1.959000E+02   1.250259E+04
 146      1.000000E+00   5.825600E+00   1.992000E+02   3.900318E+05
 147      1.000000E+00   5.884100E+00   1.993000E+02   3.900318E+05
 148      1.000000E+00   4.238000E+00   2.002000E+02   1.169499E+05
```

```
 149      1.000000E+00   1.562000E+00   2.005000E+02   1.109175E+04
 150      1.000000E+00   2.227000E+00   2.009000E+02   2.697739E+04
 151      1.000000E+00   4.144600E+00   2.015000E+02   1.059986E+05
 152      1.000000E+00   2.392000E+00   2.024000E+02   3.780071E+04
 153      1.000000E+00   3.307000E+00   2.040000E+02   7.943282E+04
 154      1.000000E+00   3.849000E+00   2.088000E+02   1.169499E+05
 155      1.000000E+00   3.828000E+00   2.091000E+02   1.059986E+05
 156      1.000000E+00   1.988000E+00   2.096000E+02   2.697739E+04
 157      1.000000E+00   3.140000E+00   2.114000E+02   7.943282E+04
 158      1.000000E+00   2.975000E+00   2.176000E+02   7.943282E+04
 159      1.000000E+00   1.695000E+00   2.222000E+02   2.697739E+04


 NONLINEAR PARAMETERS:
   1      4.784193E+01
   2      9.380365E-08
   3      3.625116E-19
   4      3.528796E+00


 NUMERICAL DERIVATIVE INCREMENTS:
   1       .000000E+00
   2       .000000E+00
   3       .000000E+00
   4       .000000E+00


 TERMS WHICH DEPEND ON NONLIN PARM 1:   1 0


 TERMS WHICH DEPEND ON NONLIN PARM 2:   2 0


 TERMS WHICH DEPEND ON NONLIN PARM 3:   2 0


 TERMS WHICH DEPEND ON NONLIN PARM 4:   2 0

 DOES DATA FOLLOW AN EVENLY SPACED TIME SERIES?
? N


   NOTE:   THE COMMAND "SC" WILL SAVE YOUR DATA FILE AT ANY TIME


 NEXT STEP? (TYPE "H" FOR HELP)
? CALF
```

```
 WHICH NONLINEAR PARAMETER IS TO BE CHANGED?
 (TYPE ITS INDEX NO. AS IT APPEARS IN THE LIST)
? 3

 ENTER NEW VALUE FOR PARAMETER   3:
? 1.0E-20

DO YOU WANT TO CHANGE ANY OTHERS?
? N


 NEXT STEP? (TYPE "H" FOR HELP)
? RV


 DO YOU WISH TO CHANGE ANY DEFAULTS IN THE LEAST SQUARES PROGRAM?
        (50: MAX. NO. OF ITERATIONS)
        (1.0E-5: CONVERG. TOLERANCE)
        (1: OUTPUT PRINTING INDEX)
? N

1                    VISCOSITY STUDY



    0  WEIGHTED NORM OF RESIDUAL =   7.8237556E+00
     NU =   .1000000E+01


   ITERATION   1    NONLINEAR PARAMETERS

    4.4009180E+01         3.7498487E-08

    1.7653158E-20         3.6340762E+00

    1  WEIGHTED NORM OF RESIDUAL =   2.8593973E+00
     NU =   .5000000E+00
     NORM(DELTA-ALF) / NORM(ALF) =   8.683E-02


   ITERATION   2    NONLINEAR PARAMETERS

    4.2417711E+01         3.2665216E-08

    2.1665495E-20         3.6639208E+00
```

```
 1  WEIGHTED NORM OF RESIDUAL =   2.0880991E+00
  NU =   .2500000E+00
  NORM(DELTA-ALF) / NORM(ALF) =   3.739E-02


ITERATION   3    NONLINEAR PARAMETERS

 4.3127340E+01          3.8470079E-08

 2.5542614E-20          3.6717600E+00

 1  WEIGHTED NORM OF RESIDUAL =   2.0585942E+00
  NU =   .1250000E+00
  NORM(DELTA-ALF) / NORM(ALF) =   1.640E-02


ITERATION   4    NONLINEAR PARAMETERS

 4.5077562E+01          5.3682115E-08

 3.7296374E-20          3.6665329E+00

 1  WEIGHTED NORM OF RESIDUAL =   2.0383975E+00
  NU =   .6250000E-01
  NORM(DELTA-ALF) / NORM(ALF) =   4.312E-02


                    .
                    .
                    .

ITERATION  17    NONLINEAR PARAMETERS

 4.7841930E+01          9.3803727E-08

 3.6250423E-19          3.5287977E+00

 1  WEIGHTED NORM OF RESIDUAL =   1.9930702E+00
  NU =   .1647949E-02
  NORM(DELTA-ALF) / NORM(ALF) =   1.424E-06


ITERATION  18    NONLINEAR PARAMETERS

 4.7841931E+01          9.3803654E-08

 3.6251113E-19          3.5287962E+00
```

```
   1  WEIGHTED NORM OF RESIDUAL =   1.9930702E+00
    NU =   .8239746E-03
    NORM(DELTA-ALF) / NORM(ALF) =   3.974E-08

 ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,

   LINEAR PARAMETERS

   .7046765E+03

   NONLINEAR PARAMETERS

   .4784193E+02   .9380365E-07   .3625111E-18   .3528796E+01

   WEIGHTED NORM OF RESIDUAL =   .1993070E+01

   WEIGHTED ESTIMATED VARIANCE =   .2579434E-01

 ,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,
 INDICATE WHICH OF THE FOLLOWING SHOULD BE PRINTED
 BY TYPING "Y":
  TABLE OF OBSERVED & PREDICTED VALUES, WTD RESIDUAL:
? Y

   COVARIANCE MATRIX:
? N

   CORRELATION MATRIX:
? Y

1


 INDEX  IND VAR 1    OBS VAL      PRED VAL     WTD RESID     WEIGHTS

   1  1.03400E+02  1.03911E+01  1.00472E+01  3.43947E-01  1.00000E+00
   2  1.03400E+02  1.04255E+01  1.00472E+01  3.78347E-01  1.00000E+00
   3  1.04400E+02  1.15790E+01  1.17734E+01 -1.94402E-01  1.00000E+00
   4  1.05500E+02  1.11142E+01  1.15357E+01 -4.21502E-01  1.00000E+00
   5  1.09200E+02  9.32570E+00  9.59673E+00 -2.71031E-01  1.00000E+00
   6  1.09200E+02  9.45850E+00  9.59673E+00 -1.38231E-01  1.00000E+00
   7  1.10100E+02  8.88180E+00  8.68219E+00  1.99613E-01  1.00000E+00
   8  1.13700E+02  9.62130E+00  1.00140E+01 -3.92717E-01  1.00000E+00
   9  1.14000E+02  8.13460E+00  8.01496E+00  1.19644E-01  1.00000E+00
  10  1.14400E+02  1.13362E+01  1.07099E+01  6.26285E-01  1.00000E+00
  11  1.18500E+02  7.44410E+00  7.33660E+00  1.07500E-01  1.00000E+00
  12  1.18500E+02  7.44930E+00  7.33660E+00  1.12700E-01  1.00000E+00
```

```
  13  1.20000E+02  6.78500E+00  6.87183E+00 -8.68340E-02  1.00000E+00
  14  1.20100E+02  7.82900E+00  8.03168E+00 -2.02682E-01  1.00000E+00
  15  1.20600E+02  7.65640E+00  7.79727E+00 -1.40873E-01  1.00000E+00

           .            .            .            .            .
           .            .            .            .            .
           .            .            .            .            .

 145  1.95900E+02  1.79200E+00  1.86556E+00 -7.35603E-02  1.00000E+00
 146  1.99200E+02  5.82560E+00  5.94568E+00 -1.20081E-01  1.00000E+00
 147  1.99300E+02  5.88410E+00  5.94261E+00 -5.85071E-02  1.00000E+00
 148  2.00200E+02  4.23800E+00  4.08523E+00  1.52767E-01  1.00000E+00
 149  2.00500E+02  1.56200E+00  1.66081E+00 -9.88084E-02  1.00000E+00
 150  2.00900E+02  2.22700E+00  2.21664E+00  1.03581E-02  1.00000E+00
 151  2.01500E+02  4.14460E+00  3.90006E+00  2.44540E-01  1.00000E+00
 152  2.02400E+02  2.39200E+00  2.49895E+00 -1.06954E-01  1.00000E+00
 153  2.04000E+02  3.30700E+00  3.40643E+00 -9.94273E-02  1.00000E+00
 154  2.08800E+02  3.84900E+00  3.83811E+00  1.08884E-02  1.00000E+00
 155  2.09100E+02  3.82800E+00  3.68392E+00  1.44076E-01  1.00000E+00
 156  2.09600E+02  1.98800E+00  1.96902E+00  1.89788E-02  1.00000E+00
 157  2.11400E+02  3.14000E+00  3.20226E+00 -6.22605E-02  1.00000E+00
 158  2.17600E+02  2.97500E+00  3.04491E+00 -6.99061E-02  1.00000E+00
 159  2.22200E+02  1.69500E+00  1.65421E+00  4.07915E-02  1.00000E+00
1

               CORRELATION MATRIX


 ROW      COLUMN    1     COLUMN    2     COLUMN    3     COLUMN    4

   1       1.000000E+00  -9.877161E-01  -9.708057E-01  -4.157271E-01
   2      -9.877161E-01   1.000000E+00   9.367497E-01   3.886600E-01
   3      -9.708057E-01   9.367497E-01   1.000000E+00   3.334069E-01
   4      -4.157271E-01   3.886600E-01   3.334069E-01   1.000000E+00
   5      -4.404127E-04   1.502759E-02   8.473789E-02  -9.063612E-01


 ROW      COLUMN    5
   1      -4.404127E-04
   2       1.502759E-02
   3       8.473789E-02
   4      -9.063612E-01
   5       1.000000E+00

 PLOT ROUTINE CURRENTLY SET NOT TO DO ANY PLOTS.
 DO YOU WANT TO START PLOTTING?
? Y
```

```
 WHICH INDEPENDENT VARIABLE SHOULD BE USED?
 (TYPE ITS NUMBER)
? 1

 IF YOU WANT TO PLOT RESIDUALS, TYPE "1"
 IF YOU WANT TO PLOT OBSERVED & PREDICTED VALUES, TYPE "2"
 IF YOU WANT TO PLOT BOTH, TYPE "3":
? 3

1               RESIDUALS
                IND VAR 1
                   1 Y DIV=  .20956E-01 AND 1 X DIV=  2.3760
                 -I---------I---------I---------I---------I---------I-
          .6263 -      *                                              -
                I
                I
                I
                I
                I
                I
                I           *
                I
                I
          .4167 -                      2                              -
                I
                I *
                I *
                I
                I
                I                             2
                I                             *      **    *
                I                                     *
          .2072 -    *                                                -
                I            *    *    *      *        *
                I                 *                        *  *
                I     *          *   *    2
                I       2    *   *    *3        * * *
                I             ******                * 
                I         *2*     ** *        2
                I             *     *     * * *                     *
                I            * ***    2 *         *        *  **
         -.0024 -          * * *     2  *     *       *               -
                I        **    2*2* * * 2         *
                I          2        * *   *
                I                     *2    22  *   * * ***    *  *
```

```
                I        *              *   * *  *  **
                I          *      *         *      *   2*  *2
                I   *                  2    * 2 *   *  *  *
                I        2   *    *                 *
                I
                I *          * *
         -.2119 -        *                                            -
                I                           *
                I             *   *
                I   *       *     *
                I                         *           *
                I
                I
                I         *
                I
                I     *
         -.4215 -  *                                                  -
                I
                 -I---------I---------I---------I---------I---------I-
               103.4000  127.1600  150.9200  174.6800  198.4400  222.2000
? C

1               OBSERVED (*) & PREDICTED (+) VALUES
                IND VAR 1
                   1 Y DIV=  .20423     AND 1 X DIV=  2.3760
                 -I---------I---------I---------I---------I---------I-
        11.7734 - +                                                   -
                I *+
                I      *
                I  *
                I        +
                I      + *
                I
                I 2
                I 2
                I     +
         9.7311 -          +                                          -
                I   3 *    **
                I   *      2   +
                I           +  *
                I    *    3
                I    +    2  +
                I         *  *
                I           +2   2   2
                I     2  +  *2
                I        2    2         2
         7.6888 -        3    +   2                                   -
                I       2     *       2
```

```
                I       2        *     4
                I            *   +2    2      +
                I        2 2*+  2 2    2      *
                I           ++   22    4
                I          2 * +  2   2      2      2
                I          4  **              2     2
                I             +2 2  2  4    + *
                I                *    22  2 * 3           4
         5.6466 -            2   +32                                  -
                I               2 *     2 +   *      *22
                I              42 2 2     *   +      +32
                I                  2   *    +
                I               22   *2+    *   2 2   *
                I                 + +         2     2  *
                I                 *  22 2   2   2   2  +
                I                   2*  2 2                2
                I                    +        2     2      +
                I                     2   2  22         + + 3
         3.6043 -                       + *             *     +       -
                I                       * + 3 2  2          2
                I                           *      2           2
                I                           4 *   2 2             2
                I                             3         +
                I                               2     2 *   +
                I                                 2         *
                I                                   + +    2
                I                                   * *+       2
                I                                      * 2          *
         1.5620 -                                          2        + -
                I
                 -I---------I---------I---------I---------I---------I-
               103.4000  127.1600  150.9200  174.6800  198.4400  222.2000
? C

 DO YOU WANT TO CONTINUE PLOTTING USING A DIFFERENT
 INDEPENDENT VARIABLE?
? Y

 WHICH INDEPENDENT VARIABLE SHOULD BE USED?
 (TYPE ITS NUMBER)
? 2

 TYPE IN ITS LABEL (MAX. OF 47 CHARACTERS)
? MOLECULAR WEIGHT

 IF YOU WANT TO PLOT RESIDUALS, TYPE "1"
 IF YOU WANT TO PLOT OBSERVED & PREDICTED VALUES, TYPE "2"
 IF YOU WANT TO PLOT BOTH, TYPE "3":
```

```
? 3

1                RESIDUALS
                 IND VAR 2
                    1 Y DIV=  .20956E-01 AND 1 X DIV=  7800.6
                  -I---------I---------I---------I---------I---------I-
          .6263 - *                                                   -
                I
                I
                I
                I
                I
                I
                I *
                I
                I
          .4167 - 2                                                   -
                I
                I *
                I *
                I
                I
                I 2
                I
                I 3                        *
                I *
          .2072 - *                                                   -
                I
                I 5
                I * *   *
                I 5
                I X
                I 7
                I 9
                I 5             *
                I 8 2   *
         -.0024 - 8                                                   -
                I X
                I 5
                I X     2       2                                   *
                I 7
                I 6 3           *
                I 8 *   *
                I 5
                I
                I 3
         -.2119 - *                                                   -
```

```
               I *
               I 2
               I 3
               I 2
               I
               I
               I *
               I
               I *
        -.4215 - *                                                 -
               I
                -I---------I---------I---------I---------I---------I-
               .000E+00  .780E+05  .156E+06  .234E+06  .312E+06  .390E+06
? C

1              OBSERVED (*) & PREDICTED (+) VALUES
               IND VAR 2
                  1 Y DIV=  .20423     AND 1 X DIV=  7800.6
                -I---------I---------I---------I---------I---------I-
       11.7734 - +                                                 -
               I 2
               I *
               I *
               I +
               I 2
               I
               I 2
               I 2
               I +
        9.7311 - +                                                 -
               I 6
               I 4
               I 2
               I 4
               I 4
               I 2
               I 7
               I 6
               I 6
        7.6888 - 6                                                 -
               I 5
               I 7
               I 7
               I X
               I X
               I X
               I X
               I X
```

```
             I X     4
     5.6466 - 8                                               -
             I X
             I X
             I 4
             I X
             I 7
             I X
             I 7 *                   *
             I 5 +
             I 8 2   *       +       +
     3.6043 - 2     +       *                                 -
             I 9 2
             I 3     2
             I 9                                            2
             I 3 +
             I 4 2
             I 2 *
             I 2 2
             I 2 +   2
             I   *           3
     1.5620 -               3                                 -
             I
              -I---------I---------I---------I---------I---------I-
             .000E+00  .780E+05  .156E+06  .234E+06  .312E+06  .390E+06
? C

 DO YOU WANT TO CONTINUE PLOTTING USING A DIFFERENT
 INDEPENDENT VARIABLE?
? N

 NEXT STEP? (TYPE "H" FOR HELP)
? RS

INDICATE WHICH OF THE FOLLOWING SHOULD BE PRINTED:
   PARAMETERS, THEIR STD DEV & T-RATIO:
? Y

   RES SUM OF SQS, RES MEAN SQ, RES STD DEV &
       COEFF OF DETERMINATION:
? Y

   TABLE OF OBS, PRED VAL, RESID & STD RESID:
? Y

   PLOT OF STD RES VS IND VAR:
? Y
```

```
   PLOT OF STD RES VS PRED VAL:
? Y

   NORMAL PROBABILITY PLOT:
? Y

1

    PARAMETER      S.D. OF PARM.     T-RATIO

     7.046765E+02    3.001868E+01    2.347460E+01
     4.784193E+01    1.903958E+00    2.512761E+01
     9.380365E-08    3.514149E-08    2.669313E+00
     3.625111E-19    3.158989E-19    1.147554E+00
     3.528796E+00    6.666115E-02    5.293632E+01


 WTD RESIDUAL SUM OF SQUARES:       3.972329E+00

 WTD RESIDUAL MEAN SQUARE:          2.579434E-02

 WTD RESIDUAL STANDARD ERROR:       1.606062E-01


 COEFFICIENT OF DETERMINATION (R-SQUARE):     9.947714E-01


1
 INDEX  IND VAR 1    OBS VAL     PRED VAL      RESID        STD RES

   1  1.03400E+02  1.03911E+01  1.00472E+01  3.43947E-01  7.73207E-02
   2  1.03400E+02  1.04255E+01  1.00472E+01  3.78347E-01  7.99518E-01
   3  1.04400E+02  1.15790E+01  1.17734E+01 -1.94402E-01 -4.14347E-01
   4  1.05500E+02  1.11142E+01  1.15357E+01 -4.21502E-01 -9.08277E-01
   5  1.09200E+02  9.32570E+00  9.59673E+00 -2.71031E-01 -6.07569E-01
   6  1.09200E+02  9.45850E+00  9.59673E+00 -1.38231E-01 -3.09873E-01
   7  1.10100E+02  8.88180E+00  8.68219E+00  1.99613E-01  4.52273E-01
   8  1.13700E+02  9.62130E+00  1.00140E+01 -3.92717E-01 -9.26535E-01
   9  1.14000E+02  8.13460E+00  8.01496E+00  1.19644E-01  2.83551E-01
  10  1.14400E+02  1.13362E+01  1.07099E+01  6.26285E-01  1.48918E+00
  11  1.18500E+02  7.44410E+00  7.33660E+00  1.07500E-01  2.69052E-01
  12  1.18500E+02  7.44930E+00  7.33660E+00  1.12700E-01  2.82066E-01
  13  1.20000E+02  6.78500E+00  6.87183E+00 -8.68340E-02 -2.21284E-01
  14  1.20100E+02  7.82900E+00  8.03168E+00 -2.02682E-01 -5.16977E-01
  15  1.20600E+02  7.65640E+00  7.79727E+00 -1.40873E-01 -3.61656E-01

           .            .            .            .            .
```

```
           .            .            .            .            .
           .            .            .            .            .

 145  1.95900E+02  1.79200E+00  1.86556E+00 -7.35603E-02 -7.09552E-01
 146  1.99200E+02  5.82560E+00  5.94568E+00 -1.20081E-01 -1.25855E+00
 147  1.99300E+02  5.88410E+00  5.94261E+00 -5.85071E-02 -6.15507E-01
 148  2.00200E+02  4.23800E+00  4.08523E+00  1.52767E-01  1.76382E+00
 149  2.00500E+02  1.56200E+00  1.66081E+00 -9.88084E-02 -1.13245E+00
 150  2.00900E+02  2.22700E+00  2.21664E+00  1.03581E-02  1.23628E-01
 151  2.01500E+02  4.14460E+00  3.90006E+00  2.44540E-01  2.99568E+00
 152  2.02400E+02  2.39200E+00  2.49895E+00 -1.06954E-01 -1.36252E+00
 153  2.04000E+02  3.30700E+00  3.40643E+00 -9.94273E-02 -1.38257E+00
 154  2.08800E+02  3.84900E+00  3.83811E+00  1.08884E-02  2.29712E-01
 155  2.09100E+02  3.82800E+00  3.68392E+00  1.44076E-01  3.14602E+00
 156  2.09600E+02  1.98800E+00  1.96902E+00  1.89788E-02  4.47527E-01
 157  2.11400E+02  3.14000E+00  3.20226E+00 -6.22605E-02 -2.03067E+00
 158  2.17600E+02  2.97500E+00  3.04491E+00 -6.99061E-02 -1.50806E+00
 159  2.22200E+02  1.69500E+00  1.65421E+00  4.07915E-02  6.21755E-01

  ENTER ANY INTEGER TO CONTINUE
? 1

1               STANDARDIZED RESIDUAL VS INDEPENDENT VARIABLE 1

                   1 Y DIV=  .10983     AND 1 X DIV=  2.3760
                 -I---------I---------I---------I---------I---------I-
         3.1460 -                                             *        -
                I                                          *
                I
                I
                I
                I
                I
                I
                I
                I
         2.0477 -                                                      -
                I                                     *
                I                                    **
                I                      2                   *
                I                             2
                I      *
                I           *                 *        *
                I
                I
                I
          .9495 -                                                      -
                I *                           *
```

```
                I                                 * *
                I                 *    *  *     *   *               *
                I                 *  * *  *
                I    *       *   *    *2                        *
                I     * 2    ****2** *        2
                I         *2* *   ***     * * *               *
                I *          * ***    2 *         *        *
                I        *** *  *2  *2* 3     *       *
         -.1488 -          2   2* * * *   *       *                   -
                I   *    * *          *2    2*
                I *      2        *     *   *** *   *
                I        *   *    *    *         *
                I   *        * *       *    2 *     ***   *
                I                             * *  *    **
                I           * *                     *
                I  *  *   *       2                    2
                I                                   *  **
                I                           *              *
        -1.2471 -                                         *           -
                I                         *                 2
                I                                                 *
                I
                I
                I
                I
                I                                              *
                I
                I
        -2.3454 -                                     *               -
                I
                 -I---------I---------I---------I---------I---------I-
               103.4000  127.1600  150.9200  174.6800  198.4400  222.2000
? C

1               STANDARDIZED RESIDUAL VS INDEPENDENT VARIABLE 2

                   1 Y DIV=  .10983     AND 1 X DIV=  7800.6
                 -I---------I---------I---------I---------I---------I-
         3.1460 -       *                                             -
                I                        *
                I
                I
                I
                I
                I
                I
                I
                I
```

```
         2.0477 -                                                     -
                I *
                I 2
                I 2 *
                I 2
                I *
                I 3
                I
                I
                I
          .9495 -                                                     -
                I 2
                I 2
                I 5             *
                I 4
                I 6     *
                I X
                I X *
                I 9 *
                I X
         -.1488 - X                                                   -
                I 9
                I X
                I 5
                I X     *
                I 3             2
                I 3
                I 7
                I * 2
                I *             *
        -1.2471 -       *                                             -
                I * 2
                I                                                   *
                I
                I
                I
                I
                I       *
                I
                I
        -2.3454 - *                                                   -
                I
                 -I---------I---------I---------I---------I---------I-
                .000E+00  .780E+05  .156E+06  .234E+06  .312E+06  .390E+06
? C

1               STANDARDIZED RESIDUAL VS. PREDICTED VALUES
```

```
           1 Y DIV=  .10983     AND 1 X DIV=  .20238
         -I---------I---------I---------I---------I---------I-
 3.1460 -           *                                        -
        I            *
        I
        I
        I
        I
        I
        I
        I
        I
 2.0477 -                                                    -
        I                  *
        I                  **
        I             *            2
        I                      2
        I                                              *
        I              *       *               *
        I
        I
        I
  .9495 -                                                    -
        I                   *                      *
        I               **
        I *             * *   **    *
        I          *  *        *    *
        I   *             *    * *   *    *  *
        I            2   2 **** 2     2  **
        I       *    2 *   * 2   ***    *     *
        I    *   *    * ** *    *  **              *
        I      *   *    2   2 2 * * *   ** 2 *
 -.1488 -     *       *** **     2     *          *          -
        I        *   2    *         *2          **
        I       *  2  * *    *    *     *               *   *
        I          *               *    * *  *
        I   *    2 *     *     *  *2            **
        I  *   *  * *                *
        I                         *     *  *
        I                    2     2          *    *       *
        I  * *  *
        I *                     *
-1.2471 -                      *                             -
        I     *    *         *
        I        *
        I
        I
```

```
             I
             I
             I         *
             I
             I
     -2.3454 -                  *                                 -
             I
              -I---------I---------I---------I---------I---------I-
              1.6542    3.6780    5.7019    7.7257    9.7496   11.7734
? C

1               NORMAL PROBABILITY PLOT

                1 Y DIV=  .10983     AND 1 X DIV=  .10564
              -I---------I---------I---------I---------I---------I-
      3.1460 -                                                  * -
             I                                               *
             I
             I
             I
             I
             I
             I
             I
             I
      2.0477 -                                                    -
             I                                             *
             I                                           **
             I                                         2*
             I                                          2
             I                                         *
             I                                      2*
             I
             I
             I
       .9495 -                                                    -
             I                                       2
             I                                      **
             I                                     33
             I                                      4
             I                                    24*
             I                                  563
             I                                57
             I                              27*
             I                            574
      -.1488 -                          262                       -
             I                           45
             I                         262
```

```
             I                 23
             I               353
             I              4*
             I             3
             I            33*
             I          *2
             I         **
     -1.2471 -        *                                    -
             I       ***
             I       *
             I
             I
             I
             I
             I    *
             I
             I
     -2.3454 - *                                           -
             I
             -I---------I---------I---------I---------I---------I-
             -2.6262   -1.5698    -.5134     .5430    1.5994    2.6558
? C

 NEXT STEP? (TYPE "H" FOR HELP)
? SO
```

10.4 The Graphical Output

The 8 DISSPLA plots generated by the run are shown in Figures 10.1-10.8. Since the fitted function defines a 2-dimensional surface, the plots of data and fit vs. the two variables T and M give projections of this surface. For the sake of simplicity, the program does not try to plot a family of curves to represent this surface, but rather evaluates the fitting function only at the observation points and plots both the observations and fits as pairs of discrete points. The various plots of the residuals are not the kind of scatter diagrams that one would hope to obtain from a really good fit, and the normal probability plot (Figure 10.8) indicates significant deviations from the diagonal distribution that one would expect if the residuals were truly normally distributed. It might be possible to remedy some or all of these problems by a proper weighting of the observations. If not, then one would be forced to conclude that the model is not quite right.

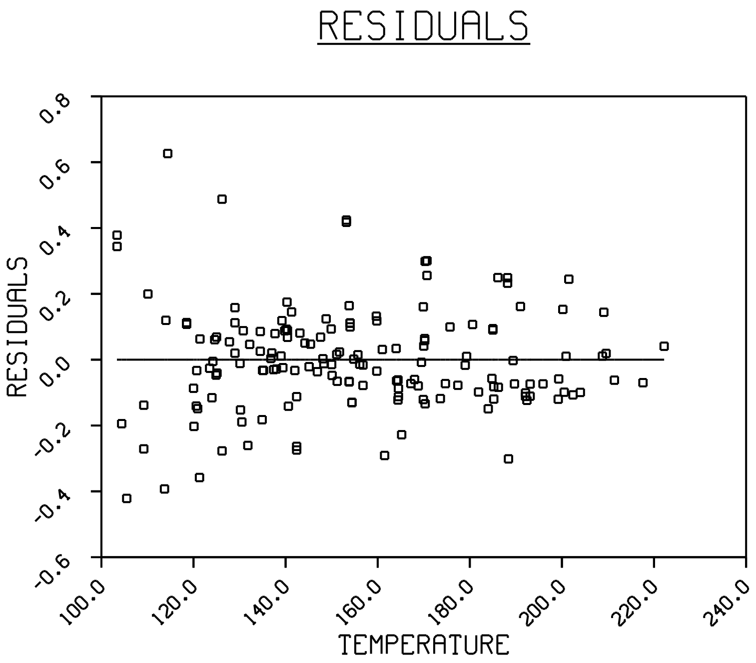


Figure 10.1: Residuals (data - model) vs. temperature

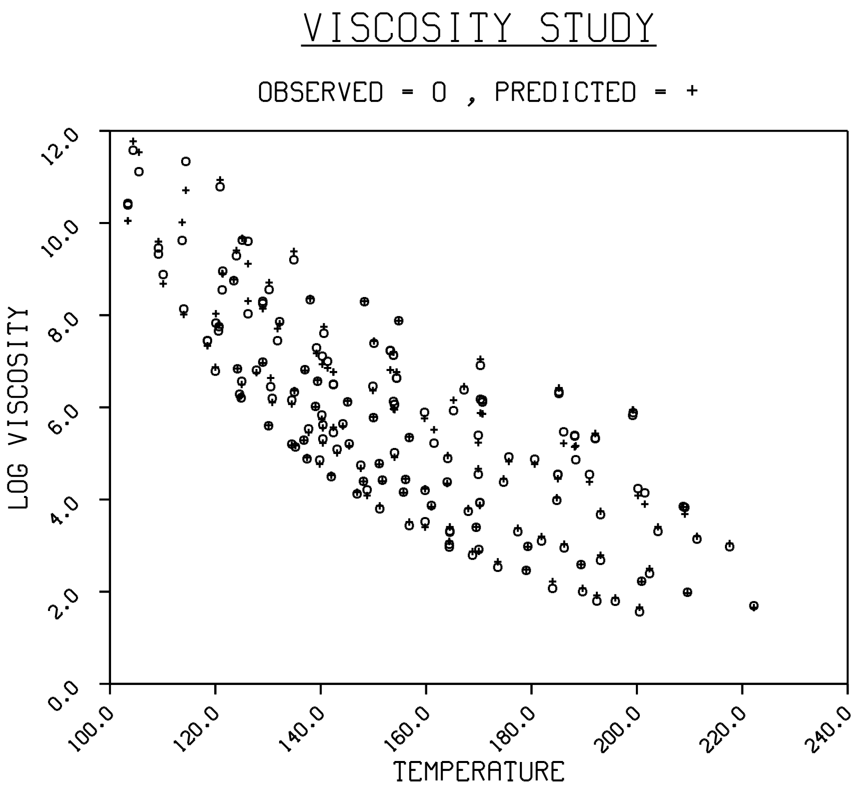


Figure 10.2: Data and fit vs. temperature

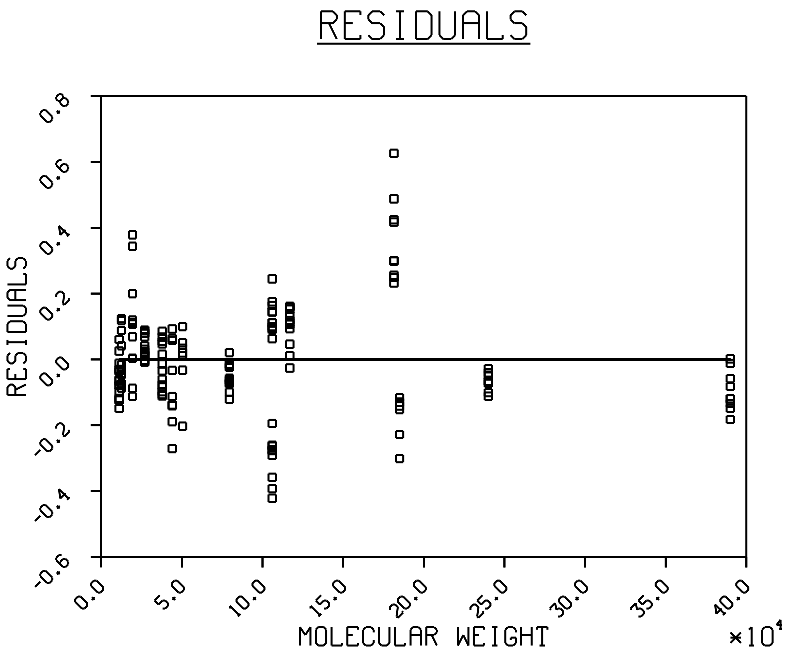


Figure 10.3: Residuals (data - model) vs. molecular weight

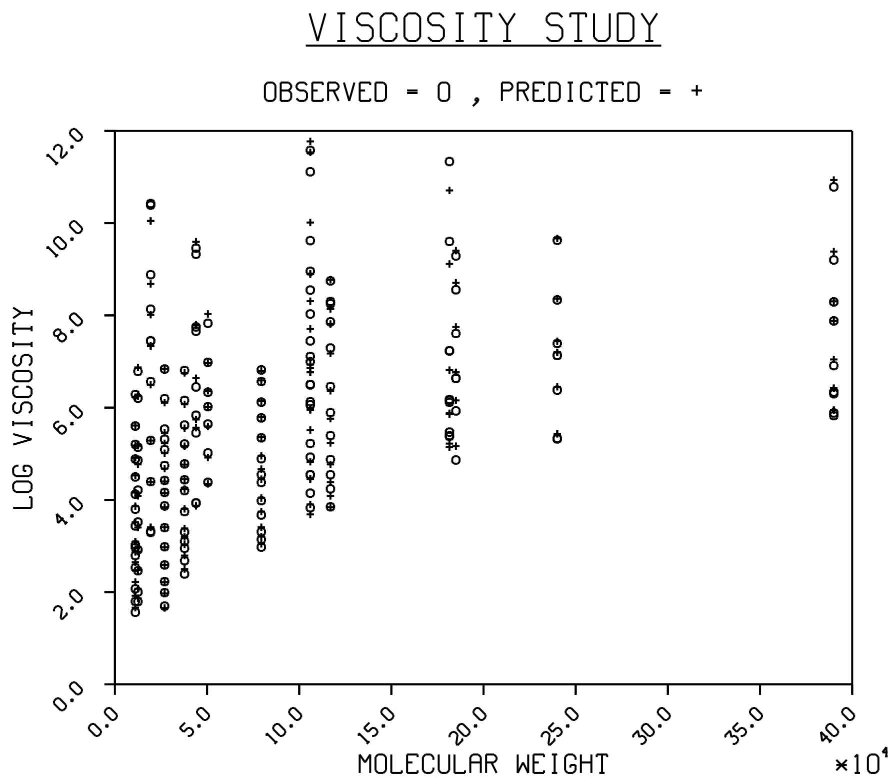


Figure 10.4: Data and fit vs. molecular weight

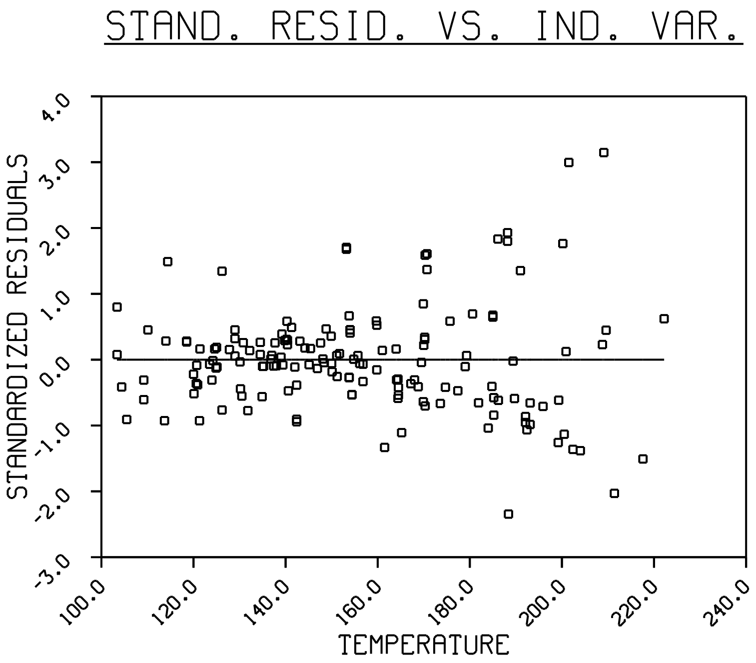


Figure 10.5: Standardized residuals vs. temperature

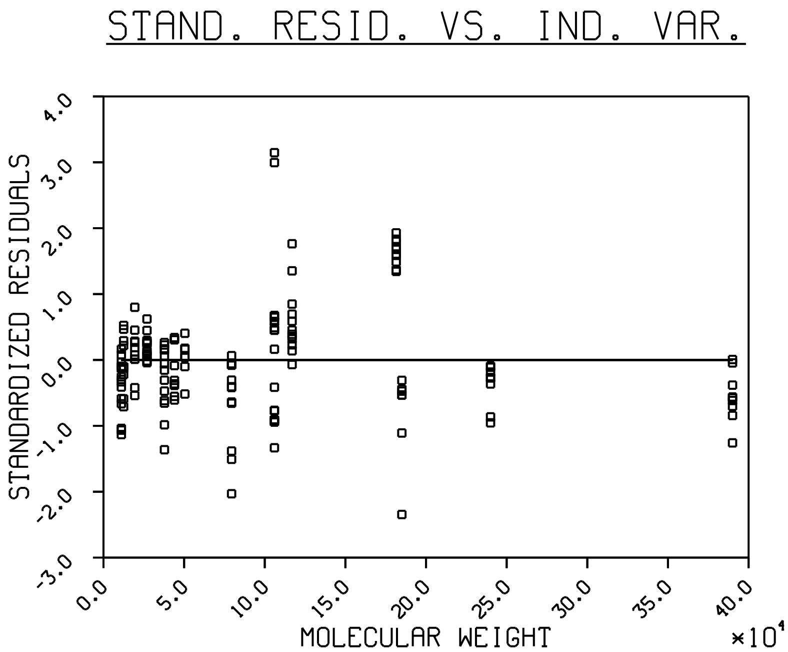


Figure 10.6: Standardized residuals vs. molecular weight

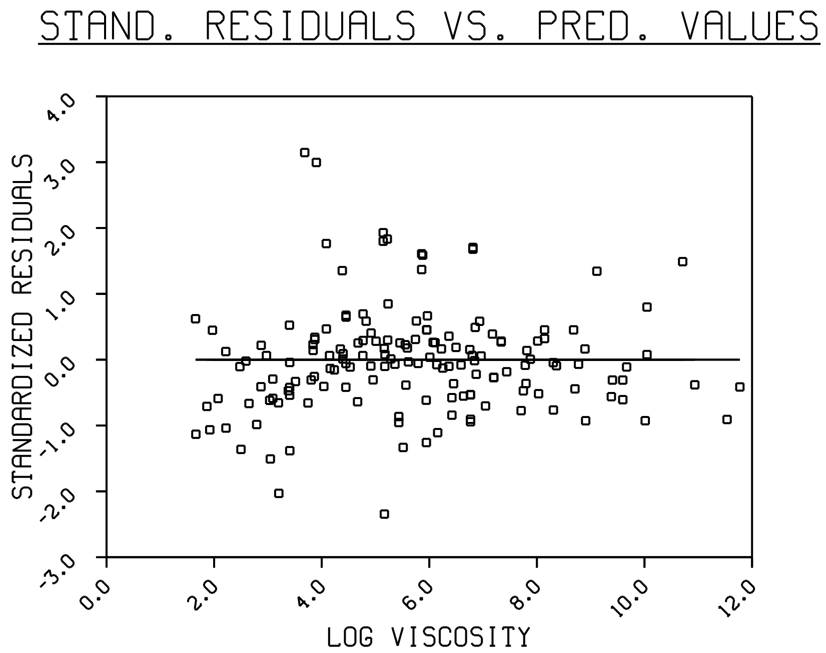


Figure 10.7: Standardized residuals vs. viscosity predicted by fit

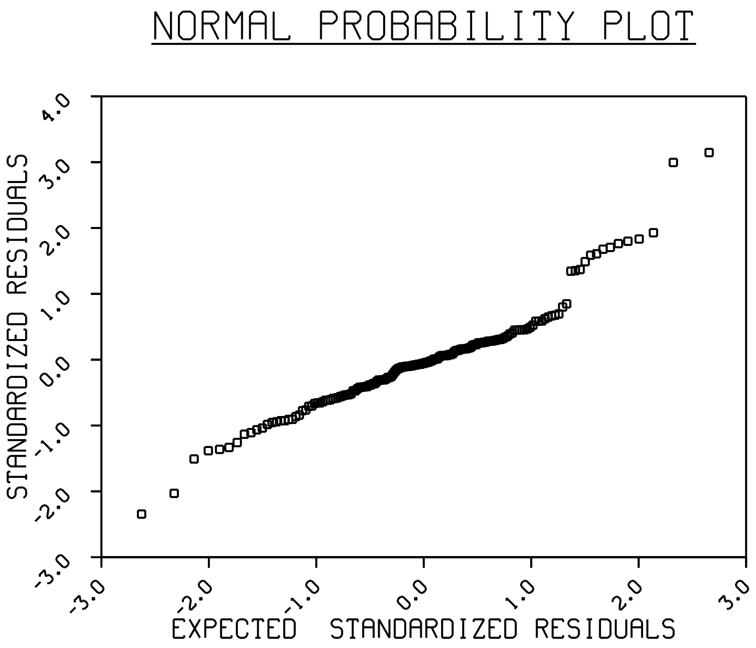


Figure 10.8: Standardized residuals versus the expected standardized residuals

Appendix A

THE SUBROUTINES IN THE INVAR CODE

Figure A.1 depicts the INVAR subroutine network. The arrows represent the directions of the subroutine CALLs. The five user supplied subroutines are written in boldface. They are described in detail in Chapter 3. The other subroutines are:

TYPE The subroutine which nominates the DISSPLA plotting devices. **PTEKAL** nominates Tektronics plotting terminals. **TK4014** and **HWSPEC** nominate the QMS laser printers.

PR The subroutine used to print out the various values requested by the user.

CH The subroutine used to change various quantities at the user's request.

ARRAYD A subroutine use to print out matrices.

VARPRO The main driver for the VARPRO subroutine package. The VARPRO subroutines **ORFAC1**, **ORFAC2**, **DPA**, **BACSUB**, **POSTPR**, **COV**, and **VARERR** are unchanged, but **ADA** was altered and **NUMBER** was added by Rall and Funderlic [12].

PLOT1, PLOT2 Subroutines used to generate the DISSPLA plots.

STAT The subroutine which generates the various statistical diagnostics obtainable with the "RS" command.

ORPLOT A sorting subroutine used by STAT.

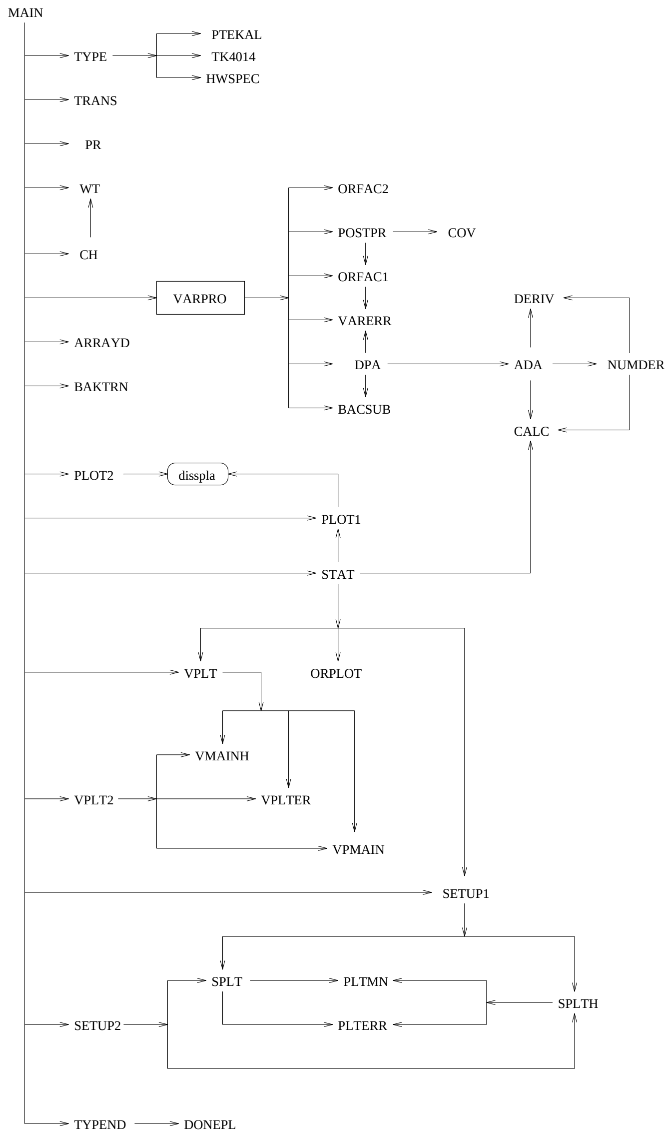


Figure A.1: The INVAR subroutine hierarchy

VPLT, VPLT2, VMAINH, VPLTER, VPMAIN Line printer plot routines.

SETUP1, SETUP2, SPLT, SPLTH, PLTMN, PLTERR Line printer plot routines.

TYPEND An entry in Subroutine TYPE which is called after the user enters any of the stop commands. It terminates the DISSPLA plotting by calling the DISSPLA subroutine **DONEPL**.

Appendix B

CHANGING THE INVAR PROGRAMS

B.1 Changing the PROGRAM Statement

The PROGRAM statement in the MAIN program has the form

```
      PROGRAM MAIN (INPUT,OUTPUT=/1000,LPOUT,INVRPL=/1000,
C
     1                 TAPE5=INPUT,TAPE6=OUTPUT,TAPE10=LPOUT)
```

which is non-standard FORTRAN specific for Cyber computers. User who want to run INVAR on some other computer will want to replace or remove this statement. TAPE5 and TAPE6 are just the standard input and output units. INVRPL is the file for the DISSPLA plots, and TAPE10 is the unit for the hardcopy line printer output. User who change this PROGRAM statement must do whatever is necessary to assign, open and close these files on their own computer.

B.2 Changing the DISSPLA Plotting Device Nomination

The DISSPLA plotting device nomination is done in Subroutine TYPE. Currently there are two ways to get the plots: in real-time on a Tektronics plotting terminal or after execution has been completed on a QMS laser printer.

To change the real-time nomination to some device other than a Tektronics terminal, change

```
IF (IDP) CALL PTEKAL
```

to

```
IF (IDP) CALL devnam
```

where "devnam" is the appropritate device name.

To change the deferred, hard-copy plotter nomination to some device other than a QMS laser printer, change

```
IF (IDCP) THEN
              CALL TK4014 (960,1)
              CALL HWSPEC ('INVRPL','FILE')
END IF
```

to

```
IF (IDCP) THEN
              CALL devnam
END IF
```

where "devnam" is the appropriate device name.

B.3 Changing the Array Dimensions

Some problems may require larger arrays than are presently available in INVAR. Arrays can easily be redimensioned by changing a few PARAMETER statements. Each of the subsections in this section lists, by subroutine, the alterations required to change one of the dimensioning parameters.

Changing the maximum number of observations

To change the maximum number of observations from 300 to m:

- In PLOT1 replace

  ```
  PARAMETER (MMAX=300)
  ```

  with

```
      PARAMETER (MMAX= m )
```

- In MAIN replace

```
      PARAMETER (MMAX=300, MMAX2=600, MIV=6, MAXN=10, MAXNP2=33,
     2           MAXN1=11, MAXNKG=18, MAXKG=8, MAXP=21)
```

  with

```
      PARAMETER (MMAX= m , MMAX2=2*m, MIV=6, MAXN=10, MAXNP2=33,
     2           MAXN1=11, MAXNKG=18, MAXKG=8, MAXP=21)
```

- In ORPLOT replace

```
      PARAMETER (MMAX=300)
```

  with

```
      PARAMETER (MMAX= m )
```

- In POSTPR replace

```
      PARAMETER (MMAX=300, MAXNKG=18)
```

  with

```
      PARAMETER (MMAX= m , MAXNKG=18)
```

- In STAT replace

```
      PARAMETER (MMAX=300, MAXN1=11, MAXNKG=18, MIV=6)
```

  with

```
      PARAMETER (MMAX= m , MAXN1=11, MAXNKG=18, MIV=6)
```

Changing the maximum number of independent variables

To change the maximum number of independent variables per observation from 6 to iv:

- In subroutine CH, the format to print the data points (FORMAT statement 60) will need to be changed.
- In MAIN replace

```
      PARAMETER (MMAX=300, MMAX2=600, MIV=6, MAXN=10, MAXNP2=33,
     2           MAXN1=11, MAXNKG=18, MAXKG=8, MAXP=21)
                 .
                 .
                 .

 1650   FORMAT (7(E14.8,2X))
```

  with

```
      PARAMETER (MMAX=300, MMAX2=600, MIV=iv, MAXN=10, MAXNP2=33,
                 MAXN1=11, MAXNKG=18, MAXKG=8, MAXP=21)
                 .
                 .
                 .

 1650   FORMAT ((iv+1)(E14.8,2X))
```

- In subroutine PR, the formats to print out data points and weights (FORMAT statements 410, 450 and 480) will need to be changed.
- In STAT replace

```
      PARAMETER (MMAX=300, MAXN1=11, MAXNKG=18, MIV=6)
```

  with

```
      PARAMETER (MMAX=300, MAXN1=11, MAXNKG=18, MIV=iv)
```

Changing the maximum number of linear parameters

To change the maximum number of linear parameters from 10 to n (k = max. no. of nonlinear parameters; p = max. no. of nonzero partials):

- In ADA replace

  ```
  PARAMETER (MAXN1=11, MAXN=10, MAXKG=8, MAXP=21)
  ```

  with

  ```
  PARAMETER (MAXN1=n+1, MAXN=n, MAXKG=8, MAXP=21)
  ```

- In CALC replace

  ```
  PARAMETER (MAXN1=11)
  ```

  with

  ```
  PARAMETER (MAXN=n+1)
  ```

- In DERIV replace

  ```
  PARAMETER (MAXN1=11, MAXKG=8)
  ```

  with

  ```
  PARAMETER (MAXN1=n+1, MAXKG=8)
  ```

- In DPA replace

  ```
  PARAMETER (MAXN1=11, MAXKG=8)
  ```

  with

```
      PARAMETER (MAXN1=n+1, MAXKG=8)
```

- In MAIN replace

```
      PARAMETER (MMAX=300, MMAX2=600, MIV=6, MAXN=10, MAXNP2=33,
     2           MAXN1=11, MAKNKG=18, MAXKG=8, MAXP=21)
                 .
                 .
                 .
 710   FORMAT (38A1,11I2)
                 .
                 .
                 .
1750  FORMAT (' TERMS WHICH DEPEND ... ',I2,':  ',11I2)
```

with

```
      PARAMETER (MMAX=300, MMAX2=600, MIV=6, MAXN=n, MAXNP2=n+p+2,
     2           MAXN1=n+1, MAXNKG=n+k, MAXKG=8, MAXP=21)
                 .
                 .
                 .
 710   FORMAT (38A1,(n+1)I2)
                 .
                 .
                 .
1750  FORMAT (' TERMS WHICH DEPEND ... ',I2,':  ',(n+1)I2)
```

- In NUMDER replace

```
      PARAMETER (MAXN=10, MAXN1=11, MAXKG=8, MAXP=21)
```

with

```
PARAMETER (MAXN=n, MAXN1=n+1, MAXKG=8, MAXP=21)
```

- In POSTPR replace

```
PARAMETER (MMAX=300, MAXNKG=18)
```

with

```
PARAMETER (MMAX=300, MAXNKG=n+k)
```

- In PR replace

```
      PARAMETER (MAXN1=11, MAXKG=8, MAXP=21)
                     .
                     .
                     .
  320   FORMAT (/' '/' TERMS WHICH DEPEND ... ',I2,':  ',11I2)
```

with

```
      PARAMETER (MAXN1=n+1, MAXKG=8, MAXP=21)
                     .
                     .
                     .
  320   FORMAT (/' '/' TERMS WHICH DEPEND ... ',I2,':  ',(n+1)I2)
```

- In STAT replace

```
PARAMETER (MMAX=300, MAXN1=11, MAXNKG=18, MIV=6)
```

with

```
PARAMETER (MMAX=300, MAXN1=n+1, MAXNKG=n+k, MIV=6)
```

Changing the maximum number of nonlinear parameters

To change the maximum number of nonlinear parameters from 8 to k (n = max. no. of linear parameters):

- In ADA replace

```
      PARAMETER (MAXN1=11, MAXN=10, MAXKG=8, MAXP=21)
```

  with

```
      PARAMETER (MAXN1=11, MAXN=10, MAXKG=k, MAXP=21)
```

- In DERIV replace

```
      PARAMETER (MAXN1=11, MAXKG=8)
```

  with

```
      PARAMETER (MAXN1=11, MAXKG=k)
```

- In DPA replace

```
      PARAMETER (MAXN1=11, MAXKG=8)
```

  with

```
      PARAMETER (MAXN1=11, MAXKG=k)
```

- In MAIN replace

```
      PARAMETER (MMAX=300, MMAX2=600, MIV=6, MAXN=10, MAXNP2=33,
     2           MAXN1=11, MAXNKG=18, MAXKG=8, MAXP=21)
                 .
```

```
                .
                .
  690   FORMAT (23A1,8E14.8)
                .
                .
                .
 1720  FORMAT (' NONLINEAR PARAMETERS:  ',8E14.8)
```

with

```
      PARAMETER (MMAX=300, MMAX2=600, MIV=6, MAXN=10, MAXNP2=33,
     2           MAXN1=11, MAXNKG=k+n, MAXKG=k, MAXP=21)
                .
                .
                .
  690   FORMAT (23A1,kE14.8)
                .
                .
                .
 1720  FORMAT (' NONLINEAR PARAMETERS:  ',kE14.8)
```

- In NUMDER replace

```
      PARAMETER (MAXN=10, MAXN1=11, MAXKG=8, MAXP=21)
```

with

```
      PARAMETER (MAXN=10, MAXN1=11, MAXKG=k, MAXP=21)
```

- In POSTPR replace

```
PARAMETER (MMAX=300, MAXNKG=18)
```

with

```
PARAMETER (MMAX=300, MAXNKG=k+n)
```

- In PR replace

```
PARAMETER (MAXN=11, MAXKG=8, MAXP=21)
```

with

```
PARAMETER (MAXN=11, MAXKG=k, MAXP=21)
```

- In STAT replace

```
PARAMETER (MMAX=300, MAXN1=11, MAXNKG=18, MIV=6)
```

with

```
PARAMETER (MMAX=300, MAXN1=11, MAXNKG=k+n, MIV=6)
```

Changing the maximum number of nonzero partial derivatives

To change the maximum number of nonzero partial derivatives from 21 to p (n = max. no. of linear parameters):

- In ADA replace

```
PARAMETER (MAXN1=11, MAXN=10, MAXKG=8, MAXP=21)
```

with

```
      PARAMETER (MAXN1=11, MAXN=10, MAXKG=8, MAXP=p)
```

- In CH replace

```
      PARAMETER (MAXP=21)
```

with

```
      PARAMETER (MAXP=p)
```

- In MAIN replace

```
      PARAMETER (MMAX=300, MMAX2=600, MIV=6, MAXN=10, MAXNP2=33,
     2           MAXN1=11, MAXNKG=18, MAXKG=8, MAXP=21)
                 .
                 .
                 .
  720   FORMAT (34A1,21E14.8)
                 .
                 .
                 .
 1770  FORMAT (' NUMERICAL DERIVATIVE INCREMENTS:  ',21E14.8)
```

with

```
      PARAMETER (MMAX=300, MMAX2=600, MIV=6, MAXN=10, MAXNP2=p+n+2,
     2           MAXN1=11, MAXNKG=18, MAXKG=8, MAXP=p)
                 .
                 .
                 .
  720   FORMAT (34A1,pE14.8)
                 .
```

.
.

```
 1770  FORMAT (' NUMERICAL DERIVATIVE INCREMENTS:  ',pE14.8)
```

- In NUMDER replace

```
      PARAMETER (MAXN=10, MAXN1=11, MAXKG=8, MAXP=21)
```

with

```
      PARAMETER (MAXN=10, MAXN1=11, MAXKG=8, MAXP=p)
```

- In PR replace

```
      PARAMETER (MAXN1=11, MAXKG=8, MAXP=21)
```

with

```
      PARAMETER (MAXN1=11, MAXKG=8, MAXP=p)
```

B.4 Changing the Iteration Specification Parameters

Changing the maximum number of iterations

To change the maximum number of iterations from 250 to i:

- In MAIN replace

```
1020 FORMAT(/' NUMBER OF ITERATIONS MUST BE GREATER '/1H ,
    2        'THAN 0 AND LESS THAN OR EQUAL TO 250.'/1H ,
    3        'HOW MANY ITERATIONS?         ')
     READ (5,*) ITMAX
     IF (ITMAX.LE.0.OR.ITMAX.GT.250) GO TO 1010
```

with

```
1020 FORMAT(/' NUMBER OF ITERATIONS MUST BE GREATER '/1H ,
    2        'THAN 0 AND LESS THAN OR EQUAL TO  i .'/1H ,
    3        'HOW MANY ITERATIONS?         ')
     READ (5,*) ITMAX
     IF (ITMAX.LE.0.OR.ITMAX.GT. i ) GO TO 1010
```

Changing the default number of iterations

To change the default number of iterations from 50 to q:

- In MAIN replace

```
      DATA ITMAX/50/, EPS1/1.0E-5/, IPRINT/1/
                 .
                 .
                 .

  980   FORMAT (/' ... (50:MAX. NO. OF ITERATIONS)' ... )')
```

with

```
      DATA ITMAX/q/, EPS1/1.0E-5/, IPRINT/1/
                 .
                 .
                 .

  980   FORMAT (/' ... ( q :MAX. NO. OF ITERATIONS)' ... )')
```

Changing the maximum value of the Marquardt parameter

To change the maximum value allowed for the Marquardt parameter from 100 to f:

- In VARPRO, for the third statement following statement number 800, replace

```
IF (NU.LE.100) GO TO 810
```

with

```
IF (NU.LE. f ) GO TO 810
```

Appendix C

DESCRIPTION OF VARIABLES USED IN INVAR

A list of variables used in INVAR follows. Each variable name and, where applicable, its dimension specifications are printed in boldface. Following that is a short description of the variable and, enclosed in brackets, a list of the subroutines in which it appears.

A(300,33) On input to VARPRO, the array contains the PH(J)'s and their derivatives. On output, the first N+KG rows and columns contain an approximation to the (weighted) covariance matrix at the solution (the first N rows correspond to the linear parameters, the last the last KG to the nonlinear ones), column N+KG+1 contains the weighted residuals, A(1,N+KG+2) contains the (Euclidean) norm of the weighted residual and A(2,N+KG+2) contains an estimate of the (weighted) variance of the observations. [ADA, COV, DPA, MAIN, POSTPR, STAT, VARPRO]

ACUM Variable used to aid in computation, e.g., accumulate a sum. [BACSUB, DPA, ORFAC1, ORFAC2, POSTPR, VARPRO]

AI Absolute value of the Ith diagonal element of A. [STAT]

AIM1 Floating point equivalent of I-1 (dummy subscript), used in computing values for the X axis label (terminal and/or line printer plots). [PLTMN]

AIROW Floating point equivalent of IROW. [PLTMN]

AJ Absolute value of the Jth diagonal element of A. [STAT]

ALF(8) Vector of nonlinear parameters. [ADA, CALC, CH, DERIV, DPA, MAIN, NUMDER, POSTPR, PR, STAT, VARPRO]

ALFNRM Norm of ALF. [VARPRO]

ALINE(103) Character vector of the current graph line (terminal and/or line printer plots). [PLTMN]

ALPHA Factor used in calculating Householder reflections. [DPA, ORFAC1, ORFAC2]

ALPHAI Axis symbol "I" (terminal and/or line printer plots). [PLTMN, VPMAIN]

ALPHAX Plotting symbol "X" (terminal and/or line printer plots). Used when more than 9 points fall in a single location. [PLTMN]

ANS User response to question asking for increment values. [MAIN]

ANUMLM NUMLAB-1. [PLTMN]

ASAVE Value of ALF(I) when computing numerical derivative. [NUMDER]

AXISCH Y axis symbol to be used on the current graph line (terminal and/or line printer plots). Symbol is either "I" or "-". [PLTMN]

A1(300,10) Triangular matrix used in solving system of equations. [BACSUB]

B(300,9) Matrix which contains the derivative portion of A. [ORFAC1, ORFAC2]

BA(1) Singly-dimensioned array to be printed as a matrix. [ARRAYD]

BB Square root of AI or AJ. [STAT]

BETA Factor used in calculating Householder reflections. [DPA, ORFAC1, ORFAC2]

BKETA Vector of the back-transformed values of the predicted Y. [BAKTRN, MAIN]

BLANK Plotting symbol (blank) (terminal and/or line printer plots). [PLTMN, VMAINH, VPMAIN]

BLIDCP Common block containing IDCP. [MAIN, STAT, TYPE]

BLKBM Common block containing BM. [POSTPR, STAT]

BLKDPH Common block containing DPH. [ADA, DERIV, MAIN, NUMDER]

BLKIDP Common block containing IDP. [MAIN, PLOT1, PLOT2, STAT, TYPE]

BLKINC Common block containing INC. [ADA, DPA, MAIN, PR]

BLKITP Common block containing ITP. [MAIN, PR, SETUP1, SETUP2, STAT]

BLKNDI Common block containing NDI. [ADA, CH, MAIN, NUMDER, PR]

BLKPH Common block containing PH. [ADA, CALC, MAIN, STAT]

BLKTS Common block containing TS. [MAIN, PLOT1, PLOT2, STAT]

BLOCKP Common block containing P. [ADA, MAIN]

BLOKIP Common block containing IP. [ARRAYD, CH, MAIN, POSTPR, PR, SETUP1, SETUP2, STAT, VARERR, VARPRO]

BM(300,18) Matrix of predictor variables used in calculating the standardized residuals. [POSTPR, STAT]

BT(300,6) Array of back-transformed independent variables. BT(I,J) contains the value of the Ith observation of the Jth independent variable. [MAIN, TRANS]

BY(300) Vector of back-transformed values of the dependent variable. [MAIN, TRANS]

B1 N+2, used to identify the first column of A which contains derivatives of PH(J). [VARPRO]

C(10) Vector of linear parameters. [ADA, CALC, MAIN, STAT, VARPRO]

CC(10) Vector used to identify which PH(J) is to be used in calculating the numerical derivative. [NUMDER]

COLUMN Character variable containing "COLUMN". [ARRAYD]

CR(18,18) Correlation matrix. [MAIN]

CTSS Corrected total sum of squares. [STAT]

D Plotting symbol "+" (terminal and/or line printer plots). [VMAINH, VPMAIN]

DALFNM Norm of the change in ALF from the previous iteration to the present one. [VARPRO]

DELR Change in the norm of the residual from the previous iteration to the present one. [VARPRO]

DELTA Distance between any 2 of the 500 points which plot the curve of the predicted Y (DISSPLA plots). [MAIN]

DELX The range of the X axis (terminal and/or line printer plots). [PLTMN]

DELY The range of the Y axis (terminal and/or line printer plots). [PLTMN]

DK Numerical derivative increment. [NUMDER]

DPH(11,8) DPH(I,J) is the derivative of PH(I) with respect to ALF(J). [ADA, DERIV, MAIN, NUMDER]

DUMMY Dummy argument in subroutine parameter list. [STAT]

DV Derivative value to be entered in A. [NUMDER]

EPS1 Absolute tolerance for the norm of the projection of the residual onto the range of the Jacobian of the variable projection functional [MAIN, VARPRO]

EPS2 Relative and absolute tolerance for the change in the norm of the residual. [VARPRO]

ERRCHK Common block containing IERROR. [PLTERR, SPLT, SPLTH, VPLT, VPLTER, VPLT2]

ERRNO Error number (absolute value of IERR). [VARERR]

ETA(300) Vector of predicted values of the dependent variable. [ADA, BAKTRN, CALC, MAIN, SETUP2, STAT]

ETAPL(600) Vector of observed and predicted values of the dependent variable in the order they are to be plotted (terminal and/or line printer plots). [MAIN, SETUP2]

EX Logical variable used in INQUIRE statement to indicate if a file name already exists or not. [MAIN]

FIRSTC First column to which Householder reflections should be applied. [DPA]

FIRSTR First row to which Householder reflections should be applied. [DPA]

FNAME Name of file conataining all initial information (data points, parameters, variables, etc.). [MAIN]

GNSTEP Step size for Gauss-Newton iteration. [VARPRO]

H Variable used in arranging indexing of IOR. [ORPLOT]

HN Variable used in arranging indexing of IOR. [ORPLOT]

HYPHEN Axis symbol "-" (terminal and/or line printer plots). [PLTMN]

I Dummy subscript. [ADA, BACSUB, CH, COV, DPA, MAIN, NUMDER, ORFAC1, ORFAC2, ORPLOT, PLOT1, PLOT2, PLTMN, POSTPR, PR, STAT, VMAINH, VPMAIN]

IA(11) Vector used in determining INC matrix. [MAIN, PR]

IANS User response to interactive questions. [CH, MAIN, PR, STAT]

IB Dummy subscript. [MAIN]

IBACK Dummy subscript. [BACSUB]

IC Number of values falling outside graph bounds (terminal and/or line printer plots). [PLTMN]

ICODE Command code chosen by the user. [CH, MAIN, PR]

ICOL Dummy subscript. [PLTMN]

ICR Flag to indicate that the correlation matrix should be printed. [MAIN]

ICV Flag to indicate that the covariance matrix should be printed. [MAIN]

IDCP Flag to indicate that DISSPLA plots should be saved in a file (META) for later access. [MAIN, STAT, TYPE]

IDP Flag to indicate that DISSPLA plots should be printed interactively on a plotting screen. [MAIN, PLOT1, PLOT2, STAT, TYPE]

IERR Integer error flag. [MAIN, ORFAC1, VARERR, VARPRO]. The returned value is interpreted as follows:

- $>$**0** successful convergence.
- **-1** terminated due to too many iterations.
- **-2** terminated for ill-conditioning (Marquardt parameter too large).
- **-4** input error in parameter M, N, KG, NPP2 or MMAX.
- **-5** INC matrix improperly specified.
- **-6** weights not nonnegative.
- **-7** "constant" column was computed more than once.
- **-8** catastrophic failure–a column of matrix A has become zero.

IERROR Flag to indicate type of error in graph (terminal and/or line printer plots). [PLTERR, SPLT, SPLTH, VPLT, VPLTER, VPLT2]

II Dummy subscript. [ADA, DPA, MAIN, STAT]

IK Subscript used to identify placement of derivative in matrix A. [ADA]

IK1 Dummy subscript. [PLTMN]

IL Dummy subscript. [CH, PR]

IMEAN Flag to indicate whether zero line is to be plotted (terminal and/or line printer plots). [VMAINH, VPLT, VPLT2, VPMAIN]

IN Subscript to identify which numerical derivative increment should be used. [ADA, NUMDER]

INC(8,11) Incidence matrix for partial derivatives. INC(K,J)=1 if nonlinear parameter ALF(K) appears in PH(J). Otherwise, INC(K,J)=0. [ADA, DPA, MAIN, PR]

INCKJ INC(K,J). [DPA]

IND Character variable containing "IND". [MAIN, PR, STAT]

INV Number of independent variable used for plotting (terminal and/or line printer plots). [MAIN, SETUP1, SETUP2]

IOR(300) Vector containing indexing of independent variable values arranged in ascending order. [ORPLOT, STAT]

IP Flag to indicate line printer output. [ARRAYD, CH, MAIN, POSTPR, PR, SETUP1, SETUP2, STAT, VARERR, VARPRO]

IPCODE Flag to indicate, during error checking, which subroutine has been called in plotting (terminal and/or line printer plots). [PLTERR, SPLT, SPLTH, VPLT, VPLTER, VPLT2]

IPI Flag to indicate whether to plot residuals or predicted and observed values. [MAIN, STAT]

IPIBLK Common block containing IPI. [MAIN, STAT]

IPIV Flag to indicate whether to plot standardized residuals versus independent variables. [STAT]

IPP Flag to indicate whether to plot probability of standardized residuals. [STAT]

IPPV Flag to indicate whether to plot standardized residuals versus predicted values. [STAT]

IPR Flag to indicate whether output is sent to terminal or to line printer. [PLTERR, PLTMN, SPLT, SPLTH, VMAINH, VPLT, VPLTER, VPLT2, VPMAIN]

IPRINT Integer used to control output printed by VARPRO. If IPRINT>0, the nonlinear parameters, norm of residual and Marquardt parameter will be printed every IPRINTth iteration. If IPRINT=0, only the final quantities will be printed. [DPA, MAIN, ORFAC1, POSTPR, VARERR, VARPRO]

IPR10 Directs line printer output into temporary file 10. [MAIN, SETUP1, SETUP2, STAT]

IPR6 Directs line printer output to be printed on terminal. [MAIN, SETUP1, SETUP2, STAT]

IPT Flag to indicate that t-ratios should be printed. [STAT]

IP1 I+1 (dummy subscript). [BACSUB, COV]

IQ Flag to indicate Command Segment. [MAIN]

IR Flag to indicate that residual sum of squares, residual mean square, residual standard error and coefficient of determination should be printed. [STAT]

IROW Line of the graph currently being printed out (terminal and/or line printer plots). [PLTMN]

ISEL Flag to indicate what (function values and/or partial derivatives) should be computed. [ADA, DPA]

ISS Integer value of the specified symbol to be plotted (terminal and/or line printer plots). [PLTMN]

ISTOP Element in ALINE vector which contains the last significant symbol to be printed (terminal and/or line printer plots). [PLTMN]

ISUB Dummy subscript. [VARPRO]

ISYM(600) Integer values of the symbols to be used in plotting data points (terminal and/or line printer plots). [MAIN, PLTMN, SETUP1, SETUP2, SPLT, SPLTH, STAT]

ITB Flag to indicate that a table should be printed. [MAIN, STAT]

ITER Number of iterations. [VARPRO]

ITERIN Control variable to determine if a step was retracted. [VARPRO]

ITERM Number of terms in model that depend on a nonlinear parameter. [MAIN]

ITEST Flag to indicate whether X axis labels are printed in E or F format (terminal and/or line printer plots). [PLTMN]

ITMAX Maximum number of iterations. [MAIN, VARPRO]

ITP Flag to indicate whether line printer plots should be printed on terminal. [MAIN, PR, SETUP1, SETUP2, STAT]

ITRN Flag to indicate that dependent and/or independent variable needs to be transformed. [MAIN]

ITWOM 2*M. [SETUP2]

ITYPE Flag to indicate which type of curve is to be drawn (DISSPLA plots). [PLOT1] The possible values are:

- **1** mean line drawn, points sometimes connected;
- **2** mean line drawn, points never connected;
- **3** mean line not drawn, points never connected.

IV Number of independent variables per observation. [ADA, CALC, CH, DERIV, DPA, MAIN, NUMDER, PR, STAT, TRANS, VARPRO]

IVP Number of columns to be printed in table. [PR]

IWT Flag to indicate that weights are calculated in subroutine WT. [MAIN]

IX Subscript used in arranging indexing of IOR. [ORPLOT]

IX1 Plotting location of Ith value of X1 vector (terminal and/or line printer plots). [VMAINH, VPMAIN]

IX2 Plotting location of Ith value of X2 vector (terminal and/or line printer plots). [VMAINH, VPMAIN]

J Dummy subscript. [ADA, ARRAYD, BACSUB, CH, COV, DPA, MAIN, NUMDER, ORFAC1, ORFAC2, ORPLOT, POSTPR, PR, STAT, VARPRO, VMAINH, VPMAIN]

JJ DUmmy subscript. [ADA, NUMDER]

JM1 J-1 (dummy subscript). [COV]

JP1 J+1 (dummy subscript). [POSTPR]

JSUB Dummy subscript. [ORFAC1, VARPRO]

K Dummy subscript. [ADA, CALC, DERIV, DPA, MAIN, NUMDER, ORFAC1, ORFAC2, PLTMN, POSTPR, PR, SETUP1, SETUP2, STAT, VARERR, VARPRO]

KBACK Dummy subscript. [POSTPR]

KG Number of nonlinear parameters. [ADA, CH, DPA, MAIN, NUMDER, ORFAC1, ORFAC2, POSTPR, PR, STAT, VARPRO]

KGPK KG+K. [ORFAC2]

KGPKM1 KG+K-1. [ORFAC2]

KGP1 KG+1. [ORFAC1, ORFAC2, VARPRO]

KG2 2*KG. [ORFAC2]

KG23 2*KG+3. [ORFAC1, ORFAC2, VARPRO]

KK Dummy subscript. [ADA, DPA]

KL Dummy subscript. [SETUP2]

KP1 K+1 (dummy subscript). [DPA, ORFAC1, ORFAC2, POSTPR]

KSS(101) Integer vector used to determine which plotting symbol is needed (terminal and/or line printer plots). [PLTMN]

KSUB Dummy subscript. [DPA, VARPRO]

L Dummy subscript. [ARRAYD, COV, DPA]

LABEL Integer value of current row (and Y label) of vertical graphs (terminal and/or line printer plots). [VMAINH, VPMAIN]

LASTC Last column to which Householder reflections should be applied. [DPA]

LI Dummy subscript. [ARRAYD]

LMSPEC Flag to indicate which set of limits are to be used for multiple, vertical graphs (terminal and/or line printer plots). [VMAINH, VPLT, VPLTER, VPLT2, VPMAIN]

LN Flag to indicate whether a label should be printed on the Y axis (terminal and/or line printer plots). [PLTMN]

LVV Integer first dimension in calling program of matrix to be printed. [ARRAYD]

M Number of observations. [ADA, BAKTRN, CH, DPA, MAIN, ORFAC1, ORPLOT, PLTMN, POSTPR, PR, SETUP1, SETUP2, SPLT, SPLTH, STAT, TRANS, VARPRO, VMAINH, VPLT, VPLTER, VPLT2, VPMAIN, WT]

MAX Index corresponding to maximum value of independent variable. [ORPLOT]

MAXKG Maximum number of nonlinear parameters. [ADA, DERIV, DPA, MAIN, NUMDER, PR]

MAXN Maximum number of linear parameters. [ADA, MAIN, NUMDER]

MAXNKG MAXN+MAXKG. [MAIN, POSTPR, STAT]

MAXNP2 MAXN+MAXP+2. [ADA, MAIN]

MAXN1 MAXN+1. [ADA, CALC, DERIV, DPA, MAIN, NUMDER, PR, STAT]

MAXP Maximum number of nonzero partials. [CH, MAIN, NUMDER, PR]

MEAN1 Plot line location of the X1 vector (terminal and/or line printer plots). [VMAINH, VPMAIN]

MH Highest column number to be printed on a given line. [ARRAYD]

MHM1 One less than the single dimension index corresponding to the first element of column MH. [ARRAYD]

MIV Maximum number of independent variables per observation. [MAIN]

ML Lowest column number to be printed on a given line. [ARRAYD]

MLM1 One less than the single dimension index corresponding to the first element of column ML. [ARRAYD]

MMAX Maximum number of observations. [ADA, BACSUB, CALC, CH, COV, DERIV, DPA, MAIN, NUMDER, ORFAC1, ORFAC2, ORPLOT, PLOT2, POSTPR, PR, STAT, TRANS, VARPRO]

MMAX2 2*MMAX. [MAIN]

MMH Single dimension index corresponding to column MH. [ARRAYD]

MML Single dimension index corresponding to column ML. [ARRAYD]

MM1 M-1. [ORPLOT]

MODIT Variable to determine whether information is to be printed at a given iteration (based on IPRINT). [VARPRO]

MP1 M+1. [SETUP2]

N Number of linear parameters. [ADA, CALC, DPA, MAIN, NUMDER, ORFAC1, POSTPR, PR, STAT, VARPRO]

NAM(40) Array which reads keywords from saved data file. [MAIN]

NC Flag to skip unnecessary computation. [ADA, MAIN, NUMDER]

NCBLK Common block containing NC. [ADA, MAIN, NUMDER]

NCC Number of columns in matrix to be printed. [ARRAYD]

NCON Number of "constant" functions in A. [DPA]

NCONP1 NCON+1. [ADA, DPA]

NDI(21) Vector of numerical derivative increments. [ADA, CH, MAIN, NUMDER, PR]

NH Highest row number to be printed on a page. [ARRAYD]

NKG1 N+KG+1. [POSTPR]

NKG2 N+KG+2. [DPA, MAIN, POSTPR, STAT, VARPRO]

NL Lowest row number to be printed on a page. [ARRAYD, CALC, DERIV]

NM1 N+KG-1. [COV]

NN The number of Y labels to be listed at the left axis (terminal and/or line printer plots). [PLTMN]

NPH Subscript to identify column number for last function PH. [ADA]

NPK N+K. [ORFAC1]

NPKG N+KG. [COV, MAIN, ORFAC1, POSTPR, STAT]

NPP1 N+P+1. [DPA]

NPP2 N+P+2. [ADA, DPA, VARPRO]

NPTS Number of pointS to be drawn on graphs (DISSPLA plots). [PLOT1, PLOT2]

NP1 N+1. [ADA, BACSUB, DERIV, DPA, MAIN, NUMDER, ORFAC1, POSTPR, PR, STAT, VARPRO]

NP2 N+2. [DPA]

NRR Number of rows in matrix to be printed. [ARRAYD]

NSER Number of vectors to be plotted (terminal and/or line printer plots). [VMAINH, VPLT, VPLTER, VPLT2, VPMAIN]

NSIZE Flag to indicate graph size (terminal and/or line printer plots). [PLTMN]

NU Marquardt parameter. [ORFAC2, VARPRO]

NUM Flag to indicate whether all initial values should be printed. [PR]

NUMCOL Number of columns per graph. 101 columns for line printer plots; 51 columns for terminal plots. [PLTMN]

NUMCP2 NUMCOL+2. [PLTMN]

NUMLAB Number of X labels to be printed at the bottom of graphs (terminal and/or line printer plots). [PLTMN]

NUMROW Number of rows in graphs (terminal and/or line printer plots). [PLTMN]

N1 Dimension of triangular matrix used in solving system of equations. [BACSUB]

ONE The plotting symbol "1" (terminal and/or line printer plots). [VMAINH, VPMAIN]

OUTPUT Unit number to determine where output should be printed. [POSTPR, VARERR, VARPRO]

P Number of nonvanishing partial derivatives of the PH(J) (i.e., number of ones in INC). [ADA, DPA, MAIN, PR]

PH(11) Vector containing the values of the functions PH(J) of the model equation. [ADA, CALC, MAIN, STAT]

PHINP1 Flag to indicate whether PH(NP1) is in the model equation. [ADA, DPA]

PI 3.141592654 [STAT]

PI4 PI/4. [STAT]

PI8 PI/8. [STAT]

PL(103) Vector of the horizontal print positions for each line of vertical graphs (terminal and/or line printer plots). [VMAINH, VPMAIN]

PP Variable used in calculating probability of standardized residuals. [STAT]

PRJRES Norm of the projection of the residual onto the range of the Jacobian of the variable projection functional. [ORFAC1, POSTPR, VARPRO]

R(300) Vector of residuals (Y-ETA). [DPA, MAIN, POSTPR, STAT]

RMS Residual mean square. [STAT]

RNEW Norm of residual after current iteration. [VARPRO]

RNORM Norm of residual. [DPA, POSTPR, VARPRO]

RSD Residual standard error. [STAT]

RSS Residual sum of squares. [STAT]

R2 Coefficient of determination. [STAT]

SAV(300) Vector used to store independent variable values. [ORPLOT]

SAVE Value of A(1,NCON), i.e., first item in last "constant" column of A. [DPA]

SAVE1 Variable used in moving values from one location to another. [POSTPR]

SCALE1 Scale of the X1 vector for vertical graphs (terminal and/or line printer plots). [VMAINH, VPMAIN]

SCALE2 Scale of the X2 vector for vertical graphs (terminal and/or line printer plots). [VMAINH, VPMAIN]

SIGMA2 Estimated variance, i.e., (RNORM**2)/(degrees of freedom). [COV]

SKIP Flag to indicate whether a given iteration should be printed out. [VARPRO]

SM Double precision variable used in computing a sum. [VMAINH, VPMAIN]

SR(300) Vector of standardized residuals. [STAT]

SRV(300) Vector of standardized residuals arranged in ascending order. [STAT]

STAR The plotting symbol "*" (terminal and/or line printer plots). [VMAINH, VPMAIN]

SUM Variable used in computing a sum. [COV, STAT]

SWS Sum of the elements of the WEIGHT vector. [STAT]

SYH(300) Vector of probabilities of standardized residuals. [STAT]

SYM(30) Vector of plot symbol assignments (terminal and/or line printer plots). [PLTMN]

SYM1(9) Vector of integer values used to indicate multiple points at same location of graphs (terminal and/or line printer plots). [PLTMN]

T(300,6) Array of independent variables. T(I,J) contains the value of the Ith observation of the JTh independent variable. [ADA, CALC, CH, DERIV, DPA, MAIN, NUMDER, ORPLOT, PR, SETUP1, SETUP2, STAT, TRANS, VARPRO]

TEMP(300) Vector of independent variables to be plotted (DISSPLA plots). [MAIN, STAT]

TITLE(40) Title given to the problem by the user. [MAIN]

TITLED(41) TITLE concatenated with "$" for use as graph lAbel (DISSPLA plots). [MAIN]

TITLE1 First line of graph title (DISSPLA plots). [PLOT1, PLOT2]

TITLE2 Second line of graph title (DISSPLA plots). [PLOT2]

TLABEL(48) Axis label given by user for the independent variable (DISSPLA plots). [MAIN, STAT]

TMAX Maximum value of TEMP vector. [MAIN]

TMIN Minimum value of TEMP vector. [MAIN] TPL(600)Vector of values of the independent variable in the order in which they are to be plotted (terminal and/or line printer plots). [MAIN, SETUP1, SETUP2]

TR T-ratios. [STAT]

TS Flag to indicate that independent variable is a time series. [MAIN, PLOT1, PLOT2, STAT]

TWO The plotting symbol "2" (terminal and/or line printer plots). [VMAINH, VPMAIN]

U(10) Vector containing information on Householder reflections; linear parameters. [DPA, POSTPR]

U1 Factor used in computing Householder reflec- tions. [ORFAC1, ORFAC2]

VAR Character variable containing "VAR". [MAIN, PR, STAT]

W(300) Vector of nonnegative weights. [DPA, MAIN, POSTPR, VARPRO]

WEIGHT(300) Vector of nonnegative weights, squared. [CH, DPA, MAIN, PR, STAT, VARPRO, WT]

WRNBEF Flag to control printing certain questions at beginning of "Command Point" only once per execution of the program. [MAIN]

WTVAL User defined value by which the weights for all data points are changed. [CH]

XARAY(300) Vector of observations for the X coordinates (DISSPLA, terminal and/or line printer plots). [PLOT1, PLTMN, SPLT, SPLTH]

XARAY1(300) Vector of X coordinates for the first curve in multiple graphs (DISSPLA plots). [PLOT2]

XARAY2(500) Vector of X coordinates for second curve in multiple graphs (DISSPLA plots). [PLOT2]

XLAB(15) Vector of X axis labels (terminal and/or line printer plots). [PLTMN]

XLBL(48) X axis label (DISSPLA plots). [PLOT1, PLOT2]

XLIM(9) Vector of the X axis labels for vertical graphs (terminal and/or line printer plots). [VMAINH, VPMAIN]

XLONG Length in inches of X axis (DISSPLA plots). [PLOT1]

XMAX Upper bound for X axis (DISSPLA plots). [PLOT1, PLOT2]

XMN1 Minimum value of X1. [VMAINH, VPMAIN]

XMN2 Minimum value of X2. [VMAINH, VPMAIN]

XMX1 Maximum value of X1. [VMAINH, VPMAIN]

XMX2 Maximum value of X2. [VMAINH, VPMAIN]

XN Minimum X value to be plotted (terminal and/or line printer plots). [PLTMN]

XORIG Lower bound for X axis (DISSPLA plots). [PLOT1, PLOT2]

XPL(500) Vector of 500 values, equally incremented, of the independent variable used to plot the predicted Y curve (DISSPLA plots). [MAIN, STAT]

XWIDTH Interval length of X axis (terminal and/or line printer plots). [PLTMN]

XX Maximum X value to be plotted (terminal and/or line printer plots). [PLTMN]

XXLONG X coordinate to determine graph placement on Versatec plotter (DISSPLA plots). [PLOT1]

XX1(300,18) Matrix product of BM and A(NPKG,NPKG) used in computing standardized residuals. [STAT]

X1(300) Vector of first series of X values to be plotted (terminal and/or line printer plots). [VMAINH, VPLT, VPLT2, VPMAIN]

X2(300) Vector of second series of X values to be plotted (terminal and/or line printer plots). [VMAINH, VPLT, VPLT2, VPMAIN]

X1MEAN Mean value of the X1 vector. [VMAINH, VPMAIN]

X2MEAN Mean value of the X2 vector. [VMAINH, VPMAIN]

Y(300) Vector of observed values of dependent variable. [CH, DPA, MAIN, PR, SETUP1, SETUP2, STAT, TRANS, VARPRO, WT]

YARAY(300) Vector of observations for Y coordinate (DISSPLA, terminal and/or line printer plots). [PLOT1, PLTMN, SPLT, SPLTH]

YB Mean of observed values, Y. [STAT]

YC Value of PH(J) using current values of ALF in computing numerical derivatives. [NUMDER]

YD Value of PH(J) using incremented values of ALF in computing numerical derivatives. [NUMDER]

YFIT(500) Vector of values for predicted Y curve (DISSPLA plots). [PLOT2]

YLAB(20) Vector of Y axis labels (terminal and/or line printer plots). [PLTMN]

YLABEL(48) Axis label given by user for the dependent variable (terminal and/or line printer plots). [MAIN, STAT]

YLBL(48) Y axis label (DISSPLA plots). [PLOT1, PLOT2]

YLONG Length in inches of Y axis (DISSPLA plots). [PLOT1]

YLOWER Lower bound for Y values to be plotted on current line (terminal and/or line printer plots). [PLTMN]

YMAX Upper bound of Y axis (DISSPLA plots). [PLOT1, PLOT2]

YN Minimum Y value to be plotted (terminal and/or line printer plots). [PLTMN]

YOBS(300) Vector of values for observed Y curve (DISSPLA plots). [PLOT2]

YORIG Lower bound of Y axis (DISSPLA plots). [PLOT1, PLOT2]

YPL(500) Vector of 500 predicted values of the dependent variable, used to plot the predicted Y curve (DISSPLA plots). [MAIN, SETUP1, STAT]

YUPPER Upper bound for Y values to be plotted on current line (terminal and/or line printer plots). [PLTMN]

YWIDTH Interval length of Y axis (terminal and/or line printer plots). [PLTMN]

YX Maximum Y value to be plotted (terminal and/or line printer plots). [PLTMN]

YYLONG Y coordinate to determine graph placement on Versatec plotter (DISSPLA plots). [PLOT1]

Y1MAX Upper bound of first curve for Y axis (DISSPLA plots). [PLOT2]

Y1ORIG Lower bound of first curve for Y axis (DISSPLA plots). [PLOT2]

Z(10) Solution vector from solving system of equations. [BACSUB]

ZERO(300) Vector of zeros used to draw the zero line on graphs (DISSPLA plots). [PLOT1]

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