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COMP - A BASIC Language Nonlinear Least-Squares Curve Fitting Program

by
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CONTENTS

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INTRODUCTION

Most mathematical models which describe biological processes contain nonlinear terms. While there are many possible nonlinear mathematical models that may describe and adequately fit biological data, usually only one (sometimes two and often none) are useful beyond descriptive purposes because they are derived from a consideration of fundamental biological principles. Parameters in these models are usually meaningful because they represent an important aspect of the process. These parameters are usually estimated using nonlinear least-squares techniques on large computers. Fitting mathematical expressions, thought to describe experimental data, is sometimes considered an art because the final parameter estimates obtained from the computer algorithm are a function of the accuracy of initial "guesstimates" for these values. Thus, computer algorithms can either fail completely, give erroneous estimates, or converge to best (true?) solutions.

The following steps typically lead to fitting a mathematical function to biological data: 1) the data are organized and cursorily examined; 2) a plot is devised (sometimes several are tried on different types of graph paper); 3) a hypothesis is generated which may express the process as a model (i.e., are the changes linear, exponential, or logistic?); 4) one model is chosen to represent the process; 5) parameters in the model which allow the best fit of the function (nonlinear least-squares estimates) to the data are calculated, usually by complicated codes on large computers. Often several runs are necessary, using different initial "guesstimates" of parameters in order to obtain a best fit (and sometimes failure); and, 6) the mathematical model and data are plotted. Sometimes residual (observed minus predicted) plots are made to evaluate the adequacy of the model.

We have developed an interactive BASIC code which runs on both a PDP 11/70 or PDP 11/34 computer to help perform the steps outlined above and to reduce the lengthy turnaround time associated with many runs on batch systems. The key to the system is the reenterant nature of the curve fitting routine (allowed only with an interpreted language such as BASIC). In general, the user supplies estimates of the parameters for a selected model (18 are currently available). The program calculates a requested number of iterative refinements (hopefully improvements) to the parameter estimates in an attempt to minimize the squared deviations between the values predicted by the model and the observed data. During program execution the user can observe whether the results are logical. If not, the process may be stopped, new parameter estimates tried, the current fit examined, the process of iteration started again, or a new model selected. Detailed users guides for running COMP on the PDP 11/34 and 11/70 are in Appendices A and B, respectively.

COMPUTER ENVIRONMENT

COMP was written in CSTS BASIC for a UNIVAC 1108 and subsequently converted to BASIC-11 on two different minicomputers. Operating parameters relative to these three machines are summarized below:

NAME	UNIVAC 1108	PDP 11/70	PDP 11/34
OPERATING SYSTEM	INFONET	IAS	RT-11
LANGUAGE	CSTS BASIC	BASIC-11[a]	BASIC-11[a]
CORE AVAILABLE TO BASIC USER	32K	8K	16K
NUMBER OF I/O DEVICES	MANY	SEVERAL	ONE VT 52
STORAGE AVAILABLE	UNLIMITED DRUMS, DISK & TAPE	MODERATE ONE 88M BYTE DISK, ONE TAPE DRIVE	LIMITED TO CAPACITY OF DISKETTE

Access to INFONET from this location was terminated in June 1977, so we have focused this document on the two PDP versions of COMP.

To reduce the size of COMP to fit available core in the 11/34, extensive use of OVERLAY was necessary. OVERLAY allows the main part of the program to reside in core, while certain segments such as the selected model, are added to the program from a diskette as needed.

This feature is not available in IAS-BASIC-11 on the 11/70. Therefore, COMP was divided into five separate programs, each containing up to five models. The User decides which program to request from the disk to run a selected individual model.

(a) Although these have the same name they are not identical.

PROGRAM DESCRIPTION

COMP is an interactive nonlinear least squares routine written in BASIC language and used to obtain estimates of parameters in nonlinear functions and to approximate their associated statistical errors. The program uses the linearizing (or Taylor Series) expansion of partial derivatives outlined in Draper and Smith, (1966, pp. 267-270). Therefore, partial derivatives must be supplied (as well as the function) by the user for any new models not currently contained in the programs. It should be noted that when a linearizing method is used to estimate parameters in a nonlinear model, all the usual procedures of linear regression theory can be applied. However, the results so obtained are only valid insofar as the linearized form approximates the true model. All of the statistics computed by COMP should be viewed with this restriction in mind.

The output of COMP includes the variance-covariance matrix, t-tests for parameters, Von Neumann's ratio [Bennett and Franklin (1954, pp. 678-679)], observed, predicted and residual values, the error mean square, and an optional procedure to evaluate heteroscedasticity. In the latter procedure the absolute values of the residuals are fit using a linear regression model. Thus, deviations which are significantly larger as X increases (usually X is time) may be detected using the linear regression. One explanation for such behavior may be multiplicative rather than additive errors.

REQUIRED INPUT

A summary of the dialogue is shown below (a return is implicit after each User entry):

COMPUTER GENERATED QUESTION	PROGRAM VARIABLE NAME	USER SUPPLIED ANSWERS
LISTING OF MODELS?	A1	0 = No. 1 = Yes. Print a list of available models and their respective code numbers.
MODEL NUMBER	K	1 = First model 2 = Second model and so on, until 18 = Eighteenth model
ENTER # OF DATA POINTS	N	N = Number of (X,Y) pairs.
ENTER # OF PARAMETERS	M	1 = Number of parameters for the model: M>6 requires program modifications.
INPUT FILE?	D1	0 = No. Input will come from keyboard. 1 = Yes. Data are on a file.
OUTPUT FILE ALSO?	Z7	0 = No 1 = Yes
SAVE ORIGINAL DATA OR RESIDUALS	Z8	1 = Yes. Save a file of the original X, Y pairs. 2 = Save a file of the residuals and corresponding X values.

When using input or output files, their names will be requested, i.e.:

INPUT FILE NAME?	------.DAT
OUTPUT FILE NAME?	------.OUT

If an input file is not used the following questions will be asked:

LIST OBSERVATIONS ON Y	Y(1) Y(2) Y(3) ---- ---- Y(N)

```
LIST SAMPLING TIMES
  (Corresponding to X)        T(1)
                              T(2)
                              T(3)
                              ----
                              ----
                              T(N)
```

After data input (either via files or keyboard) the following questions will be asked:

```
ENTER PARAMETER GUESSES       P(1)
                              P(2)
                              P(3)
                              ----
                              ----
                              P(M)

ENTER # OF ITERATIONS         N2        Zero will result in a check on
                                        "guesstimates" if entered at the
                                        first iteration (i.e., observed
                                        and predicted values are printed).
                                        After one or more iterations, the
                                        program will give summary statistics
                                        as well, if zero is entered.
```

BASIC CODING FOR A MODEL SECTION OF COMP

To add a model to COMP, the User must write BASIC statements for the model, the partial derivative(s), residuals and convergence criteria. We illustrate this with the Gompertz Growth Model which is found on page 8 in Appendix C.

For the Gompertz Growth Model: $Y_i = ae^{-be^{-cX_i}}$

The BASIC representation is:

```
F(I,1) = P(1)*EXP(-P(2)*EXP(-P(3)*T(I)))
```

Where F(I,1) = Y
P(1) = a
P(2) = b
P(3) = c
T(I) = X or in this case -- time.

The partial derivatives of the parameters with respect to Y are:

$$1) = \frac{\partial a}{\partial Y_i} = e^{-be^{-cX_i}}$$

$$2) = \frac{\partial b}{\partial Y_i} = -ae^{-be^{-cX_i}} * e^{-cX_i}$$

$$3) = \frac{\partial c}{\partial Y_i} = ae^{-be^{-cX_i}} * bX_i * e^{-cX_i}$$

The BASIC representations are:

```
1) X(1,I) = EXP(-P(2)*EXP(-P(3)*T(I)))
2) X(2,I) = -F(I,1)*EXP(-P(3)*T(I))
3) X(3,I) = F(I,1)*P(2)*T(I)*EXP(-P(3)*T(I))
```

For the residuals:

$$R_i = Y_{i\ (OBS)} - Y_{i\ (PREDICTED)}$$

The BASIC statement always is:

```
R(I,1) = Y(I,1)-F(I,1)
```

To compute the convergence criterion:

$$C = \sum_{i=1}^{n} R_i(\partial a/\partial Y_i + \partial b/\partial Y_i + \partial c/\partial Y_i)$$

The BASIC statement is:

```
C = C + R(I,1) * (X(1,I) + X(2,I) + X(3,I))
```

For another model, the appropriate partials would be included in the area bracketed.

All of the above BASIC statements are included in a FOR loop (I = 1 to N) terminated by NEXT I and RETURN.

AVAILABLE MODELS

Description	Equation	Page Number in Appendix C
One Compartment Exponential	$Y = ae^{-bt}$	6
Two Compartment Exponential	$Y = a_1e^{-b_1t} + a_2e^{-b_2t}$	7
Three Compartment Exponential	$Y = a_1e^{-b_1t} + a_2e^{-b_2t} + a_3e^{-b_3t}$	11
Exponential Turnover	$Y = ate^{-bt}$	8
Exponential Uptake (Starts at y = 0, t = 0)	$Y = a(1 - e^{-bt})$	7
Power Function	$Y = at^b$	7
Gompertz Growth Curve	$Y = ae^{-be^{-ct}}$	8
Laird Reformulation of Gompertz Growth Curve	$Y = ae^{[b/c(1 - e^{-ct})]}$	12
Logistic Growth Curve	$Y = \frac{a}{1 + e^{(b - ct)}}$	12
Mitscherlich	$Y = a + be^{-ct}$	6
Gamma Uptake	$Y = a[1 - (1 + t/b)^{-c + 1}]$	9
Gamma Decay	$Y = a[1 + (t/b)]^{-c}$	9
Log Gamma Uptake	$\text{Log } Y = \text{Log } a + \text{Log } [1 - (1 + t/b)^{-c + 1}]$	10
Log Gamma Decay	$\text{Log } Y = \text{Log } a - c\,[\text{Log } (1 + t/b)]$	10
Log Exponential Uptake (Model Number 5)	$\text{Log } Y = \text{Log } a + \text{Log } (1 - e^{-bt})$	10

One Compartment with Exponential Input	$Y = \frac{a}{(b-c)} [e^{-ct} - e^{-bt}]$	6
Quadratic	$Y = a + bt + ct^2$	8
Linear	$Y = a + bt$	5

AN EXAMPLE OF COMP RUN ON A PDP 11/70

LOGIN PROCEDURE

```
        IAS  PROGRAM DEVELOPMENT SYSTEM   VERSION 1.1
                09:47:59            16-SEP-77

PDS> LOGIN/NO MICB46001
PASSWORD?
USER MICB46001   UIC [300,200] TT16:   TASK 16   09:48:31 16-SEP-77
```

LIST PREVIOUSLY CREATED DATA FILE

```
PDS> TYPE EXPTWO.DAT
1,91.3
5,64.0
10,41.7
15,27.9
20,19.2
30,10.2
40,6.3
50,4.2
60,3.25
70,2.60
```

INVOKE BASIC INTERPRETER

```
PDS> BASIC
IAS BASIC V01

READY
```

RUN COMP VERSION WHICH CONTAINS NEEDED MODEL

```
RUN COMP2.BAS
NON-LINEAR LEAST SQUARES USING FIRST TERM OF TAYLOR SERIES
MAXIMUM NUMBER OF DATA POINTS IS 50, MAX PARAMS = 6
```

ANSWER 1=YES, 0=NO	
MODEL LIST?	Obtain list of models in COMP2
? 1	
MODELS:	
1 FOR LINEAR	
2 FOR THREE COMPARTMENT EXPONENTIAL	
3 FOR TWO COMPARTMENT EXPONENTIAL	
4 FOR QUADRATIC	
MOD #	
? 3	Select two compartment exponential model.
# OF DATA POINTS	
? 10	There are 10 data pairs; see file listing above.
# OF PARAMETERS	
? 4	The model contains four parameters to estimate.
INPUT FILE?	
? 1	Data are from an input file; see above.
OUTPUT FILE ALSO?	
? 0	No output file will be created.
INPUT FILE NAME	
? EXPTWO.DAT	Name of previously created data file.
PARAMETER GUESSES	
? 90	Users initial guesses at the four unknown parameters in:
? .1	
? 10	
? .02	$Y = ae^{-bt} + ce^{-dt}$
# ITERATIONS	
? 5	Allow five "passes," through the algorithm seeking better (improved) estimates of the parameters.

PARAMETER VALUES, CONVERGENCE CRITERION

(5) Successive Estimates of

a = P(1)	b = P(2)	c = P(3)	d = P(4)	the convergence criterion
89.4524	.100471	11.0953	.0217557	-721.405
89.3733	.100538	11.1773	.0217887	-44.6721
89.3722	.100539	11.1784	.0217902	-.01577
89.3722	.100539	11.1784	.0217902	-7.08199E-03
89.3722	.100539	11.1784	.0217902	-4.76360E-03

The fitting process is proceeding well because:

a) The parameter estimates stabilized (to 6 significant digits) at iteration 3.

b) The convergence criterion is steadily approaching zero. Usually a steady decline toward zero, but oscillating between plus and minus values is desirable.

The following four additional (but probably not needed) iterations illustrate this behavior for the convergence criterion:

```
ITERATIONS
? 2
 69.3722        .100539        11.1784        .0217902        1.34754E-03
 69.3722        .100539        11.1784        .0217902       -3.17574E-03
ITERATIONS
? 2
 69.3723        .100539        11.1784        .0217902       -4.97618E-04
 69.3723        .100539        11.1783        .0217902        5.55597E-03
```

Since satisfactory convergence has been obtained enter zero to obtain the final results.

```
ITERATIONS
? 0
Input X-values   Input Y-values   Calculated Y-values   Input Y-calculated Y
 TIME             OBSERVED          EXPECTED              DEVIATIONS
 1                 91.8             91.7612               .0388336
 5                 64               64.0855              -.0854721
 10                41.7             41.691                8.98635E-03
 15                27.9             27.8427               .0573406
 20                19.2             19.195                5.02777E-03
 30                10.2             10.1922               7.82108E-03
 40                6.3              6.27763               .0223699
 50                4.2              4.34635              -.146347
 60                3.25             3.23843               .0115671
 70                2.6              2.51036               .0896432
```

The estimated variance - covariance matrix is arranged as follows:

	P(1)	P(2)	P(3)	P(4)
P(1)	$S^2p(1)$	$S^2p(1)p(2)$	$S^2p(1)p(3)$	$S^2p(1)p(4)$
P(2)		$S^2p(2)$	$S^2p(2)p(3)$	$S^2p(2)p(4)$
P(3)			$S^2p(3)$	$S^2p(3)p(4)$
P(4)				$S^2p(4)$

and the blanks below the diagonal values would simply be repeats of the above diagonal values. The square root of the diagonal parameter variances (i.e., the standard deviations) are used to calculate the t-tests for the parameters which are printed below (i.e., parameter estimate/standard deviation = t). Parameter covariances can be interpreted "somewhat" like a simple correlation coefficient. The sign indicates the direction of joint relationship and the size indicates the strength of the joint relationship among the two parameters. Small covariances allow "easier" fits. In this example parameters a and c [P(1) and P(3)] are jointly related. Since they enter linearly the association did not cause extreme difficulty.

VARIANCE-COVARIANCE MATRIX

.461678	-5.01326E-04	-.483221	-7.77393E-04
-5.01326E-04	6.40914E-07	5.51226E-04	8.50702E-07
-.483221	5.51226E-04	.516341	8.25350E-04
-7.77393E-04	8.50702E-07	8.25350E-04	1.37291E-06

The Von Neumann ratio is a statistic used to detect runs and is computed using squared successive differences in residuals (labeled deviations above) and the variance about regression. To determine statistical significance of the calculated ratio compare it to the critical values in Table 1. The expected value for a random series of runs is two, but as can be seen from Table 1 a statistically significant value depends on sample size. In this example (n=10) a calculated statistic less than 1.06 or greater than 2.94 would be statistically significant ($P<0.05$). A statistically high ratio indicates short-term oscillations and significantly small values indicate longer-term trends or nearly stable conditions (i.e. nonrandomness). For ratios based on more than 25 observations the t-statistic is computed. High positive t-values indicate long-term trends, high negative values indicate

TABLE 1. Critical Values for the Von Neumann Ratio[a]

Sample Size	Upper Critical Values		Lower Critical Values	
	α = 0.01	α = 0.05	α = 0.01	α = 0.05
4	0.63	0.78	3.37	3.22
5	0.54	0.82	3.46	3.18
6	0.56	0.89	3.44	3.11
7	0.61	0.94	3.39	3.06
8	0.66	0.98	3.34	3.02
9	0.71	1.02	3.29	2.98
10	0.75	1.06	3.25	2.94
11	0.79	1.10	3.21	2.90
12	0.83	1.13	3.17	2.87
15	0.92	1.21	3.08	2.99
20	1.04	1.30	2.96	2.70
25	1.13	1.37	2.87	2.63

(a) Adapted from Bennett and Franklin, p. 679, 1954.

short, rapid oscillations. For practical purposes, a value for t of ±2 can be considered statistically significant ($P<0.05$). In the example, the ratio (1.40) indicates no significant departure from expected "residual runs."

The calculated variance about the regression is the traditional error mean square.

```
  VON NEUMANN RATIO           CALCULATED VARIANCE
 CALCULATED     N>25=T          ABOUT REGRESSION
  1.40342         0             7.05932E-03
```

The parameter values and convergence criterion are repeated from above. The t-test calculation was discussed in conjunction with the variance-covariance matrix and a discussion of their validity is in the section on program description. The statistical significance of each parameter should be assessed using a t-table and N-M degrees of freedom. In this case, all four parameters are significantly different ($p < 0.01$) from zero (i.e., H_o: parameter = 0, H_a: parameter $\neq$ 0).

```
PARAMETERS, CONVERGENCE CRITERION
 69.3723          .100539         11.1763         .0217902        5.55697E-03
T-TESTS OF PARAMETERS
 131.533
 125.585
 13.5564
 18.5969
```

A residual test for heteroscedasticity is requested. A zero would have terminated this run. Using this procedure the absolute values of residuals are fit using a linear regression model. Linearly increasing residual values as a function of time (X) may be detected. A statistically significant relationship may indicate that a multiplicative rather than an additive error model should have been assumed. Two iterations are always necessary if this option is selected.

```
TEST RESIDUALS?
? 1
# ITERATIONS
? 2

PARAMETER VALUES, CONVERGENCE CRITERION
 .0318146       5.16109E-04   -29240.4
 .0317796       5.16926E-04    1.01280E-03
```

All of the output previously discussed is recalculated using the two parameter linear regression model. The t-tests for the two parameters are not statistically significant indicating the additive model assumption may have been correct. Any interpretation of the variance-covariance matrix and Von Neumann ratio in this section should be carefully considered and requires the help of a professional statistician.

ITERATIONS
? 0

TIME	OBSERVED	EXPECTED	DEVIATIONS
1	.0388336	.0322965	6.53709E-03
5	.0854721	.0343642	.0511079
10	8.96835E-03	.0369489	-.0279805
15	.0573406	.0395335	.0178071
20	5.02777E-03	.0421131	-.0370904
30	7.82108E-03	.0472874	-.0394663
40	.0223699	.0524567	-.0300868
50	.146347	.0576259	.0887211
60	.0115671	.0627952	-.0512281
70	.0896432	.0679644	.0216788

VARIANCE-COVARIANCE MATRIX
6.36893E-04 -1.34520E-05
-1.34520E-05 4.46911E-07
VON NEUMANN RATIO CALCULATED VARIANCE
CALCULATED N>25=T ABOUT REGRESSION
5.82910E-03 0 2.31987E-03

PARAMETERS, CONVERGENCE CRITERION

.0317796 5.16926E-04 1.01280E-03
T-TESTS OF PARAMETERS
1.25926
.773246

EXIT COMP

TEST RESIDUALS?
? 0

READY

EXIT BASIC

BYE

10:56:51 TASK TERMINATION
CORE SIZE 18K CPU TIME 13.10

EXIT SYSTEM

PDS> LOGO
USER MICB46631 UIC [300,200] TT16: TASK 101 10:56:59 16-SEP-77
CONNECT TIME 11 M SYSTEM UTILIZATION 14 MCTS

BYE

REFERENCES

Bennett, C. and N. A. Franklin. 1954. Statistical Analysis in Chemistry and the Chemical Industry. John Wiley & Sons, N.Y.

Draper, N. R. and H. Smith. 1967. Applied Regression Analysis. John Wiley & Sons, N.Y.

APPENDIX A

USER'S GUIDE FOR COMP ON A DEDICATED PDP 11/34

APPENDIX A. USER'S GUIDE FOR COMP ON A DEDICATED PDP 11/34

A diskette labeled 'COMP' contains all the BASIC programs necessary for using the overlayed version of COMP. A second diskette (labeled 'SYSTEMS') contains the computer operating system (RT-11). Assuming the 'System' diskette is loaded in the left slot (labeled DK-0) and the 'COMP' is loaded in the right slot (labeled DK-1) the following procedure should be followed:

I. DEAD START — If the computer is on, skip to step II. Turn computer power switch to ON (located on computer). Turn the CRT (Descope) power ON (switch on right side of CRT). Depress the BOOT-INIT switch (on computer). The CRT should respond by displaying four meaningless six-digit numbers and a dollar sign. Depress the Caplock key (on CRT) and enter DX on the CRT followed by (R).[a] The CRT will display: RT-11SJ V02C-02. Enter today's date, i.e., DATE 19-OCT-77 (R)[a] (do not fail to enter the word DATE).

II. RUNNING BASIC

Enter: R BASIC (R)
CRT will display: BASIC V01B-02
Enter another (R).
CRT will display: READY

III. STARTING COMP (If a data file must be created skip to Section V.)

Enter: OLD 'DX1:COMP'
CRT will display: READY
Enter: RUN

IV. RUNNING COMP

COMP is interactive, and generally self-explanatory (see preceeding sections for more details). Remember that overlays are used to save computer core, so if a model is chosen, then later a different model is wanted, return to Step III. Failure to do this will result in

---

(a)Carriage return

subjecting the data to two models simultaneously and unexpected results will be obtained. The following hints may be useful:

a) If data are to be read from a file, the file must have been previously created (see Section V). COMP will request the data file name, and it should be supplied without quote marks (i.e., JOHN.DAT).

b) Getting back to READY - to interrupt the program enter two consecutive Control-C's. The screen will display a period. Enter: RE This latter step returns the BASIC mode with program intact. Note: Control-S stops and Control-Q resumes output.

c) Iterations - an answer greater than 0 (zero) will cause the program to try that many iterations. An answer of 0 (zero) will either display a check on your guesstimates or go on to the next step depending on how far the analysis has progressed. An answer of less than zero (a minus number) causes the program to branch back to line 500 which will print the question:

    ENTER PARAMETER GUESSES
    ?

(Note: Line 500 may be referenced when re-entering the program from READY, i.e., GO TO 500)

Parameter guesses can be re-entered and the program run again.

V. CREATING A DATA FILE

On our configuration the only way to create data files is through the CRT keyboard. Those not familiar with PIP or RT-EDIT may use the BASIC program 'DX1:COMPIN' - which will interactively lead one through the file building process.

VI. ADDING NEW MODELS

1. New models are easy to add to COMP. Assume a four compartment exponential model, model 20, is to be added to COMP. Return to BASIC (see Section IVb above) and enter:

    NEW 'DX1:COMP20'

Now enter model 20 with the following conventions:

a) Line 305 must be of the form:

```
305 PRINT 'FOUR COMPARTMENT EXPONENTIAL MODEL'
```

b) Line 320 must contain the number of parameters to be estimated:

```
320 M = 8
```

c) The model must be inserted between lines 2000-4000 but the line number incrementation is optional.

d) No RETURN or END statement should be used.

e) When finished enter:

```
SAVE 'DX1:COMP20'.
```

2. The Main Program - COMP - will need three changes to accept the new model. Change lines:

   240 - to list the new model when a model list is requested

   266 - to increase the maximum number of models (K)

   285 - to overlay the new model when it is requested

a) To make these changes return to BASIC (Section IVb above) and enter:

```
OLD 'DX1:COMP'
```

b) Type in the new lines 240, 266, and 285.

c) Enter:

```
REPLACE 'DX1:COMP'
```

d) Test the changes (make sure there are no errors) by entering:

```
RUN
```

e) WARNING: If the new model does not run properly and you make changes while in COMP, DO NOT fix it and use the REPLACE command!!! If you do, COMP will contain the model which you called via OVERLAY. Make a note of successful changes, then enter the OLD command and use the REPLACE command as outlined in the previous steps.

APPENDIX B

USER'S GUIDE FOR INTERACTIVE USE OF COMP ON A REMOTE PDP 11/70

APPENDIX B. USER'S GUIDE FOR INTERACTIVE USE OF COMP ON A REMOTE PDP 11/70

I. DEAD START (Using a DTC-300 equipped with Microfile)

On the DTC-300 Teletypewriter:	Depress the POWER and LINE buttons. Depress the CAP button on the lower right hand side of the keyboard so that all alphabetic characters received and sent are in capital letters.
On the Microfile:	Depress both the POWER and middle top white (labeled HOST) buttons.
On the Coupler:	Make sure POWER is on (red button on) and duplex is set to FULL.
Dial the Computer number:	942-7601. When whistling signal is heard, insert handset in coupler, and check that green light is on. When a PDS is received on the teletypewriter, enter: LOGIN USER ID PASSWORD[a] If extraneous material is unwanted, login as shown below: LOGIN/NO USER ID PASSWORD The /NO indicates that no user messages are desired.[b]
List Files:	For a listing of all the BASIC files, or programs, enter [after the PDS]: DIRECTORY *.BAS;* or DIR *.BAS;* To list all data files, enter: DIRECTORY *.DAT;* or DIR *.DAT;*

(a) An example USER ID is MICB46681 and an example PASSWORD is GEORGE.
(b) See example on page 13.

II. RUNNING BASIC:

To invoke the BASIC interpreter enter:

BA [after a PDS]

The computer will return:

IAS BASIC V01

READY

Enter:

RUN and the name of the program selected for execution (i.e., RUN COMP1).

III. STARTING COMP

Use the procedure in Section II to run BASIC. The appropriate program to request will depend on the model chosen, (see Table B-1 and also the Chapter on available models for the mathematical representation of each model).

IV. RUNNING COMP

The program is self-explanatory but some detail of its operation is included in Chapters 2 and 3. Some further operational details peculiar to running COMP on the PDP 11/70 are given below.

a) Data files are created by entering EDIT after a PDS. In the following example, words underlined are User replies while the other material is printed from the computer.

ENTER EDIT	PDS> <u>EDIT</u>
NAME FILE	FILE? <u>EXPONE.DAT</u>
	[EDI -- CREATING NEW FILE]
	INPUT
ENTER DATA	<u>9.0, 2</u> (R)
	<u>8.0, 2</u> (R)
	<u>6.2, 5</u> (R)(R) [Two carriage returns terminate data entry.]
TOP OF FILE	*<u>TOF</u>
	[PAGE 1]

TABLE B.1. Models in Various COMP Versions Used on PDP 11/70

Name of Version	Models
COMPØ.BAS	1 Gamma Decay Model
	2 Gamma Uptake Model
	3 Linear
	4 Log Gamma Uptake
	5 Log Gamma Decay
COMP1.BAS	1 One Compartment Exponential
	2 One Compartment With Exponential Input
	3 Mitscherlich
	4 Linear
	5 Log Exponential Uptake (starts at zero)
COMP2.BAS	1 Linear
	2 Three Compartment Exponential
	3 Two Compartment Exponential
	4 Quadratic
COMP3.BAS	1 Power Function
	2 Gompertz Growth Curve
	3 A*T*EXP(-BT) Exponential Turnover
	4 Linear
COMPADD.BAS	1 Linear
	2 Laird Gompertz Growth Curve
	3 Logistic Growth Curve
COMPBIGB.BAS (runs only on BIG BASIC)	1 One Compartment Exponential
	2 One Compartment With Exponential Input
	3 Mitscherlich
	4 Linear
	5 Three Compartment Exponential
	6 Two Compartment Exponential
	7 Quadratic

```
PRINT FILE      * P*
                9.0, 2
                8.0, 2
                6.2, 5
                [EDIT -- *EOB*]
TOP OF FILE     * TOF
                [PAGE 1]
OUT OF EDIT     * EXIT
                [ED--EXIT]
                PDS>
```

Other uses of EDIT are in appropriate PDP manuals.

b) To restart the program at the question ENTER # OF PARAMETERS, type: GO TO 460.

ADDING NEW MODELS TO COMP ON THE PDP 11/70

In order to add new models to the program COMP.BAS a new copy of the existing program called COMPADD.BAS should be made. This version was specifically constructed to facilitate adding new models. A new copy of COMPADD.BAS is created by issuing the command COPY:

```
PDS>   COPY
FROM?  COMPADD.BAS
TO?    COMPLOGI.BAS
```

Note: The name COMPLOGI.BAS is an example name, any logical name can be used. the .BAS portion of the command tells the computer that this file is a BASIC file.

As previously stated, underlined characters are typed by the User. This sequence of commands produces a new version of the program COMPADD called COMPLOGI. Additional models can be added to COMPLOGI without changing the orginal program. This is a safety step used in case something goes wrong in changing the new version. If errors are made, delete the new program and start over with the COPY command.

In order to change the file and add new models, put the file into EDIT mode. This is done by issuing the command:

PDS> EDIT COMPLOGI.BAS

Lines 244-246 contain:

```
244 PRINT " MODELS:"
246 PRINT "        1 FOR LINEAR"
```

and can be printed by typing the FIND command:

* FIND 244

When the contents of line 244 are typed, give an (R) to inform the computer to print the next line also. In this case just after line 248 is the place to insert the model name being added to the program. This is done by the INSERT command:

*I

The I is a sufficient part of the command. After printing the I the CRT or TTY will drop down one line leaving no characters, just a blank line. The line to be inserted is then typed:

250 PRINT " 4 FOR USER SELECTED NEW MODEL"

When through adding lines, issue two (R)s to return to asterisk, then the next command can be keyed in.

Check a current listing to see where the calculations should be added. In this case, the new model calculations are added at line 6040. REMARK (REM) statements should be inserted just ahead of the lines of calculations. In the COMP version COMPADD, line 8000 was used for the END statement so the INSERT command needs to be implemented just after the line number prior to line 8000.

After the last line of the calculations have been added, enter an (R) which causes an asterisk to print. Enter:

*TOF

This command causes EDIT to take the program back to Top of File. At line 260 the model # is requested using the variable K. To implement the new model, add a line number to the statement at line 620. First find line 620:

*FIND 620

The computer prints:

620 ON K GOTO 900, 910, 915

Use the CHANGE command to add a new line number:

*CH/915/915, 925/

The computer prints:

620 ON K GOTO 900, 910, 915, 925

A correct GOSUB statement for the new model should be placed at line 925. Once again use the FIND command:

*FIND 920

The computer prints:

920 GOTO 940

Input the letter I after the asterisk:

*I

Then type:

925 GOSUB 6040
930 GOTO 940

To EXIT the EDIT mode the letters ED are typed in after the asterisk:

*ED

This will save the present version and delete the unchanged program. If you use the EXIT command:

*EX

both versions will be saved, but only version 2 will have the changes, so the first copy must be manually deleted. When the computer returns:

PDS>

A successful EXIT from EDIT has been made.

To disconnect the teletype from the computer type LOGOUT. If the BASIC interpreter is being used, enter BYE and the computer will return a PDS.

APPENDIX C

PROGRAM LISTINGS

VARIABLES USED IN COMP

(n = number of pairs of points, m = number of parameters)

VARIABLE NAME	USE OF VARIABLE
A(m,m)	Inverse of S(m,m).
B(n,m)	Transpose of X(m,n).
D(m,1)	Product of X(m,n) * R(n,1).
E(m,1)	Product of A(m,m) * D(m,1) and change in parameter value(s) for the current iteration.
F(n,1)	Expected values for Y based on the selected model.
H(1,2*m)	H(1,I) = New (refined) parameter estimates. H(1,m+1) = Convergence criterion.
P(m)	Initial parameter guesstimates and new (calculated) parameter values.
Q(m)	Temporary storage for previous P(m) values.
R(n,1)	Residuals, Y-F.
S(m,m)	Product of X(m,n) * B(n,m).
T(n)	Observations on X (usually sampling times).
V(m,m)	Variance-Covariance matrix.
X(m,n)	Partial derivative of each parameter with respect to Y, evaluated at each sampling time.
Y(n,1)	Observations on Y
C	Convergence Criterion
K	Model Selected
N	Number of Pairs of Points
M	Number of Parameters
N1	Number of Iterations
N3	Set to 0 (zero) when N2 is entered as zero. Result in printing check on guesstimates.
E1	Von Neumann Ratio (Test for residual runs) Use Table 11.5 on page 679 in Bennett and Franklin, 1954, for Table 1, page 17, this report.
T1	If N>25 this t-test approximation for significant residual runs is printed. Use an ordinary t-table.
V1	Residual Variance

LISTING OF COMP FOR PDP 11/34

```
60 PRINT 'NON-LINEAR LEAST SQUARES USING FIRST TERM OF TAYLOR SERIES'
70 PRINT 'MAXIMUM NUMBER OF POINTS IS 50'
80 FOR I=1 TO 10\PRINT \NEXT I
100 PRINT 'TO ANSWER YES, ENTER 1'
110 PRINT 'TO ANSWER NO, ENTER 0'
130 DIM X(3,50),B(50,3),F(50),R(50),T(50),Y(50)
140 DIM S(6,6),V(6,6),A(6,6)
150 DIM D(6),Q(6),H(12),P(6),E(6)
155 G1=50\G2=3
160 PRINT 'MOD LIST';\INPUT A1\IF A1=0 THEN 260
190 PRINT 'MODELS:'\PRINT '1 = EXPONENTIAL'
195 PRINT '2 = COMPARTMENT WITH EXPONENTIAL INPUT'\PRINT '3 = MITSCHERLICH'
200 PRINT '4 = TWO COMPARTMENT EXPONENTIAL'\PRINT '5 = UPTAKE'
205 PRINT '6 = POWER FUNCTION'\PRINT '7 = GOMPERTZ'\PRINT '8 = QUADRATIC'
210 PRINT '9 = A*T*EXP(-BT)'\PRINT '10 = CUSHING DECAY GAMMA'
220 PRINT '11 = CUSHING UPTAKE-GAMMA'\PRINT '12 = LOG CUSHING DECAY-GAMMA'
225 PRINT '13 = LOG UPTAKE-GAMMA'\PRINT '14 = LOG UPTAKE (=5)'
230 PRINT '15 = LINEAR'\PRINT '16 = 3 COMPARTMENT EXPONENTIAL'
240 PRINT '17 = 4 COMPARTMENT EXPONENTIAL (4TH NEGATIVE)'
241 PRINT '18 = LOGISTIC GROWTH (Y=B1/(1+EXP(B2-B3*T))'
242 PRINT '19 = LAIRD REFORMULATION OF GOMPERTZ'
243 PRINT '20 = TWO COMPARTMENT EXP. FORCING P3 = 1 - P1'
245 REM
260 PRINT 'MODEL NUMBER';\INPUT K
265 IF K>=1 THEN 266 \PRINT K;' IS NOT A VALID MODEL #'\GO TO 190
266 IF K<=19 THEN 270 \PRINT K;' IS NOT A VALID MODEL #'\GO TO 190
270 IF K<>1 THEN 271 \OVERLAY 'DX1:COMP1.BAS'\GO TO 300
271 IF K<>2 THEN 272 \OVERLAY 'DX1:COMP2.BAS'\GO TO 300
272 IF K<>3 THEN 273 \OVERLAY 'DX1:COMP3.BAS'\GO TO 300
273 IF K<>4 THEN 274 \OVERLAY 'DX1:COMP4.BAS'\GO TO 300
274 IF K<>5 THEN 275 \OVERLAY 'DX1:COMP5.BAS'\GO TO 300
275 IF K<>6 THEN 276 \OVERLAY 'DX1:COMP6.BAS'
276 IF K<>7 THEN 277 \OVERLAY 'DX1:COMP7.BAS'
277 IF K<>8 THEN 278 \OVERLAY 'DX1:COMP8.BAS'
278 IF K<>9 THEN 279 \OVERLAY 'DX1:COMP9.BAS'
279 IF K<>10 THEN 280 \OVERLAY 'DX1:COMP10.BAS'
280 IF K<>11 THEN 281 \OVERLAY 'DX1:COMP11.BAS'
281 IF K<>12 THEN 282 \OVERLAY 'DX1:COMP12.BAS'
282 IF K<>13 THEN 283 \OVERLAY 'DX1:COMP13.BAS'
283 IF K<>14 THEN 284 \OVERLAY 'DX1:COMP14.BAS'
284 IF K<>16 THEN 285 \OVERLAY 'DX1:COMP16.BAS'
285 IF K<>17 THEN 290 \OVERLAY 'DX1:COMP17.BAS'
290 IF K<>18 THEN 291 \OVERLAY 'DX1:COMP18.BAS'
291 IF K<>19 THEN 292 \OVERLAY 'DX1:COMP19.BAS'
292 IF K<>20 THEN 300 \OVERLAY 'DX1:COMP20.BAS'
300 PRINT 'MODEL ';K;' HAS BEEN ADDED TO PROGRAM'
320 M=2
330 PRINT 'DATA ON FILE';\INPUT D1\IF D1=0 THEN 350 \OVERLAY 'DX1:COMP99.BAS'
340 GO TO 160
350 PRINT '# OF DATA POINTS';\INPUT N\IF N<=50 THEN 370
360 PRINT 'TOO MANY'\GO TO 350
370 PRINT 'ENTER OBSERVATIONS ON Y'
380 FOR I=1 TO N\INPUT Y(I)\NEXT I
420 PRINT 'ENTER SAMPLING TIMES'
430 FOR I=1 TO N\INPUT T(I)\NEXT I
500 REM COME HERE TO START OVER  ------- ZERO OUT ARRAYS
501 FOR I=1 TO G1
502 F(I)=0\FOR J=1 TO G2
503 X(J,I)=0\B(I,J)=0
504 NEXT J
```

```
505 NEXT I
506 FOR I=1 TO G2
507 F(I)=0\Q(I)=0\P(I)=0\E(I)=0
508 FOR J=1 TO G2
509 S(I,J)=0\V(I,J)=0\A(I,J)=0
510 NEXT J
511 NEXT I
512 FOR I=1 TO 2*G2
513 H(I)=0
514 NEXT I
515 PRINT 'ENTER ';M;' PARAMETER GUESSES'
519 FOR I=1 TO M\INPUT P(I)\NEXT I
520 PRINT '# OF ITERATIONS';\INPUT N2\IF N2<0 THEN 500 \IF N2>0 THEN 560
530 N3=0\N1=1\GO TO 610
560 N1=N2\N3=1\PRINT
570 IF M>5 THEN 600
580 FOR I=1 TO M\PRINT 'PARAM';I;'  ';\NEXT I\PRINT 'CONVERG'\PRINT \GO TO 610
600 FOR I=1 TO M\PRINT 'PARAMETER',\NEXT I\PRINT 'CONVERGENCE'
605 FOR I=1 TO M\PRINT I,\NEXT I\PRINT 'CRITERION'\PRINT
610 FOR J=1 TO N1
620 IF K=15 THEN 1300
630 GO TO 6000
640 IF N2=0 THEN 1180
950 FOR I=1 TO N
954 FOR I1=1 TO M\B(I,I1)=X(I1,I)\NEXT I1
958 NEXT I
959 FOR I=1 TO M
960 FOR I1=1 TO M\S(I,I1)=0
961 FOR I2=1 TO N\S(I,I1)=S(I,I1)+X(I,I2)*B(I2,I1)\NEXT I2
964 NEXT I1
966 NEXT I
976 FOR I=1 TO M
978 FOR J1=1 TO M\A(I,J1)=0\NEXT J1
982 A(I,I)=1\NEXT I
991 T2=1\REM T2 IS THE DETERMINANT.
993 REM CALCULATE INVERSE
994 FOR I=1 TO M\J9=S(I,I)
1000 FOR J1=1 TO M\S(I,J1)=S(I,J1)/J9\A(I,J1)=A(I,J1)/J9\NEXT J1
1014 FOR J1=1 TO M\IF I-J1=0 THEN 1028 \I3=S(J1,I)
1017 FOR J8=1 TO M\S(J1,J8)=S(J1,J8)-I3*S(I,J8)
1022 A(J1,J8)=A(J1,J8)-I3*A(I,J8)\NEXT J8
1028 NEXT J1
1030 NEXT I
1042 FOR I=1 TO M\D(I)=0
1044 FOR J1=1 TO N\D(I)=D(I)+X(I,J1)*R(J1)\NEXT J1
1048 NEXT I
1051 FOR I=1 TO M\E(I)=0
1053 FOR J1=1 TO M\E(I)=E(I)+A(I,J1)*D(J1)\NEXT J1
1056 NEXT I
1076 FOR I=1 TO M\Q(I)=P(I)\P(I)=0\P(I)=Q(I)+E(I)\NEXT I
1085 FOR I=1 TO M\H(I)=P(I)\NEXT I
1092 H(M+1)=C
1095 IF M>4 THEN 1097 \FOR I=1 TO M+1\PRINT H(I),\NEXT I\PRINT \GO TO 1100
1097 FOR I=1 TO M+1\PRINT H(I);\NEXT I\PRINT
1100 NEXT J
1105 FOR I=1 TO 4\PRINT '  ';\NEXT I
1110 PRINT 'ITERATIONS';\INPUT N2\IF N2<0 THEN 500
1130 IF N3=0 GO TO 1160
1140 [illegible]
1160 [illegible]
```

```
1180 IF N3 OGO TO 1200
1190 PRINT 'CHECK ON GUESSTIMATES'
1200 PRINT ' '
1210 PRINT ' TIME           OBSERVED        EXPECTED      DEVIATIONS'
1220 FOR I=1 TO N
1230 IF K=1200 TO 1260
1240 IF K=1300 TO 1260 \IF K=1400 TO 1260
1250 GO TO 1270
1260 Y(I)=ABS(Y(I))
1270 PRINT T(I),Y(I),F(I),R(I)
1280 IF Z7=OGO TO 1360
1290 IF I 100 TO 1310
1300 OPEN "LP:" FOR OUTPUT AS FILE #2
1302 PRINT #2,F$
1310 IF J= TO 1350
1320 PRINT #2,T(I),Y(I),D$
1330 GO TO 1360
1340 IF I=NGO TO 1380
1350 PRINT #2,T(I),R(I),D$
1360 IF I=NGO TO 1380
1370 V2=V2+(R(I)-R(I1))^2
1380 V1=V1+R(I)^2
1390 NEXT I
1400 IF Z7=OGO TO 1420
1410 PRINT #2,999,999,D$
1420 IF N3=0 THEN 520
1430 V1=V1/(N-M)
1440 REM REPLACES MAT V(M,M) = (V1) * A(M,M)
1441 FOR I=1 TO M
1442 FOR J=1 TO M
1444 V(I,J)=V1*A(I,J)
1446 NEXT J
1448 NEXT I
1450 PRINT \PRINT 'VARIANCE-COVARIANCE MATRIX'
1462 FOR I=1 TO M
1464 FOR J=1 TO M\PRINT V(I,J),\NEXT J\PRINT
1467 NEXT I\PRINT
1470 V2=V2/(N-1)\E1=V2/V1
1490 IF N 2560 TO 1550
1500 E2=N-1\E3=N-2\E4=N+1
1530 T1=(1-(V2/(2*V1)))/SQR(E3/(E2*E4))
1540 GO TO 1560
1550 T1=0
1560 PRINT '  VON NEUMANN RATIO         CALCULATED VARIANCE'
1570 PRINT 'CALCULATED      N 25=T          ABOUT REGRESSION'
1580 PRINT E1,T1,V1
1590 V1=0
1600 V2=0
1610 PRINT ' '
1620 FOR I=1 TO M\PRINT 'PARAMETER',\NEXT I\PRINT 'CONVERGENCE'
1625 FOR I=1 TO M\PRINT I,\NEXT I\PRINT 'CRITERION'\PRINT
1630 FOR I=1 TO M\PRINT H(I),\NEXT I\PRINT H(I+1)\PRINT
1650 PRINT "T-TESTS OF PARAMETERS"
1660 FOR I=1 TO M\PRINT H(I)/SQR(V(I,I)),\NEXT I\PRINT \PRINT
1700 REM
1710 PRINT 'TEST RESIDUALS TO CHECK HETEROSCEDASTICITY'
1720 INPUT Q2\IF Q2 0 THEN 500
1730 IF Q2=OGO TO 3000
1740 FOR I=1 TO N
1750 [illegible]
```

```
1[illegible]
1[illegible] [illegible] PROGRAM CALLS LINEAR MODEL
1[illegible]80 [illegible] 2
1[illegible] [illegible] TO [illegible]
1800 REM COME HERE TO PROCESS MODEL
5[illegible] GO TO 940  REM END OF MODEL
5000 REM LINEAR MODEL
5[illegible]0 C=0
5020 FOR I=1 TO N
50[illegible]0 [illegible]
5030 [illegible]
50[illegible] X(1,I)=1
50[illegible] X(2,I)=T(I)
50[illegible] [illegible]R(I)*(X(1,I)+X(2,I))
5080 NEXT I
[illegible] GO TO 940
[illegible] REM CLOSE FILES HERE
[illegible] [illegible]
*
```

OVERLAID MODELS FOR COMP (PDP 11/34)

COMP1.BAS

```
305 PRINT 'EXPONENTIAL MODEL F = P1*EXP(-P2*T)'
320 M=2
1810 REM SUBROUTINE FOR EXPONENTIAL MODEL
1820 C=0
1830 FOR I=1 TO N
1840 F(I)=P(1)*EXP(-P(2)*T(I))
1850 R(I)=Y(I)-F(I)
1860 X(1,I)=EXP(-P(2)*T(I))
1870 X(2,I)=-P(1)*T(I)*EXP(-P(2)*T(I))
1880 C=C+R(I)*(X(1,I)+X(2,I))
1890 NEXT I
```

COMP2.BAS

```
305 PRINT 'COMPARTMENT WITH EXPONENTIAL INPUT'
320 M=3
1920 REM SUBROUTINE FOR COMPARTMENT WITH EXPONENTIAL INPUT
1930 C=0
1940 FOR I=1 TO N
1950 K1=(EXP(-P(3)*T(I))-EXP(-P(2)*T(I)))/(P(2)-P(3))
1960 R(I)=Y(I)-(P(1)*K1)
1970 F(I)=P(1)*K1
1980 X(1,I)=K1
1990 X(2,I)=(P(1)*T(I)*EXP(-P(2)*T(I)))/(P(2)-P(3))-P(1)*K1/(P(2)-P(3))
2000 X(3,I)=(P(1)*K1)/(P(2)-P(3))-(P(1)*T(I)*EXP(-P(3)*T(I)))/(P(2)-P(3))
2010 C=C+R(I)*(X(1,I)+X(2,I)+X(3,I))
2020 NEXT I
```

COMP3.BAS

```
305 PRINT 'MITSCHERLICH MODEL'
320 M=3
2050 REM SUBROUTINE FOR MITSCHERLICH MODEL
2060 C=0
2070 FOR I=1 TO N
2080 F(I)=P(1)+P(2)*EXP(-P(3)*T(I))
2090 R(I)=Y(I)-F(I)
2100 X(1,I)=1
2110 X(2,I)=EXP(-P(3)*T(I))
2120 X(3,I)=-P(2)*T(I)*EXP(-P(3)*T(I))
2130 C=C+R(I)*(X(1,I)+X(2,I)+X(3,I))
2140 NEXT I
```

COMP4.BAS

```
305 PRINT 'TWO-COMPONENT EXPONENTIAL'
320 M=4
2170 REM TWO-COMPONENT EXPONENTIAL
2180 C=0
2190 FOR I=1 TO N
2200 F(I)=P(1)*EXP(-P(2)*T(I))+P(3)*EXP(-P(4)*T(I))
2210 R(I)=Y(I)-F(I)
2220 X(1,I)=EXP(-P(2)*T(I))
2230 X(2,I)=-P(1)*T(I)*EXP(-P(2)*T(I))
2240 X(3,I)=EXP(-P(4)*T(I))
2250 X(4,I)=-P(3)*T(I)*EXP(-P(4)*T(I))
2290 C=C+R(I)*(X(1,I)+X(2,I)+X(3,I)+X(4,I))
2300 NEXT I
```

COMP5.BAS

```
305 PRINT 'CUSHING UPTAKE  Y = A - A*EXP(-B*T)'
320 M=2
2330 REM SUBROUTINE FOR CUSHING UPTAKE MODEL
2340 C=0
2350 FOR I=1 TO N
2360 F(I)=P(1)*(1-EXP(-P(2)*T(I)))
2370 R(I)=Y(I)-F(1)
2380 X(1,I)=1-EXP(-P(2)*T(I))
2390 X(2,I)=P(1)*T(I)*EXP(-P(2)*T(I))
2400 C=C+R(I)*(X(1,I)+X(2,I))
2410 NEXT I
```

COMP6.BAS

```
305 PRINT 'Y+(A*W^B); W CORRES TO T(I)'
320 M=2
2720 REM SUBROUTINE TO FIT Y=(A*W^B); W CORRES TO T(I)
2730 C=0
2740 FOR I=1 TO N
2750 F(I)=P(1)*(T(I)^P(2))
2760 R(I)=Y(I)-F(I)
2770 X(1,I)=T(I)^P(2)
2780 X(2,I)=F(I)*LOG(T(I))
2790 C=C+R(I)*(X(1,I)+X(2,I))
2800 NEXT I
```

COMP7.BAS

```
305 PRINT 'GOMPERTZ'
320 M=3
2830 REM SUBROUTINE TO FIT GOMPERTZ
2840 C=0
2850 FOR I=1 TO N
2860 F(I)=P(1)*EXP(-P(2)*EXP(-P(3)*T(I)))
2870 R(I)=Y(I)-F(I)
2880 X(1,I)=EXP(-P(2)*EXP(-P(3)*T(I)))
2890 X(2,I)=-F(I)*EXP(-P(3)*T(I))
2900 X(3,I)=F(I)*P(2)*T(I)*EXP(-P(3)*T(I))
2910 C=C+R(I)*(X(1,I)+X(2,I)+X(3,I))
2920 NEXT I
```

COMP8.BAS

```
305 PRINT 'QUADRATIC MODEL'
320 M=3
2950 REM SUBROUTINE TO FIT QUADRATIC
2960 C=0
2970 FOR I=1 TO N
2980 F(I)=P(1)+P(2)*T(I)+P(3)*(T(I)^2)
2990 R(I)=Y(I)-F(I)
3000 X(1,I)=1
3010 X(2,I)=T(I)
3020 X(3,I)=T(I)^2
3030 C=C+R(I)*(X(1,I)+X(2,I)+X(3,I))
3040 NEXT I
```

COMP9.BAS

```
305 PRINT 'F=P1*T*EXP(-B*T)'
320 M=2
3070 REM SUBROUTINE TO FIT ATEXP(-BT)
3080 C=0
3090 FOR I=1 TO N
3100 F(I)=P(1)*T(I)*EXP(-P(2)*T(I))
3110 R(I)=Y(I)-F(I)
3120 X(1,I)=T(I)*EXP(-P(2)*T(I))
3130 X(2,I)=-T(I)*F(I)
3140 C=C+R(I)*(X(1,I)+X(2,I))
3150 NEXT I
```

COMP10.BAS

```
305 PRINT 'DECAY FROM ALGAE'
320 M=3
3340 REM SUBROUTINE TO FIT--DECAY FROM ALGAE Y=A(1+T/B)^-C
3350 REM C=ALPHA; A=(LAMBDA*B)/(ALPHA-1)
3360 C=0
3370 FOR I=1 TO N
3380 A1=1+(T(I)/P(2))
3390 A2=A1^(-P(3))
3400 A3=A1^(-P(3)-1)
3410 F(I)=P(1)*A2
3420 R(I)=Y(I)-F(I)
3430 X(1,I)=A2
3440 X(2,I)=(P(1)*T(I)*P(3)/P(2)^2)*(A3)
3450 X(3,1)=-P(1)*A2*LOG(A1)
3460 C=C+R(I)*(X(1,I)+X(2,I)+X(3,I))
3470 NEXT I
```

COMP11.BAS

```
305 PRINT 'ALGAE UPTAKE  Y=A(1-(1+T/B))-(ALPHA-1)'
320 M=3
3180 REM SUBROUTINE TO FIT ALGAE UPTAKE--Y=A(1-(1+T/B))-(ALPHA-1)
3190 REM A+LAMBDA*B/(ALPHA-1)
3200 C=0
3210 FOR I=1 TO N
3220 A1=1+(T(I)/P(2))
3230 A2=A1^(-P(3))
3240 A3=A1^(-P(3)+1)
3250 F(I)=P(1)*(1-A3)
3260 R(I)=Y(I)-F(I)
3270 X(1,I)=1-A3
3280 X(2,I)=((-P(3)+1)*P(1)*T(I)/(P(2)^2))*(A2)
3290 X(3,I)=P(1)*A3*LOG(A1)
3300 C=C+R(I)*(X(1,I)+X(2,I)+X(3,I))
3310 NEXT I
```

COMP12.BAS

```
305 PRINT 'LOG FORM OF DECAY MODEL'
320 M=3
3500 REM LOG FORM OF DECAY MODEL  LOGY=LOGA-ALPHA*LOG(1+T/B)
3510 REM WHERE A=LAMBDA*T/(ALPHA-1.)
3520 C=0
3530 FOR I=1 TO N
3540 A1=(1+T(I)/P(2))
3550 A2=P(2)^2
3560 F(I)=LOG(P(1))-P(3)*LOG(A1)
3570 R(I)=LOG(Y(I))-F(I)
3580 X(1,I)=1/P(1)
3590 X(2,I)=P(3)*T(I)/(A1*A2)
3600 X(3,I)=-LOG(A1)
3610 C=C+R(I)*(X(1,I)+X(2,I)+X(3,I))
3620 NEXT I
```

COMP13.BAS

```
305 PRINT 'LNY=LNA+LN (1-(T/B)^(ALP-1)'
320 M=3
3650 REM LOG OF CUSH. UPTK. MOD.-- LNY=LNA+LN (1-(1+T/B)^(ALP-1)
3660 C=0
3670 FOR I=1 TO N
3680 A1=1+(T(I)/P(2))
3690 A2=A1^(-P(3))
3700 A3=A1^(-P(3)+1)
3710 F(I)=LOG(P(1))+LOG(1-(A3))
3720 R(I)=LOG(Y(I))-F(I)
3730 X(1,I)=1/P(1)
3740 X(2,I)=(-P(3)+1)*T(I)*A2/((1-(A3))*P(2)^2
3750 X(3,I)=A3*LOG(A1)/(A-(A3))
3760 C=C+R(I)*(X(1,I)+X(2,IX(3,I))
3770 NEXT I
```

COMP14.BAS

```
305 PRINT 'LOG FORM OF UPTAKE MODEL'
320 M=2
3820 REM LOG FORM OF UPTAKE MODEL
3840 C=0
3850 FOR I=1 TO N
3870 F(I)=P(1)+LOG(1-EXP(-P(2)*T(I)))
3880 R(I)=Y(I)-F(I)
3890 X(1,I)=1
3900 X(2,I)=(T(I)*EXP(-P(2)*T(I)))/(1-EXP(-P(2)*T(I)))
3930 C=C+R(I)*(X(1,I)+X(2,I))
3940 NEXT I
```

COMP15.BAS

Model 15 is LINEAR in main program COMP (see lines 6000-6090 page C.5)

COMP16.BAS

```
305 PRINT '3 COMPARTMENT EXPONENTIAL  Y=A*EXP(-B*T)+C*EXP(-D*T)+E*EXP(-F*T)'
320 M=6
2000 C=0
2010 FOR I=1 TO N
2015 C1=0
2020 F(I)=P(1)*EXP(-P(2)*T(I))+P(3)*EXP(-P(4)*T(I))+P(5)*EXP(-P(6)*T(I))
2030 R(I)=Y(I)-F(I)
2040 X(1,I)=EXP(-P(2)*T(I))
2050 X(2,I)=-P(1)*T(I)*EXP(-P(2)*T(I))
2060 X(3,I)=EXP(-P(4)*T(I))
2070 X(4,I)=-P(3)*T(I)*EXP(-P(4)*T(I))
2080 X(5,I)=EXP(-P(6)*T(I))
2090 X(6,I)=-P(5)*T(I)*EXP(-P(6)*T(I))
3000 FOR J1=1 TO 6\C1=C1+X(J1,I)\NEXT J1
3010 C=C+R(I)*C1
3020 NEXT I
```

COMP17.BAS

Model 17 is unavailable for publication

COMP18.BAS

```
305 PRINT 'LOGISTIC GROWTH CURVE'
320 M=3
2000 REM LOGISTIC GROWTH CURVE
2010 REM Y=B1/(1+E^(B2-B3*T)
2020 REM B1=ASYMPTOTE; AT T=0; Y=B1/(1+E^B2)
2030 C=0
2040 FOR I=1 TO N
2050 A1=EXP(P(2)-P(3)*T(I))
2060 F(I)=P(1)/(1+A1)
2070 R(I)=Y(I)-F(I)
2080 X(1,I)=1/(1+A1)
2090 X(2,I)=(-P(1)*A1)/(1+A1)^2
2100 X(3,I)=(P(1)*T(I)*A1)/(1+A1)^2
2110 C=C+R(I)*(X(1,I)+X(2,I)+X(3,I))
2120 NEXT I
```

COMP19.BAS

```
305 PRINT 'LAIRD FORM OF GOMPERTZ'
320 M=3
2000 REM LAIRD FORM OF GOMPERTZ
2010 REM WHERE B1 = EGG WEIGHT
2020 REM Y = V1 EXP^B2/B3(1-EXP B3*T)
2030 C=0
2035 FOR I=1 TO N
2040 A1=P(2)/P(3)
2050 A2=EXP(-P(3)*T(I))
2060 A3=EXP(A1*(1-A2))
2070 A4=P(3)*T(I)*A2
2080 A5=P(1)*P(2)/(P(3))^2
2090 F(I)=P(1)*A3
2100 X(1,I)=A3
2110 X(2,I)=((P(1)/P(3)/*A3)*(1-A2)
2120 X(3,I)=A5*A3*(A2+A4-1)
2130 R(I)=Y(I)-F(I)
2140 C=C+R(I)*(X(1,I)+X(2,I)+X(3,I))
2150 NEXT I
*
```

OVERLAY TO READ DATA FILES (PDP 11/34)

COMP99.BAS

```
160 REM GET FILE NAME AND READ DATA
190 PRINT 'ENTER NAME OF DATA FILE (NO QUOTE MARKS!!!!!!)';\INPUT B$
195 OPEN B$ FOR INPUT AS FILE #1
200 FOR I=1 TO 1000
205 IF END #1 THEN 225
210 N=N+1\INPUT #1:T(I),Y(I)\NEXT I
220 NEXT I
225 PRINT 'HAVE READ ';N;' ITEMS'\PRINT 'VIEW';\INPUT D1
230 IF D1=0 THEN 270
240 REM
241 REM
242 REM
243 REM
244 REM
245 REM
250 REM
260 FOR J=1 TO N\PRINT T(J),Y(J)\NEXT J
265 REM
266 REM
270 GO TO 500
8005 CLOSE #1
```

<u>LISTING OF COMP FOR PDP 11/70</u>

```
5 REM * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * *
6 REM REVISION OF COMP                    /CALLED COMPADD.BAS
8 REM THIS VERSION HAS THREE MODELS WHICH ALLOWS ROOM FOR
9 REM  ADDITIONAL MODELS TO BE ADDED
12 REM THIS NEXT LINE SPACES DOWN ON PAGE - COSMETICS ONLY.
13 FOR I = 1 TO 4     \ PRINT     \ NEXT I
15 REM CHECK LINES 260,1230,1240,1770 FOR VARIABLE K (MODEL #)
16 REM FOR STATEMENTS - CHANGE FOR APPROPRIATE MODELS FOR LOG
60 PRINT "NON-LINEAR LEAST-SQUARES USING FIRST TERM OF TAYLOR SERIES"
70 PRINT "MAXIMUM NUMBER OF DATA POINTS IS 50, MAXIMUM PARAMETERS = 6"
75 REM THIS NEXT LINE SPACES DOWN ON PAGE AFTER HEADING
80 FOR I=1 TO 4 \ PRINT  \ NEXT I
120 PRINT "ANSWER 1=YES, 0=NO"
130 DIM Y(50,1),T(50),P(6),X(6,50),F(50,1),E(6,1),S(6,6)
150 DIM V(6,6),B(50,6),A(6,6),D(6,1),Q(6),R(50,1),H(1,6)
160 PRINT "MODEL LIST?"      \ INPUT A1
180 IF A1=0 GO TO 260
244 PRINT"  MODELS:"
246 PRINT        "    1 FOR LINEAR"
247 PRINT        "    2 FOR LOGISTIC GROWTH CURVE"
248 PRINT        "    3 FOR LAIRD FORM OF GOMPERTZ"
260 PRINT "MOD #"       \ INPUT K
280 PRINT "# OF DATA POINTS"      \INPUT N
300 PRINT "# OF PARAMETERS"      \INPUT M
320 PRINT "INPUT FILE?"      \INPUT D1
340 IF D1=0 GO TO 370
350 GOSUB 2450
360 GO TO 460
370 PRINT "LIST OBSERVATIONS ON Y"
380 FOR I=1 TO N \ INPUT Y(I,1) \ NEXT I
420 PRINT "LIST SAMPLING TIMES"
430 FOR I=1 TO N \ INPUT T(I) \ NEXT I
460 PRINT "PARAMETER GUESSES"
470 FOR I=1 TO M \ INPUT P(I) \ NEXT I
500 PRINT "# ITERATIONS"
510 INPUT N2 \ IF N2=0 GO TO 560
550 N1=N2    \ N3 = 1     \ GOTO 600
560 N3=0 \ N1=1 \ GO TO 610 \ PRINT    \ PRINT
600 PRINT  \PRINT "PARAMETER VALUES, CONVERGENCE CRITERION"
610 FOR J=1 TO N1
620 ON K GO TO 900,910,915
900 GOSUB 3970      \REM LINEAR
905 GOTO 940
910 GOSUB 4040       \ REM LOGISTIC GROWTH CURVE
912 GOTO 940
915 GOSUB 5040        \ REM LAIRD FORM OF GOMPERTZ
920 GOTO 940
940 IF N2=0 GO TO 1160
950 REM  REPLACES MAT B(N,M) = TRN(X(M,N))   'X TRANSPOSE
952 FOR I=1 TO N \ FOR I1=1 TO M \ B(I,I1)=X(I1,I)
957 NEXT I1 \ NEXT I \ FOR I=1 TO M \ FOR I1=1 TO M
960 REM  REPLACES MAT S(M,M) = X(M,N) * B(N,M)
962 S(I,I1)=0 \ FOR I2=1 TO N
964 S(I,I1)=S(I,I1)+X(I,I2)*B(I2,I1)
965 NEXT I2 \ NEXT I1 \ NEXT I
970 REM MAT A(M,M) = INV(S(M,M))                'INVERSE
971 REM FROM P. 142 OF 'STATISTICS AND DATA ANALYSIS IN GEOLOGY' BY DAVIS
972 REM SET A TO IDENTIFY MATRIX AND TO SAVE ORIGINAL S MATRIX
976 FOR I=1 TO M \ FOR J1=1 TO M \ A(I,J1)=0
982 NEXT J1 \ A(I,I)=1 \ NEXT I
991 REM T2 = THE DETERMINANT  \ T2=1
994 REM CALCULATE INVERSE  \ FOR I=1 TO M
998 REM DIVIDE ITH ROW OF S AND A BY S(I,I)
1000 J9=S(I,I) \ FOR J1=1 TO M
```

```
1008 S(I,J1)=(I,J1)/J9
1010 A(I,J1)=A(I,J1)/J9 \ NEXT J1
1012 REM REDUCE THE ITH COLUMN OF S TO ZERO
1014 FOR J1=1 TO M \ IF (I-J1)=0 GO TO 1026
1017 REM I3 = RATIO  \ I3=S(J1,I) \ FOR J8=1 TO M
1021 S(J1,J8)=S(J1,J8)-I3*S(I,J8)
1022 A(J1,J8)=A(J1,J8)-I3*A(I,J8)
1025 NEXT J8
1026 NEXT J1
1030 NEXT I
1040 REM MAT D(M,1) = X(M,N)*R(N,1)
1042 FOR I = 1 TO M     \ D(I,1) = 0      \ FOR J1 = 1 TO N
1046 D(I,1)=D(I,1)+X(I,J1)*R(J1,1)
1047 NEXT J1       \NEXT I
1050 REM REPLACES E(M,1) = A(M,M) * D(M,1)      'ESTIMATES OF REG. COEF.
1051 FOR I=1 TO M     \E(I,1)= 0     \ FOR J7 = 1 TO M
1054 E(I,1)=E(I,1)+A(I,J7)*D(J7,1)
1055 NEXT J7       \NEXT I
1076 FOR I=1 TO M      \ Q(I) = P(I)       \ P(I) = 0
1082 P(I)=Q(I)+E(I,1)       \ NEXT I
1086 FOR I=1 TO M       \ H(1,I) = P(I)
1090 NEXT I       \ H(1,M+1) = C
1093 ON M GO TO 1094,1094,1096,1098,1100
1094 PRINT H(1,1),H(1,2),H(1,3)        \ GOTO 1105
1096 PRINT H(1,1),H(1,2),H(1,3),H(1,4)        \ GOTO 1105
1098 PRINT H(1,1),H(1,2),H(1,3),H(1,4),H(1,5)     \ GOTO 1105
1100 PRINT H(1,1);H(1,2);H(1,3);H(1,4);H(1,5);H(1,6);H(1,7)
1105 NEXT J
1110 PRINT "ITERATIONS"       \INPUT N2     \ IF N2=0 GOTO 1160
1140 N1=N2       \GOTO 610
1160 N1=1        \GOTO 610
1180 IF N3<>0 GO TO 1210
1190 PRINT "CHECK ON GUESSTIMATES"        \PRINT
1210 PRINT \PRINT " TIME            OBSERVED           EXPECTED          DEVIATIONS"
1212 F$ = "######.######'######.######"
1220 FOR I=1 TO N
1270 PRINT T(I),Y(I,1),F(I,1),R(I,1)
1280 IF Z7=0 GO TO 1380
1290 IF I>1 GO TO 1310
1300 PRINT #2, F$
1310 IF Z8=2 GO TO 1350
1320 PRINT #2,USING F$,T(I),Y(I,1)       \ GOTO 1360
1340 IF I=N GO TO 1380
1350 PRINT #2,USING F$,T(I),R(I,1)
1360 IF I=N GO TO 1380
1370 V2=V2+(R(I+1,1)-R(I,1))^2
1380 V1=V1+R(I,1)^2
1390 NEXT I
1400 IF Z7=0 GO TO 1420
1410 PRINT #2,USING F$,999;',';999
1420 IF N3=0 GO TO 8000
1430 V1=V1/(N-M)
1440 REM REPLACES MAT V(M,M) = (V1) * A(M,M)
1441 FOR I=1 TO M      \FOR J = 1 TO M
1444 V(I,J)=V1*A(I,J)
1446 NEXT J       \NEXT I
1450 PRINT "VARIANCE-COVARIANCE MATRIX"
1460 REM REPLACES MAT PRINT V(M,M)
1462 FOR I=1 TO M      \FOR J = 1 TO M
1464 PRINT V(I,J)
1465 NEXT J       \PRINT      \NEXT I
1470 V2=V2/(N-1)        \E1 = V2/V1
1490 IF N<25 GO TO 1550
1500 E2=N-1     \ E3 = N-2      \ E4 = N+1
```

```
1530 T1=(1-(V2/(2*V1)))/[illegible]
1540 GO TO 1560
1550 T1 = 0
1560 PRINT "  VON NEUMANN RATIO          CALCULATED VARIANCE"
1570 PRINT "CALCULATED     ...ED=1          ABOUT REGRESSION"
1580 PRINT E1,T1,V1       \ V1 = 0       \ V2 = 0
1620 PRINT \PRINT "PARAMETERS, CONVERGENCE CRITERION" \PRINT
1630 REM REPLACES MAT PRINT H(1,M+1)
1640 ON M GO TO 1644,1644,1646,1648,1650
1644 PRINT H(1,1),H(1,2),H(1,3)          \GOTO 1655
1646 PRINT H(1,1),H(1,2),H(1,3),H(1,4)        \GOTO 1655
1648 PRINT H(1,1),H(1,2),H(1,3),H(1,4),H(1,5)       \ GOTO 1655
1650 PRINT H(1,1);H(1,2);H(1,3);H(1,4);H(1,5);H(1,6);H(1,7)
1655 PRINT "T-TESTS OF PARAMETERS"      \ FOR I = 1 TO M
1670 B5=H(1,I)/SQR(V(I,I))      \ PRINT B5       \ NEXT I
1700 REM TEST FOR HETEROSCEDASTICITY
1710 PRINT "TEST RESIDUALS"        \ INPUT B2
1730 IF B2=0 GO TO 1500
1740 FOR I=1 TO N       \ Y(I,1) = ABS(R(I,1))         \ NEXT I
1770 K=1 \ REM CALLS LINEAR MODEL
1780 M=2
1790 GO TO 500
1800 GO TO 6000
2450 REM  THIS IS A SUBROUTINE TO READ INPUT FROM FILES
2460 PRINT "OUTPUT FILE ALSO?"       \ INPUT B7
2480 IF B7=0 GO TO 2570
2490 PRINT "ENTER OUTPUT FILE NAME"      \ INPUT C$
2530 PRINT "ENTER PLOT TITLE"      \ LINPUT F$
2550 PRINT "LINE ARE (1=OBS Y; OR 2= RESIDS.)"      \ INPUT B8
2570 PRINT "ENTER FILE NAME"       \ INPUT B$
2590 IF B7=0 GO TO 2620
2600 OPEN B$ FOR INPUT AS FILE #1
2605 OPEN C$ FOR OUTPUT AS FILE #2    \ GOTO 2660
2620 OPEN B$ FOR INPUT AS FILE #1
2660 FOR I=1 TO N       \ IF END #1 GOTO 2700
2680 INPUT #1,T(I),Y(I,1)      \ NEXT I
2700 RETURN    \ GOTO [illegible]
3970 REM * * * * * * * * * * * * * * * * *
3975 REM          LINEAR MODEL
3985 C = 0       \ FOR I = 1 TO N
3995 F(I,1) = P(1)+P(2)*T(I)
4000 R(I,1) = Y(I,1)-F(I,1)
4005 X(1,I) = 1       \ X(2,I) = T(I)
4015 C = C+R(I,1)*(X(1,I)+X(2,I))
4020 NEXT I       \ RETURN      \ GOTO 6000
4030 REM * * * * * * * * * * * * * * * * *
4031 REM  LOGISTIC GROWTH CURVE
4040 REM Y = B1/(1+EXP(B2-B3T))
4045 REM B1 = ASYMPTOTE; AT T = 0; Y = B1/(1+EXPB2)
4050 C = 0   \FOR I = 1 TO N
4055 A1 = EXP(P(2)-P(3)*T(I))
4059 F(I,1) = P(1)/(1+A1)
4060 R(I,1) = Y(I,1)-F(I,1)
4065 X(1,I) = 1/(1+A1)
4070 X(2,I) = (-P(1)*A1)/(1+A1)^2
4075 X(3,I) = (P(1)*T(I)*A1)/(1+A1)^2
4080 C = C + R(I,1)*(X(1,I)+X(2,I)+X(3,I))
4085 NEXT I [illegible]     \GOTO 6000
5000 REM * * * * * * * * * * * * * * * * *
5010 REM LAIRD FORM OF GOMPERTZ
5015 REM WHERE B1 = EGG WEIGHT
5020 REM Y = B1EXP^B2/B3(1-EXP^B3T)
5040 C = 0         \     FOR I = 1 TO N
5045 A1 = P(2)/P(3)
```

```
5050 A2 = EXP(-P(3)*T(I))
5055 A3 = EXP(A1*(1.-A2))
5060 A4 = P(3)*T(I)*A2
5065 A5 = P(1)*P(2)/(P(3))^2
5070 F(I,1) = P(1) *A3
5075 X(1,I) = A3
5080 X(2,I) = ((P(1)/P(3))*A3)*(1-A2)
5085 X(3,I) = A5 *A3 *(A2+A4-1.)
5090 R(I,1) = Y(I,1)-F(I,1)
6000  C = C+R(I,1)*(X(1,I)+X(2,I)+X(3,I))
6010 NEXT I
6020 RETURN
6030 END
```

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