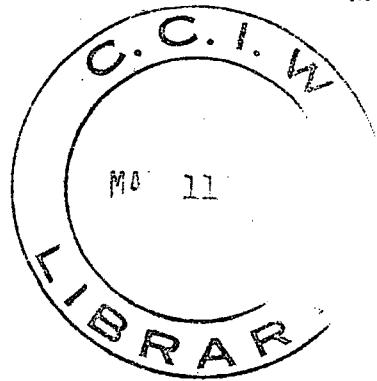


CANADA. Inland Waters Directorate.
Report Series
#11 Vol. 1



INLAND WATERS BRANCH

DEPARTMENT OF ENERGY, MINES AND RESOURCES



*Computer Programs in Use in the
Water Quality Division, Vol. 1.*

A. DEMAYO

REPORT SERIES NO.11

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Programs AD0001 to AD0004 do not give the correct results when X=0. There are two solutions to overcome this problem:

- (1) Instead of using X=0 use very small value.
For example, when the smallest, non zero X value is, say 1,
then X=1E-7 can be used instead of X=0.

OR:

- (2) Apply the following patch to the programs AD0001 to AD0004:

02.23 F J1=1,L1;D 16

16.10 I (X(J1))16.3,16.2,16.3
16.20 S SX(1)=1;S YX(1)=Y(J1)
16.30 R



REPORT SERIES NO.11

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A. DEMAYO

**INLAND WATERS BRANCH
DEPARTMENT OF ENERGY, MINES AND RESOURCES
OTTAWA, CANADA, 1971**

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Preface

This is the first in a series of reports presenting computer programs in use in Water Quality Division.

The present volume contains several "Least square fit" programs, and a program for finding the real or imaginary roots of a polynomial equation. These programs can be also used as subroutines in other programs.

All the programs presented in this report were written in FOCAL-69 and are used on a PDP-8/L - 8K computer.

Computer Programs in Use in the Water Quality Division, Vol. I.

A. DEMAYO

1. LEAST SQUARE FIT TO VARIOUS TYPES OF POLYNOMIAL EXPRESSIONS

1.1. Program AD0001

1.1.1. Abstract

Given L1 pairs of points X_j , Y_j , the adjustable coefficients B_i of:

$$Y_j(\text{obs}) = \sum_{i=1}^L B_i X_j^{i-1}(\text{obs}), \text{ where } j=1 \dots L1 \text{ and } L=NA \dots NB$$

are calculated. NA, NB, L1, X_j and Y_j are entered via Teletype ASR-33. (Keyboard or punched paper tape). After the coefficients B_i are obtained the program calculates $Y_j(\text{calc})$, compares it to $Y_j(\text{obs})$ and then calculates the mean square deviation from:

$$SD = \left[\frac{\sum_{j=1}^{L1} [Y_j(\text{obs}) - Y_j(\text{calc})]^2}{L1-L} \right]^{\frac{1}{2}}$$

1.1.2. Theory

Given L1 pairs of points $X_j(\text{obs})$, $Y_j(\text{obs})$ ($j=1 \dots L1$) this program calculates the coefficients B_i of expression:

$$Y_j(\text{calc}) = \sum_{i=1}^L B_i X_j^{i-1}(\text{obs}) \quad \begin{matrix} L = NA \dots NB \\ j = 1 \dots L1 \end{matrix} \quad \dots (1)$$

which minimizes the sum:

$$\sum_{j=1}^{L1} [Y(\text{obs}) - Y(\text{calc})]^2$$

The coefficients B_i are found by solving a linear system of L equations given in a general form by:

$$\sum_{j=1}^{L1} [Y_j(\text{obs}) * X_j^m(\text{obs})] = \sum_{i=1}^L \left[B_i * \sum_{j=1}^{L1} X_j^{i+m-1}(\text{obs}) \right] \quad \dots (2)$$

$m = 0, 1, \dots, L-1.$

In an expanded form, the equations are shown in (3).

$$\begin{aligned} \sum_{j=1}^{L1} Y_j(\text{obs}) * X_j^0(\text{obs}) &= B_1 * \sum_{j=1}^{L1} X_j^0(\text{obs}) + B_2 * \sum_{j=1}^{L1} X_j(\text{obs}) + \dots \\ &\quad + B_1 * \sum_{j=1}^{L1} X_j^{i-1}(\text{obs}) + \dots + B_L * \sum_{j=1}^{L1} X_j^{L-1}(\text{obs}) \\ \sum_{j=1}^{L1} Y_j(\text{obs}) * X_j(\text{obs}) &= B_1 * \sum_{j=1}^{L1} X_j(\text{obs}) + B_2 * \sum_{j=1}^{L1} X_j^2(\text{obs}) + \dots \\ &\quad + B_1 * \sum_{j=1}^{L1} X_j^i(\text{obs}) + \dots + B_L * \sum_{j=1}^{L1} X_j^L(\text{obs}) \\ &\dots \quad \dots (3) \\ \sum_{j=1}^{L1} Y_j(\text{obs}) * X_j^m(\text{obs}) &= B_1 * \sum_{j=1}^{L1} X_j^m(\text{obs}) + B_2 * \sum_{j=1}^{L1} X_j^{m+1}(\text{obs}) + \dots \\ &\quad + B_1 * \sum_{j=1}^{L1} X_j^{i+m-1}(\text{obs}) + \dots + B_L * \sum_{j=1}^{L1} X_j^{L+m-1}(\text{obs}) \\ &\dots \\ \sum_{j=1}^{L1} Y_j(\text{obs}) * X_j^{L-1}(\text{obs}) &= B_1 * \sum_{j=1}^{L1} X_j^{L-1}(\text{obs}) + B_2 * \sum_{j=1}^{L1} X_j^L(\text{obs}) + \dots \\ &\quad + B_1 * \sum_{j=1}^{L1} X_j^{i+L-2}(\text{obs}) + \dots + B_L * \sum_{j=1}^{L1} X_j^{2(L-1)}(\text{obs}) \end{aligned}$$

L , the number of adjustable coefficients B_i , can vary between two limits, NA and NB (NA can also equal NB) which are specified in the input of the program. Thus:

$$L = NA, NA+1, \dots, NB$$

NB and the corresponding maximum value for $L1$ are given in Table 1.

TABLE 1

NB Memory size:	Maximum value for L1	
	4K#	8K#
2	22	64
3	19	61
4	16	58
5	12	54
6	7	49
7	-	44
8	-	38
9	-	31
10	-	24
11	-	15

PDP-8/L computer, FOCAL-69 language, extended functions deleted.

The program contains a subroutine for the solution of a system of linear equations (Statements 14.05 to 15.30). The system is solved by Gauss-Jordan reduction method. The steps of this method which the program follows very closely are as follows. Given the systems of equations:

$$\begin{aligned}
 A_{11}X_1 + A_{12}X_2 + \dots + A_{1i}X_i + \dots + A_{1L}X_L &= C_1 \\
 A_{21}X_1 + A_{22}X_2 + \dots + A_{2i}X_i + \dots + A_{2L}X_L &= C_2 \\
 \dots & \\
 A_{n1}X_1 + A_{n2}X_2 + \dots + A_{ni}X_i + \dots + A_{nL}X_L &= C_n \\
 \dots & \\
 A_{L1}X_1 + A_{L2}X_2 + \dots + A_{Li}X_i + \dots + A_{LL}X_L &= C_L
 \end{aligned} \quad \dots \quad (4)$$

Consider the L by (L+1) matrix formed by the coefficients A and terms C:

$$\begin{array}{cccccc}
 A_{11} & A_{12} & \dots & A_{1i} & \dots & A_{1L} & C_1 \\
 A_{21} & A_{22} & \dots & A_{2i} & \dots & A_{2L} & C_2 \\
 \dots & & & & & & \\
 A_{n1} & A_{n2} & \dots & A_{ni} & \dots & A_{nL} & C_n \\
 \dots & & & & & & \\
 A_{L1} & A_{L2} & \dots & A_{Li} & \dots & A_{LL} & C_L
 \end{array} \quad \dots \quad (5)$$

- Divide the 1st row by A_{11} . This makes element $A_{11}=1$.
- Perform the subtraction: 2nd row - 1st row * A_{21} . This operation makes $A_{21}=0$.

* Denotes multiplication sign.

c. Perform the subtraction: n th row - 1st row * A_{n1} . This operation makes $A_{n1}=0$.

d. Repeat c until $n=L$.

Now the matrix 1.1.5 has the following aspect:

$$\begin{array}{cccccc} 1 & A_{12} & A_{13} & \dots & A_{1i} & \dots & A_{1L} & C_1 \\ 0 & A_{22} & A_{23} & \dots & A_{2i} & \dots & A_{2L} & C_2 \\ \dots & & & & & & & \dots(6) \\ 0 & A_{n2} & A_{n3} & \dots & A_{ni} & \dots & A_{nL} & C_n \\ \dots & & & & & & & \\ 0 & A_{L2} & A_{L3} & \dots & A_{Li} & \dots & A_{LL} & C_L \end{array}$$

It must be pointed out that, though the same notation has been used, the elements of matrix (6) have different values from those of matrix (5):

e. Operations a - d are repeated starting this time with element A_{22} and row 2 and leaving the 1st row alone. At the end of this series of calculations, matrix (6) has become:

$$\begin{array}{cccccc} 1 & A_{12} & A_{13} & \dots & A_{1i} & \dots & A_{1L} & C_1 \\ 0 & 1 & A_{23} & \dots & A_{2i} & \dots & A_{2L} & C_2 \\ 0 & 0 & A_{33} & \dots & A_{3i} & \dots & A_{3L} & C_3 \\ \dots & & & & & & & \dots(7) \\ 0 & 0 & A_{n3} & \dots & A_{ni} & \dots & A_{nL} & C_n \\ \dots & & & & & & & \\ 0 & 0 & A_{L3} & \dots & A_{Li} & \dots & A_{LL} & C_L \end{array}$$

The same operations are repeated for each diagonal element and for each row except the last row. At the end, the matrix of coefficients has become:

$$\begin{array}{cccccc} 1 & A_{12} & A_{13} & \dots & A_{1i} & \dots & A_{1L} & C_1 \\ 0 & 1 & A_{23} & \dots & A_{2i} & \dots & A_{2L} & C_2 \\ \dots & & & & & & & \dots(8) \\ 0 & 0 & 0 & \dots & 0 & \dots & 1 & A_{L-1,L} & C_{L-1} \\ 0 & 0 & 0 & \dots & 0 & \dots & 0 & A_{LL} & C_L \end{array}$$

* Denotes multiplication sign.

Thus, from the last row, X_L can be obtained immediately. This value is substituted in row L-1 and X_{L-1} obtained, and so on, until all the X's are obtained.

1.1.3. Input data

The input parameters are (in the order in which they must be entered): NA,NB,L1, and X-Y pairs. (Refer to the above write-up for the meaning of these symbols).

An example of a set of input data is shown in Figure 1.1.

1.1.4. Output data

The output consists, initially, of a table of X-Y values. Then, as they are calculated by the program, the adjustable coefficients, B_i , are typed out. Finally, a table of $Y_{(obs)}$, $Y_{(calc)}$, and the difference between $Y_{(obs)}$ and $Y_{(calc)}$ is typed out. The last line of the output contains the value of the mean square deviation calculated from expression:

$$SD = \sqrt{\frac{\sum_{j=1}^{L1} [Y_j(\text{obs}) - Y_j(\text{calc})]^2}{L1-L}} \quad \dots (9)$$

Note that this treatment assumes that the Y coordinates are subject to error while the X coordinates are free of error.

A typical output is shown in Figure 1.1. For this example seven X-Y points were calculated from the relation:

$$Y = 2 + 3X - 0.55X^2 + 0.043X^3$$

The calculated relation was (4 adjustable coefficients):

$$Y = 2.006 + 2.996X - 0.5494X^2 + 0.04297X^3$$

1.1.5. The computer program

The listing of the program is reproduced in Figure 1.2. The program is written in FOCAL 69 language (Digital Equipment Corporation, 1969), and can be run in its present form on any PDP-8 series computer.

The memory requirements are listed in Table 1 on page 2.

As far as the computer time is concerned, when the number of adjustable coefficients ≤ 6 , then the limiting factor is the speed of the ASR-33 Teletype. As a typical example, approximately four minutes on a PDP-8/L is required to fit ten points to polynomials with two to five adjustable coefficients.

1.1.6. References:

1. Deming, W.E. 1964. Statistical adjustment of data. Dover Publications Inc., New York, N.Y.
2. Digital Equipment Corporation. 1969. Advanced FOCAL. Publ. No. DEC-08-AJBB-DL.

Figure 1.1. Program AD0001 - input and output.

```

*G
2 5 7
1.50 5.41
3.00 7.21
4.50 8.28
6.00 9.49
7.50 11.70
9.00 15.80
10.50 22.64

DATA POINTS :
NO.          X           Y
= 1 = 0.150000E+01 = 0.541000E+01
= 2 = 0.300000E+01 = 0.721000E+01
= 3 = 0.450000E+01 = 0.828000E+01
= 4 = 0.600000E+01 = 0.949000E+01
= 5 = 0.750000E+01 = 0.117000E+02
= 6 = 0.900000E+01 = 0.158000E+02
= 7 = 0.105000E+02 = 0.226400E+02

NO. OF ADJUSTABLE COEFFICIENTS= 2
BC= 1) = 0.117714E+01
BC= 2) = 0.172119E+01

NO.          Y OBS.        Y CALC.        DIF
= 1 = 0.541000E+01 = 0.375893E+01 = 0.165107E+01
= 2 = 0.721000E+01 = 0.634071E+01 = 0.869289E+00
= 3 = 0.828000E+01 = 0.892250E+01 = -0.642496E+00
= 4 = 0.949000E+01 = 0.115043E+02 = -0.201428E+01
= 5 = 0.117000E+02 = 0.140861E+02 = -0.238607E+01
= 6 = 0.158000E+02 = 0.166679E+02 = -0.867849E+00
= 7 = 0.226400E+02 = 0.192496E+02 = 0.339036E+01

MEAN SQUARE DEVIATION= 0.227565E+01

NO. OF ADJUSTABLE COEFFICIENTS= 3
BC= 1) = 0.722713E+01
BC= 2) = -0.967694E+00
BC= 3) = 0.224074E+00

NO.          Y OBS.        Y CALC.        DIF
= 1 = 0.541000E+01 = 0.627975E+01 = -0.869752E+00
= 2 = 0.721000E+01 = 0.634071E+01 = 0.869293E+00
= 3 = 0.828000E+01 = 0.741000E+01 = 0.870005E+00
= 4 = 0.949000E+01 = 0.948762E+01 = 0.238419E-02
= 5 = 0.117000E+02 = 0.125736E+02 = -0.873568E+00
= 6 = 0.158000E+02 = 0.166679E+02 = -0.867846E+00
= 7 = 0.226400E+02 = 0.217705E+02 = 0.869534E+00

MEAN SQUARE DEVIATION= 0.106553E+01

NO. OF ADJUSTABLE COEFFICIENTS= 4
BC= 1) = 0.200623E+01
BC= 2) = 0.299632E+01
BC= 3) = -0.549392E+00
BC= 4) = 0.429703E-01

NO.          Y OBS.        Y CALC.        DIF
= 1 = 0.541000E+01 = 0.540960E+01 = 0.396729E-03
= 2 = 0.721000E+01 = 0.721086E+01 = -0.856400E-03
= 3 = 0.828000E+01 = 0.828015E+01 = -0.144959E-03
= 4 = 0.949000E+01 = 0.948762E+01 = 0.238419E-02
= 5 = 0.117000E+02 = 0.117034E+02 = -0.341797E-02
= 6 = 0.158000E+02 = 0.157977E+02 = 0.229454E-02
= 7 = 0.226400E+02 = 0.226406E+02 = -0.610352E-03

MEAN SQUARE DEVIATION= 0.282348E-02

NO. OF ADJUSTABLE COEFFICIENTS= 5
BC= 1) = 0.198266E+01
BC= 2) = 0.302125E+01
BC= 3) = -0.557395E+00
BC= 4) = 0.439578E-01
BC= 5) = -0.411387E-04

NO.          Y OBS.        Y CALC.        DIF
= 1 = 0.541000E+01 = 0.540853E+01 = 0.146771E-02
= 2 = 0.721000E+01 = 0.721336E+01 = -0.336075E-02
= 3 = 0.828000E+01 = 0.827979E+01 = 0.209808E-03
= 4 = 0.949000E+01 = 0.948547E+01 = 0.452805E-02
= 5 = 0.117000E+02 = 0.117031E+02 = -0.304985E-02
= 6 = 0.158000E+02 = 0.158002E+02 = -0.192642E-03
= 7 = 0.226400E+02 = 0.226396E+02 = 0.457764E-03

MEAN SQUARE DEVIATION= 0.466606E-02*

```

Figure 1.2. Program AD0001 - listing.

```

*C-8K FOCAL 01969
*
*01.06 E
*01.07 A NA,NB,L1
*01.09 F J1=1,L1;A X(J1),Y(J1)
*01.10 T !!!"DATA POINTS :",!,," NO.           X                   Y",!
*01.11 F J1=1,L1;T %2,J1,"   ",%,X(J1),"   ",Y(J1),!
*01.15 F L=NA,NB;D 2
*01.20 Q
*
*02.17 S N2=2*L-1
*02.20 F J1=1,N2;S SX(J1)=0
*02.22 F J1=1,L;S YX(J1)=0
*02.25 F J2=1,N2;F J1=1,L1;S SX(J2)=SX(J2)+X(J1)*(J2-1)
*02.27 F J2=1,L;F J1=1,L1;S YX(J2)=YX(J2)+Y(J1)*(X(J1)*(J2-1))
*02.28 T !!!"NO. OF ADJUSTABLE COEFFICIENTS",%2,L
*02.30 F J2=1,L;F J1=1,L;S A(J2+J1*L)=SX(J1+(J2-1))
*02.35 D 15.0
*02.78 F K=1,L; T !"B(",%2,K,")   ",%,B(K)
*02.80 F J1=1,L1;S YX(J1)=0
*02.82 S SD=0
*02.84 T !!!" NO.           Y OBS.           Y CALC.           DIF",!
*02.85 F J1=1,L1;S YX=B(1);D 8.0
*02.86 S SD=FSQT(SD/(L1-L))
*02.88 T !"MEAN SQUARE DEVIATION",SD;R
*
*08.10 F J2=2,L;S YX=YX+B(J2)*(X(J1)+(J2-1))
*08.15 S D=Y(J1)-YX;S SD=SD+D*D
*08.20 T %2,J1,"   ",%,Y(J1),"   ",YX,"   ",D,!;R
*
*14.05 S N=K+1; S DD=A(N+II*L)/A(II+II*L)
*14.10 F J=II,L; S A(N+J*L)=A(N+J*L)-A(II+J*L)*DD
*14.15 S YX(N)=YX(N)-YX(II)*DD; R
*
*15.05 S MM=L-1
*15.10 F II=1,MM; F K=II,MM; D 14.0
*15.15 S B(L)=YX(L)/A(L+L*L)
*15.20 F M=2,L;S N=L+1-M;S KK=N+1;S B(N)=YX(N)/A(N+N*L);D 15.25
*15.21 G 15.30
*15.25 F K=KK,L; S B(N)=B(N)-A(N+K*L)*B(K)/A(N+N*L)
*15.30 R
*

```

Program AD0001 can be slightly modified so that it can be used with polynomial expressions, which by substitution can be reduced to the form of expression (1):

$$Y = \sum_{i=1}^L B_i X^{i-1}$$

Programs AD0002, AD0003, and AD0004 are examples of such modifications.

1.2. Program AD0002

1.2.1. Theory

Given L_1 pairs of points $X_j(\text{obs})$, $Z_j(\text{obs})$, where $j = 1 \dots L_1$; this program calculates the coefficients B_i of expression:

$$Z_j(\text{calc}) = \left[\sum_{i=1}^L B_i X_j^{i-1} (\text{obs}) \right]^{-1} \quad \dots \dots (10)$$

where $L = NA \dots NB$

$$j = 1 \dots L_1$$

which minimize the expression:

$$\sum_{j=1}^{L_1} [Z_j(\text{obs}) - Z_j(\text{calc})]^2$$

By performing the substitution:

$$Y_j = 1/Z_j \quad \dots \dots (11)$$

the problem becomes identical to that of program AD0001.

1.2.2. Input and output parameters

The input and the output are identical to those of program AD0001. A typical example is shown in Figure 1.3. In this example, six X-Z points were calculated from:

$$Z = (1.1 - 0.65X + 0.1X^2 - 0.078X^3)^{-1}$$

Then the six points were fitted to an expression of the type (10) with L taking values of 2, 3, 4, and 5. For $L = 4$ the results were:

$$Z = (1.111 - 0.6740X + 0.1131X^2 - 0.0800X^3)^{-1}$$

1.2.3. The computer program

The listing of the program is reproduced in Figure 1.4.

The program is identical to that of Figure 1.2 except for minor modifications in the printout (Y substituted by Z), and of course, the substitution:

$$Y = 1/Z$$

in the statement 01.09.

Figure 1.3. Program AD0002 - input and output.

*G
 2 5 6
 0.700 1.499
 1.420 6.439
 2.140 -1.674
 2.860 -0.566
 3.580 -0.284
 4.300 -0.165

DATA POINTS :

NO.	X	Z
= 1	= 0.700000E+00	= 0.149900E+01
= 2	= 0.142000E+01	= 0.643900E+01
= 3	= 0.214000E+01	=-0.167400E+01
= 4	= 0.286000E+01	=-0.566000E+00
= 5	= 0.358000E+01	=-0.284000E+00
= 6	= 0.430000E+01	=-0.165000E+00

NO. OF ADJUSTABLE COEFFICIENTS= 2

B(= 1) = 0.269343E+01
 B(= 2) =-0.181894E+01

NO.	Z OBS.	Z CALC.	DIF
= 1	= 0.149900E+01	= 0.704139E+00	= 0.794862E+00
= 2	= 0.643900E+01	= 0.904651E+01	=-0.260751E+01
= 3	=-0.167400E+01	=-0.533962E+00	=-0.840039E+00
= 4	=-0.566000E+00	=-0.398608E+00	=-0.167392E+00
= 5	=-0.284000E+00	=-0.261892E+00	=-0.221081E-01
= 6	=-0.165000E+00	=-0.195008E+00	= 0.300077E-01

MEAN SQUARE DEVIATION= 0.142881E+01

NO. OF ADJUSTABLE COEFFICIENTS= 3

B(= 1) = 0.384862E+00
 B(= 2) = 0.617298E+00
 B(= 3) =-0.487248E+00

NO.	Z OBS.	Z CALC.	DIF
= 1	= 0.149900E+01	= 0.172945E+01	=-0.230450E+00
= 2	= 0.643900E+01	= 0.358503E+01	= 0.285398E+01
= 3	=-0.167400E+01	=-0.190287E+01	= 0.228871E+00
= 4	=-0.566000E+00	=-0.544912E+00	=-0.210883E-01
= 5	=-0.284000E+00	=-0.273975E+00	=-0.100257E-01
= 6	=-0.165000E+00	=-0.167505E+00	= 0.250501E-02

MEAN SQUARE DEVIATION= 0.165843E+01

NO. OF ADJUSTABLE COEFFICIENTS= 4

B(= 1) = 0.111171E+01
 B(= 2) =-0.674031E+00
 B(= 3) = 0.113103E+00
 B(= 4) =-0.800462E-01

NO.	Z OBS.	Z CALC.	DIF
= 1	= 0.149900E+01	= 0.149734E+01	= 0.166607E-02
= 2	= 0.643900E+01	= 0.651672E+01	=-0.777178E-01
= 3	=-0.167400E+01	=-0.167439E+01	= 0.390053E-03
= 4	=-0.566000E+00	=-0.567067E+00	= 0.106704E-02
= 5	=-0.284000E+00	=-0.283729E+00	=-0.271440E-03
= 6	=-0.165000E+00	=-0.165028E+00	= 0.274778E-04

MEAN SQUARE DEVIATION= 0.549736E-01

NO. OF ADJUSTABLE COEFFICIENTS= 5

B(= 1) = 0.107701E+01
 B(= 2) =-0.589551E+00
 B(= 3) = 0.492221E-01
 B(= 4) =-0.612582E-01
 B(= 5) =-0.187801E-02

NO.	Z OBS.	Z CALC.	DIF
= 1	= 0.149900E+01	= 0.149930E+01	=-0.302315E-03
= 2	= 0.643900E+01	= 0.640780E+01	= 0.312052E-01
= 3	=-0.167400E+01	=-0.166958E+01	=-0.442267E-02
= 4	=-0.566000E+00	=-0.566510E+00	= 0.509620E-03
= 5	=-0.284000E+00	=-0.283937E+00	=-0.633001E-04
= 6	=-0.165000E+00	=-0.165004E+00	= 0.405312E-05

MEAN SQUARE DEVIATION= 0.315227E-01*

*

Figure 1.4. Program AD0002 - listing.

```

*W
C-8K FOCAL @1969

01.06 E
01.07 A NA,NB,L1
01.09 F J1=1,L1;A X(J1),Z(J1);S Y(J1)=1/Z(J1)
01.10 T !!!"DATA POINTS :",!,," NO.           X           Z",!
01.11 F J1=1,L1;T %2,J1,"   ",%,X(J1),"   ",Z(J1),!
01.15 F L=NA,NB;D 2
01.20 Q

02.17 S N2=2*L-1
02.20 F J1=1,N2;S SX(J1)=0
02.22 F J1=1,L;S YX(J1)=0
02.25 F J2=1,N2;F J1=1,L1;S SX(J2)=SX(J2)+X(J1)*(J2-1)
02.27 F J2=1,L;F J1=1,L1;S YX(J2)=YX(J2)+Y(J1)*(X(J1)*(J2-1))
02.28 T !!!"NO. OF ADJUSTABLE COEFFICIENTS",%2,L
02.30 F J2=1,L;F J1=1,L;S A(J2+J1*L)=SX(J1+(J2-1))
02.35 D 15.0
02.78 F K=1,L; T !!!"B()",%2,K,"    ",%,B(K)
02.80 F J1=1,L1;S YX(J1)=0
02.82 S SD=0
02.84 T !!!" NO.           Z OBS.           Z CALC.           DIF",!
02.85 F J1=1,L1;S YX=B(1);D 8.0
02.86 S SD=FSQT(SD/(L1-L))
02.88 T !!!"MEAN SQUARE DEVIATION",SD;R

08.10 F J2=2,L;S YX=YX+B(J2)*(X(J1)*(J2-1))
08.12 S YX=1/YX
08.15 S D=Z(J1)-YX;S SD=SD+D*D
08.20 T %2,J1,"   ",%,Z(J1),"   ",YX,"   ",D,!;R

14.05 S N=K+1; S DD=A(N+II*L)/A(II+II*L)
14.10 F J=II,L; S A(N+J*L)=A(N+J*L)-A(II+J*L)*DD
14.15 S YX(N)=YX(N)-YX(II)*DD; R

15.05 S MM=L-1
15.10 F II=1,MM; F K=II,MM; D 14.0
15.15 S B(L)=YX(L)/A(L+L*L)
15.20 F M=2,L;S N=L+1-M;S KK=N+1;S B(N)=YX(N)/A(N+N*L);D 15.25
15.21 G 15.30
15.25 F K=KK,L; S B(N)=B(N)-A(N+K*L)*B(K)/A(N+N*L)
15.30 R
*

```

1.3. Program AD0003

1.3.1. Theory

Given L_1 pairs of points $Y_j(\text{obs})$, $Z_j(\text{obs})$, where $j = 1 \dots L_1$, this program calculates the coefficients B_i of expression:

$$Y_j(\text{calc}) = B_0 + \sum_{i=1}^L B_i Z_j^{1-i}(\text{obs}) \quad \dots (12)$$

where $L = NA \dots NB$

$$j = 1 \dots L_1$$

which minimize the sum:

$$\sum_{j=1}^{L_1} [Y_j(\text{calc}) - Y_j(\text{obs})]^2$$

By substituting:

$$Z_j = 1/X_j \quad \dots (13)$$

the problem becomes identical to that of program AD0001.

1.3.2. Input and output parameters

The input and the output are identical to those of program AD0001. A typical example is shown in Figure 1.5. In this example, seven Y-Z points which were calculated from:

$$Y = 8.7 - 5.2/Z + 1/Z^2$$

were fitted to an expression of the form (12).

The results for $L = 3$ were:

$$Y = 8.700 - 5.197/Z + 0.9973/Z^2$$

1.3.3. The computer program

The listing of the program is reproduced in Figure 1.6. The program is almost identical to program AD0001. The differences consist of a minor modification in the printout (statement 01.10) and the substitution:

$$X = 1/Z$$

in the statement 01.09.

*G Figure 1.5. Program AD0003 - input and output.

2 5 7
 1.30 5.292
 2.55 6.815
 3.80 7.401
 5.05 7.710
 6.30 7.900
 7.55 8.029
 8.800 8.122

DATA POINTS :

NO.	Z	Y
= 1	= 0.130000E+01	= 0.529200E+01
= 2	= 0.255000E+01	= 0.681500E+01
= 3	= 0.380000E+01	= 0.740100E+01
= 4	= 0.505000E+01	= 0.771000E+01
= 5	= 0.630000E+01	= 0.790000E+01
= 6	= 0.755000E+01	= 0.802900E+01
= 7	= 0.880000E+01	= 0.812200E+01

NO. OF ADJUSTABLE COEFFICIENTS= 2

B(= 1) = 0.857340E+01
 B(= 2) = -0.431335E+01

NO.	Y OBS.	Y CALC.	DIF
= 1	= 0.529200E+01	= 0.525544E+01	= 0.365658E-01
= 2	= 0.681500E+01	= 0.688189E+01	= -0.668869E-01
= 3	= 0.740100E+01	= 0.743830E+01	= -0.373039E-01
= 4	= 0.771000E+01	= 0.771927E+01	= -0.926685E-02
= 5	= 0.790000E+01	= 0.788874E+01	= 0.112629E-01
= 6	= 0.802900E+01	= 0.800209E+01	= 0.269108E-01
= 7	= 0.812200E+01	= 0.808324E+01	= 0.387573E-01

MEAN SQUARE DEVIATION= 0.439125E-01

NO. OF ADJUSTABLE COEFFICIENTS= 3

B(= 1) = 0.869983E+01
 B(= 2) = -0.519735E+01
 B(= 3) = 0.997298E+00

NO.	Y OBS.	Y CALC.	DIF
= 1	= 0.529200E+01	= 0.529199E+01	= 0.143051E-04
= 2	= 0.681500E+01	= 0.681503E+01	= -0.247955E-04
= 3	= 0.740100E+01	= 0.740117E+01	= -0.169754E-03
= 4	= 0.771000E+01	= 0.770976E+01	= 0.244141E-03
= 5	= 0.790000E+01	= 0.789998E+01	= 0.209808E-04
= 6	= 0.802900E+01	= 0.802893E+01	= 0.686646E-04
= 7	= 0.812200E+01	= 0.812210E+01	= -0.972748E-04

MEAN SQUARE DEVIATION= 0.161135E-03

NO. OF ADJUSTABLE COEFFICIENTS= 4

B(= 1) = 0.869882E+01
 B(= 2) = -0.518591E+01
 B(= 3) = 0.962922E+00
 B(= 4) = 0.276245E-01

NO.	Y OBS.	Y CALC.	DIF
= 1	= 0.529200E+01	= 0.529200E+01	= -0.286102E-05
= 2	= 0.681500E+01	= 0.681488E+01	= 0.123978E-03
= 3	= 0.740100E+01	= 0.740129E+01	= -0.288963E-03
= 4	= 0.771000E+01	= 0.770988E+01	= 0.126839E-03
= 5	= 0.790000E+01	= 0.790003E+01	= -0.247955E-04
= 6	= 0.802900E+01	= 0.802890E+01	= 0.106812E-03
= 7	= 0.812200E+01	= 0.812198E+01	= 0.190735E-04

MEAN SQUARE DEVIATION= 0.206037E-03

NO. OF ADJUSTABLE COEFFICIENTS= 5

B(= 1) = 0.868578E+01
 B(= 2) = -0.497176E+01
 B(= 3) = -0.193418E+00
 B(= 4) = 0.243348E+01
 B(= 5) = -0.160668E+01

NO.	Y OBS.	Y CALC.	DIF
= 1	= 0.529200E+01	= 0.529199E+01	= 0.858307E-05
= 2	= 0.681500E+01	= 0.681508E+01	= -0.820160E-04
= 3	= 0.740100E+01	= 0.740067E+01	= 0.333786E-03
= 4	= 0.771000E+01	= 0.771011E+01	= -0.109673E-03
= 5	= 0.790000E+01	= 0.790045E+01	= -0.446320E-03
= 6	= 0.802900E+01	= 0.802903E+01	= -0.286102E-04
= 7	= 0.812200E+01	= 0.812161E+01	= 0.392914E-03

MEAN SQUARE DEVIATION= 0.492261E-03*

Figure 1.6. Program AD0003 - listing.

```

*W
C-8K FOCAL 01969

01.06 E
01.07 A NA,NB,L1
01.09 F J1=1,L1;A Z(J1),Y(J1);S X(J1)=1/Z(J1)
01.10 T !!!"DATA POINTS :",!,," NO.           Z           Y",!
01.11 F J1=1,L1;T %2,J1,"   ",%,Z(J1),"   ",Y(J1),!
01.15 F L=NA,NB;D 2
01.20 Q

02.17 S N2=2*L-1
02.20 F J1=1,N2;S SX(J1)=0
02.22 F J1=1,L;S YX(J1)=0
02.25 F J2=1,N2;F J1=1,L1;S SX(J2)=SX(J2)+X(J1)*(J2-1)
02.27 F J2=1,L;F J1=1,L1;S YX(J2)=YX(J2)+Y(J1)*(X(J1)*(J2-1))
02.28 T !!!"NO. OF ADJUSTABLE COEFFICIENTS",%2,L
02.30 F J2=1,L;F J1=1,L;S A(J2+J1*L)=SX(J1+(J2-1))
02.35 D 15.0
02.78 F K=1,L; T !!!"B(",%2,K,")   ",%,B(K)
02.80 F J1=1,L1;S YX(J1)=0
02.82 S SD=0
02.84 T !!!" NO.      Y OBS.          Y CALC.          DIF",!
02.85 F J1=1,L1;S YX=B(1);D 8.0
02.86 S SD=FSQT(SD/(L1-L))
02.88 T !!!"MEAN SQUARE DEVIATION",SD;R

08.10 F J2=2,L;S YX=YX+B(J2)*(X(J1)*(J2-1))
08.15 S D=Y(J1)-YX;S SD=SD+D*D
08.20 T %2,J1,"   ",%,Y(J1),"   ",YX,"   ",D,!;R

14.05 S N=K+1; S DD=A(N+II*L)/A(II+II*L)
14.10 F J=II,L; S A(N+J*L)=A(N+J*L)-A(II+J*L)*DD
14.15 S YX(N)=YX(N)-YX(II)*DD; R

15.05 S MM=L-1
15.10 F II=1,MM; F K=II,MM; D 14.0
15.15 S B(L)=YX(L)/A(L+L*L)
15.20 F M=2,L;S N=L+1-M;S KK=N+1;S B(N)=YX(N)/A(N+N*L);D 15.25
15.21 G 15.30
15.25 F K=KK,L; S B(N)=B(N)-A(N+K*L)*B(K)/A(N+N*L)
15.30 R
*

```

1.4. Program AD0004

1.4.1. Theory

Given L_1 pairs of Z-X values ($j = 1 \dots L_1$) this program calculates the coefficients B_i of:

$$Z_j(\text{calc}) = \exp \left[\sum_{i=1}^L B_i X_j^{i-1}(\text{obs}) \right] \quad \dots (14)$$

where $L = NA \dots NB$

$j = 1 \dots L_1$

By making the substitution:

$$Y_j = \ln Z_j \quad \dots (15)$$

the problem becomes identical to that of program AD0001.

1.4.2. Input and output parameters

The input and the output are identical to those of program AD0001. An example is shown in Figure 1.7. In this example six Z-X points obtained from:

$$Z = \exp(1.2 - X + 1.2X^2 - 3X^3)$$

were fitted to an expression of the form (14).

The results obtained for $L = 4$ were:

$$Z = \exp(1.200 - 0.9981X + 1.198X^2 - 3.001X^3)$$

1.4.3. The computer program

The listing of program AD0004 is reproduced in Figure 1.8. This program is identical to program AD0001 except for minor modifications in the headings of the tables and for the substitution:

$$Y = \ln Z$$

in the statement 01.09.

*G Figure 1.7. Program AD0004 - input and output.

```
2 5 6
0.1 3.031
0.2 2.784
0.3 2.527
0.4 2.226
0.5 1.868
0.6 1.468
```

DATA POINTS :

NO.	X	Z
= 1	= 0.100000E+00	= 0.303100E+01
= 2	= 0.200000E+00	= 0.278400E+01
= 3	= 0.300000E+00	= 0.252700E+01
= 4	= 0.400000E+00	= 0.222600E+01
= 5	= 0.500000E+00	= 0.186800E+01
= 6	= 0.600000E+00	= 0.146800E+01

NO. OF ADJUSTABLE COEFFICIENTS= 2

```
B(= 1) = 0.130635E+01
B(= 2) = -0.141395E+01
```

NO.	Z OBS.	Z CALC.	DIF
= 1	= 0.303100E+01	= 0.320577E+01	= -0.174768E+00
= 2	= 0.278400E+01	= 0.278308E+01	= 0.925064E-03
= 3	= 0.252700E+01	= 0.241612E+01	= 0.110883E+00
= 4	= 0.222600E+01	= 0.209754E+01	= 0.128457E+00
= 5	= 0.186800E+01	= 0.182098E+01	= 0.470235E-01
= 6	= 0.146800E+01	= 0.158087E+01	= -0.112874E+00

MEAN SQUARE DEVIATION= 0.136283E+00

NO. OF ADJUSTABLE COEFFICIENTS= 3

```
B(= 1) = 0.112404E+01
B(= 2) = -0.466709E-01
B(= 3) = -0.195325E+01
```

NO.	Z OBS.	Z CALC.	DIF
= 1	= 0.303100E+01	= 0.300370E+01	= 0.273056E-01
= 2	= 0.278400E+01	= 0.281955E+01	= -0.355525E-01
= 3	= 0.252700E+01	= 0.254530E+01	= -0.182996E-01
= 4	= 0.222600E+01	= 0.220969E+01	= 0.163078E-01
= 5	= 0.186800E+01	= 0.184484E+01	= 0.231569E-01
= 6	= 0.146800E+01	= 0.148122E+01	= -0.132239E-01

MEAN SQUARE DEVIATION= 0.332742E-01

NO. OF ADJUSTABLE COEFFICIENTS= 4

```
B(= 1) = 0.119967E+01
B(= 2) = -0.998071E+00
B(= 3) = 0.119812E+01
B(= 4) = -0.300135E+01
```

NO.	Z OBS.	Z CALC.	DIF
= 1	= 0.303100E+01	= 0.303086E+01	= 0.142574E-03
= 2	= 0.278400E+01	= 0.278423E+01	= -0.233173E-03
= 3	= 0.252700E+01	= 0.252704E+01	= -0.343323E-04
= 4	= 0.222600E+01	= 0.222567E+01	= 0.330925E-03
= 5	= 0.186800E+01	= 0.186825E+01	= -0.247002E-03
= 6	= 0.146800E+01	= 0.146795E+01	= 0.545979E-04

MEAN SQUARE DEVIATION= 0.353113E-03

NO. OF ADJUSTABLE COEFFICIENTS= 5

```
B(= 1) = 0.120078E+01
B(= 2) = -0.101716E+01
B(= 3) = 0.130086E+01
B(= 4) = -0.321699E+01
B(= 5) = 0.154058E+00
```

NO.	Z OBS.	Z CALC.	DIF
= 1	= 0.303100E+01	= 0.303094E+01	= 0.643730E-04
= 2	= 0.278400E+01	= 0.278401E+01	= -0.119209E-04
= 3	= 0.252700E+01	= 0.252717E+01	= -0.166416E-03
= 4	= 0.222600E+01	= 0.222579E+01	= 0.213623E-03
= 5	= 0.186800E+01	= 0.186810E+01	= -0.972748E-04
= 6	= 0.146800E+01	= 0.146798E+01	= 0.164509E-04

MEAN SQUARE DEVIATION= 0.295547E-03*

*

Figure 1.8. Program AD0004 - listing

```

*W
C-8K FOCAL 81969

01.06 E
01.07 A NA,NB,L1
01.09 F J1=1,L1;S X(J1),Z(J1);S Y(J1)=FLOG(Z(J1))
01.10 T !!!"DATA POINTS :",!!," NO.           X          Z",!
01.11 F J1=1,L1;T Z2,J1,"  ",%X(J1),"  ",Z(J1),!
01.15 F L=NA,NB;D 2
01.20 Q

02.17 S N2=2*L-1
02.20 F J1=1,N2;S SX(J1)=0
02.22 F J1=1,L;S YX(J1)=0
02.25 F J2=1,N2;F J1=1,L1;S SX(J2)=SX(J2)+X(J1)*(J2-1)
02.27 F J2=1,L;F J1=1,L1;S YX(J2)=YX(J2)+Y(J1)*(X(J1)*(J2-1))
02.28 T !!!"NO. OF ADJUSTABLE COEFFICIENTS",%2,L
02.30 F J2=1,L;F J1=1,L;S A(J2+J1*L)=SX(J1+(J2-1))
02.35 D 15.0
02.78 F K=1,L; T !!"B()",%2,K,)  ",%,B(K)
02.80 F J1=1,L1;S YX(J1)=0
02.82 S SD=0
02.84 T !!" NO.           Z OBS.           Z CALC.          DIF",!
02.85 F J1=1,L1;S YX=B(1)*D 8.0
02.86 S SD=FSQT(SD/(L1-L))
02.88 T !!"MEAN SQUARE DEVIATION",SD;R

03.10 F J2=2,L;S YX=YX+B(J2)*(X(J1)+(J2-1))
03.12 S YX=FEXP(YX)
03.15 S D=Z(J1)-YX;S SD=SD+D*D
03.20 T %2,J1,"  ",%,Z(J1),"  ",YX,"  ",D,!;R

14.05 S N=K+1; S DD=A(N+II*L)/A(II+II*L)
14.10 F J=II,L; S A(N+J*L)=A(N+J*L)-A(II+J*L)*DD
14.15 S YX(N)=YX(N)-YX(II)*DD; R

15.05 S MM=L-1
15.10 F II=1,MM; F K=II,MM; D 14.0
15.15 S B(L)=YX(L)/A(L+L*L)
15.20 F M=2,L;S N=L+1-M;S KK=N+1;S B(N)=YX(N)/A(N+N*L);D 15.25
15.21 G 15.30
15.25 F K=KK,L; S B(N)=B(N)-A(N+K*L)*B(K)/A(N+N*L)
15.30 R
*

```

2. LEAST SQUARE FIT TO A LINEAR EXPRESSION WITH TWO OR THREE VARIABLES.

2.1. Programs AD0005

2.1.1. Abstract.

Given L1 pairs of X_j , Y_j values the constant coefficients A_i of expressions:

$$Y = A_0 + A_1 Z \quad \text{and} \quad \dots (16)$$

$$Y = A_0 + A_1 Z + A_2 V \quad \dots (17)$$

are calculated by the method of least squares.

The variables Z and V can be equal to X or be known functions of X . In this program $Z = \ln X$ and $V = X$; therefore expressions (16) and (17) take the form of:

$$Y = A_0 + A_1 \ln(X) \quad \text{and} \quad \dots (18)$$

$$Y = A_0 + A_1 \ln(X) + A_2 X \quad \dots (19)$$

2.1.2. Theory

The coefficients A_i of expression (17) are obtained from the following system of linear equations.

$$\begin{aligned} \sum_{j=1}^{L1} Y_j &= A_0 L1 + A_1 \sum_{j=1}^{L1} Z_j + A_2 \sum_{j=1}^{L1} V_j \\ \sum Y_j Z_j &= A_0 \sum Z_j + A_1 \sum Z_j^2 + A_2 \sum V_j Z_j \\ \sum Y_j V_j &= A_0 \sum V_j + A_1 \sum V_j Z_j + A_2 \sum V_j^2 \end{aligned} \quad \dots (20)$$

For expression (16), all the sums containing V_j become zero resulting in a system with two equations and two unknowns.

The program contains a subroutine (statements 12.10 to 15.20) which solves a linear system of equations. In a matrix form the system of equations (20) can be written as:

$$ZA = Y$$

where matrix Z is:

$$\begin{array}{lll} Z_{11} & Z_{12} & Z_{13} \\ Z_{21} & Z_{22} & Z_{23} \\ Z_{31} & Z_{32} & Z_{33} \end{array} \quad \begin{array}{lll} L1 & \sum Z_j & \sum V_j \\ \sum Z_j & \sum Z_j^2 & \sum V_j Z_j \\ \sum V_j & \sum V_j Z_j & \sum V_j^2 \end{array}$$

Matrix A is:

$$A_{11} \quad A_0$$

$$A_{21} \equiv A_1$$

$$A_{22} \quad A_2$$

and, finally, matrix Y is:

$$Y_{11} \quad \sum Y_j$$

$$Y_{21} \equiv \sum Y_j Z_j$$

$$Y_{31} \quad \sum Y_j V_j$$

The problem is to find matrix A when matrices Z and Y are known. The elements of the two known matrices are entered in the following order:

$Z_{11}, Z_{12}, Z_{13}, Y_{11}, Z_{21}, \dots Y_{21}, Z_{31}, \dots Y_{31}$

2.1.3. Input data

The input data consist of L_1 , the number of pairs of X-Y points, and the actual X-Y values. A set of input data is shown at the top of Figure 2.1. It consists of seven points calculated from the relation:

$$Y = 1.23 - 0.9 \ln X + 2.34 X \quad \dots (21)$$

2.1.4. Output data

The typical output is shown in Figure 2.1. It consists of a table of initial values, and a table of observed and calculated values, and the difference between them for each of relations (16) and (17). The mean square deviation corresponding to each relation is also calculated.

The calculated relation corresponding to (21) was:

$$Y = 1.228 - 0.902 \ln X + 2.342 X \quad \dots (22)$$

2.1.5. The computer program

A listing of the program is reproduced in Figure 2.2. The program is written in FOCAL-69 and it requires the extended functions (actually it requires only the logarithmic function).

Figure 2.1. Program AD0005 - input and output.

```

*G
7
0.60 3.0937
0.72 3.2105
0.84 3.3525
0.96 3.5131
1.08 3.6879
1.20 3.8739
1.32 4.0689

NO.= 1 X= 0.600000E+00 Y= 0.309370E+01 Z=-0.510825E+00
NO.= 2 X= 0.720000E+00 Y= 0.321050E+01 Z=-0.328504E+00
NO.= 3 X= 0.840000E+00 Y= 0.335250E+01 Z=-0.174353E+00
NO.= 4 X= 0.960000E+00 Y= 0.351310E+01 Z=-0.408218E-01
NO.= 5 X= 0.108000E+01 Y= 0.368790E+01 Z= 0.769610E-01
NO.= 6 X= 0.120000E+01 Y= 0.387390E+01 Z= 0.182322E+00
NO.= 7 X= 0.132000E+01 Y= 0.406890E+01 Z= 0.277632E+00

EQUATION : Y = A+B*LN(X) OR Y = A+B*Z
A(= 0) = 0.363412E+01
A(= 1) = 0.123331E+01
Y OBS.= 0.309370E+01 Y CALC.= 0.300411E+01 DIF.= 0.895882E-01
Y OBS.= 0.321050E+01 Y CALC.= 0.322897E+01 DIF.= -0.184717E-01
Y OBS.= 0.335250E+01 Y CALC.= 0.341909E+01 DIF.= -0.665870E-01
Y OBS.= 0.351310E+01 Y CALC.= 0.358377E+01 DIF.= -0.706735E-01
Y OBS.= 0.368790E+01 Y CALC.= 0.372904E+01 DIF.= -0.411363E-01
Y OBS.= 0.387390E+01 Y CALC.= 0.385898E+01 DIF.= 0.149212E-01
Y OBS.= 0.406890E+01 Y CALC.= 0.397653E+01 DIF.= 0.923739E-01
MEAN SQUARE DEVIATION= 0.751579E-01

EQUATION : Y = A+B*LN(X)+C*X OR Y = A+B*Z+C*X
A(= 0) = 0.122791E+01
A(= 1) = -0.901866E+00
A(= 2) = 0.234202E+01
Y OBS.= 0.309370E+01 Y CALC.= 0.309381E+01 DIF.= -0.112057E-03
Y OBS.= 0.321050E+01 Y CALC.= 0.321042E+01 DIF.= 0.758171E-04
Y OBS.= 0.335250E+01 Y CALC.= 0.335244E+01 DIF.= 0.572205E-04
Y OBS.= 0.351310E+01 Y CALC.= 0.351306E+01 DIF.= 0.419617E-04
Y OBS.= 0.368790E+01 Y CALC.= 0.368788E+01 DIF.= 0.252724E-04
Y OBS.= 0.387390E+01 Y CALC.= 0.387390E+01 DIF.= 0.333786E-05
Y OBS.= 0.406890E+01 Y CALC.= 0.406898E+01 DIF.= -0.810623E-04
MEAN SQUARE DEVIATION= 0.874083E-04*

```

Figure 2.2. Program AD0005 - listing.

```

*W
C-8K FOCAL @1969

01.05 E
01.09 A L13F J1=1,L13A X(J1),Y(J1);S Z(J1)=FLLOG(X(J1))
01.12 F J1=1,L13T !"NO.",%Z,J1," X",%X(J1)," Y",Y(J1)," Z",Z(J1)
01.15 S SX=0;S SY=0;S SZ=0;S XX=0;S XY=0;S XZ=0;S YZ=0;S ZZ=0
01.20 F J1=1,L13D0 2
01.21 S L=2;T !!!"EQUATION : Y = A+B*LN(X) OR Y = A+B*Z"
01.22 S A(0)=L13S A(1)=SZ;S A(2)=SZ;S A(3)=ZZ;S A(4)=SY;S A(5)=YZ
01.26 D 12;I (L-3)1.28,1.30,1.28
01.28 S B(2)=0
01.30 S SD=0;F J1=1,L13D 3
01.35 S SD=FSQRT(SD/(L1-L));T !!!"MEAN SQUARE DEVIATION",%,SD
01.38 I (2-L)1.50;
01.40 S L=3;T !!!"EQUATION : Y = A+B*LN(X)+C*X OR Y = A+B*Z+C*X"
01.42 S A(0)=L13S A(1)=SZ;S A(2)=SX;S A(3)=SZ;S A(4)=ZZ;S A(5)=XZ
01.44 S A(6)=SX;S A(7)=XZ;S A(8)=XX;S A(9)=SY;S A(10)=YZ;S A(11)=XY
01.48 G 1.26
01.50 Q

02.10 S SX=SX+X(J1);S SY=SY+Y(J1);S SZ=SZ+Z(J1)
02.12 S XX=XX+X(J1)*X(J1);S XY=XY+X(J1)*Y(J1)
02.15 S XZ=XZ+X(J1)*Z(J1);S YZ=YZ+Y(J1)*Z(J1);S ZZ=ZZ+Z(J1)*Z(J1)

03.10 S YC=B(0)+B(1)*Z(J1)+B(2)*X(J1)
03.20 S DI=Y(J1)-YC;S SD=SD+DI*DI
03.30 T !!!"Y OBS.",%,Y(J1)," Y CALC.",%,YC," DIF.",%,DI

12.10 S N=L-1;S I=-1;F K=0,N;S R(K)=K+1
12.14 S M=1E-6;F J=0,N;F K=0,N;D 13
12.18 S R(P)=0;F K=0,L;S A(P+L*K)=A(P+L*K)/M
12.20 F J=0,N;D 14
12.23 S I=I+1;I (I-N)12.14,12.26,12.14
12.26 F J=0,N;F K=0,N;D 15
12.28 F K=0,N;T !!!"A(",%1,K,") ",%,B(K)

13.05 I (R(J))0,13.3,13.1
13.10 I (FABS(A(J+L*K))-FABS(M))13.3;S M=A(J+L*K);S P=J;S Q=K
13.30 R

14.10 I (J-P)14.2,14.4,14.2
14.20 S D=A(J+L*Q)
14.30 F K=0,L;S A(J+L*K)=A(J+L*K)-A(P+L*K)*D
14.40 R

15.10 I (1E-6-FABS(A(J+L*K)))15.20;R
15.20 S B(K)=A(J+L*L)
*
```

2.2. Program AD0006 and AD0007

By setting $Z = \ln(1/X)$ and $V = 1/X$ the following two expressions are obtained:

$$Y = A_0 + A_1 \ln(1/X) \quad \dots (23)$$

$$Y = A_0 + A_1 \ln(1/X) + A_2/X \quad \dots (24)$$

The program AD0006 calculates the coefficients A_0 , A_1 and A_2 when a series of X, Y values are given.

The input and the output of the program are shown in Figure 2.3. The input consists of six X, Y values calculated from:

$$Y = 3.45 + 6.54 \ln(1/X)$$

The calculated expressions were:

$$Y = 3.450 + 6.540 \ln(1/X) \quad \text{and}$$

$$Y = 3.451 + 6.540 \ln(1/X) - 4.865 \times 10^{-4}/X$$

The program itself is reproduced in Figure 2.4.

In program AD0007, $Z = \ln X$ and $V = 1/X$. The corresponding relations are:

$$Y = A_0 + A_1 \ln X \quad \dots (25)$$

$$Y = A_0 + A_1 \ln X + A_2/X \quad \dots (26)$$

The input - output and the listing of this program are reproduced in Figures 2.5 and 2.6 respectively.

The input consists of six points calculated from:

$$Y = 6.7 + 0.89 \ln X - 5.43/X$$

The calculated relation was:

$$Y = 6.698 + 0.8906 \ln X - 5.428/X$$

Figure 2.3. Program AD0006 - input and output.

```

*G
6
1 3.45
2 -1.083
3 -3.735
4 -5.616
5 -7.076
6 -8.268

NO.= 1 W= 0.100000E+01 Y= 0.345000E+01 Z= 0.000000E+00
NO.= 2 W= 0.200000E+01 Y=-0.108300E+01 Z=-0.693147E+00
NO.= 3 W= 0.300000E+01 Y=-0.373500E+01 Z=-0.109861E+01
NO.= 4 W= 0.400000E+01 Y=-0.561600E+01 Z=-0.138630E+01
NO.= 5 W= 0.500000E+01 Y=-0.707601E+01 Z=-0.160944E+01
NO.= 6 W= 0.600000E+01 Y=-0.826801E+01 Z=-0.179176E+01

EQUATION : Y = A+B*LN(1/W) OR Y = A+B*Z
A(= 0) = 0.345007E+01
A(= 1) = 0.654002E+01
Y OBS.= 0.345000E+01 Y CALC.= 0.345007E+01 DIF.= -0.672340E-04
Y OBS.= -0.108300E+01 Y CALC.= -0.108313E+01 DIF.= 0.128269E-03
Y OBS.= -0.373500E+01 Y CALC.= -0.373488E+01 DIF.= -0.125408E-03
Y OBS.= -0.561600E+01 Y CALC.= -0.561633E+01 DIF.= 0.322342E-03
Y OBS.= -0.707601E+01 Y CALC.= -0.707569E+01 DIF.= -0.316620E-03
Y OBS.= -0.826801E+01 Y CALC.= -0.826807E+01 DIF.= 0.667572E-04
MEAN SQUARE DEVIATION= 0.247644E-03

EQUATION : Y = A+B*LN(1/W)+C/W OR Y = A+B*Z+C/W
A(= 0) = 0.345051E+01
A(= 1) = 0.654024E+01
A(= 2) = -0.486511E-03
Y OBS.= 0.345000E+01 Y CALC.= 0.345002E+01 DIF.= -0.233650E-04
Y OBS.= -0.108300E+01 Y CALC.= -0.108308E+01 DIF.= 0.822544E-04
Y OBS.= -0.373500E+01 Y CALC.= -0.373484E+01 DIF.= -0.161648E-03
Y OBS.= -0.561600E+01 Y CALC.= -0.561631E+01 DIF.= 0.308991E-03
Y OBS.= -0.707601E+01 Y CALC.= -0.707570E+01 DIF.= -0.304222E-03
Y OBS.= -0.826801E+01 Y CALC.= -0.826811E+01 DIF.= 0.104904E-03
MEAN SQUARE DEVIATION= 0.278372E-03*

```

Figure 2.4. Program AD0006 - listing.

```

*W
C-8K FOCAL @1969

01.05 E
01.09 A L1;F J1=1,L1;A W(J1),Y(J1);S X(J1)=1/W(J1);S Z(J1)=FLOG(X(J1))
01.12 F J1=1,L1;T !"NO.",%2,J1," W",%,W(J1)," Y",Y(J1)," Z",Z(J1)
01.15 S SX=0;S SY=0;S SZ=0;S XX=0;S XY=0;S XZ=0;S YZ=0;S ZZ=0
01.20 F J1=1,L1;DO 2
01.21 S L=2;T !!!"EQUATION : Y = A+B*LN(1/W) OR Y = A+B*Z"
01.22 S A(0)=L1;S A(1)=SZ;S A(2)=SZ;S A(3)=ZZ;S A(4)=SY;S A(5)=YZ
01.26 D 12;I (L-3)1.28,1.30,1.28
01.28 S B(2)=0
01.30 S SD=0;F J1=1,L1;D 3
01.35 S SD=FSQT(SD/(L1-L));T !!!"MEAN SQUARE DEVIATION",%,SD
01.38 I (2-L)1.50;
01.40 S L=3;T !!!"EQUATION : Y = A+B*LN(1/W)+C/W OR Y = A+B*Z+C/W"
01.42 S A(0)=L1;S A(1)=SZ;S A(2)=SX;S A(3)=SZ;S A(4)=ZZ;S A(5)=XZ
01.44 S A(6)=SX;S A(7)=XZ;S A(8)=XX;S A(9)=SY;S A(10)=YZ;S A(11)=XY
01.46
01.48 G 1.26
01.50 Q

02.10 S SX=SX+X(J1);S SY=SY+Y(J1);S SZ=SZ+Z(J1)
02.12 S XX=XX+X(J1)*X(J1);S XY=XY+X(J1)*Y(J1)
02.15 S XZ=XZ+X(J1)*Z(J1);S YZ=YZ+Y(J1)*Z(J1);S ZZ=ZZ+Z(J1)*Z(J1)

03.10 S YC=B(0)+B(1)*Z(J1)+B(2)*X(J1)
03.20 S DI=Y(J1)-YC;S SD=SD+DI*DI
03.30 T !!!"Y OBS.",%,Y(J1)," Y CALC.",%,YC," DIF.",%,DI

12.10 S N=L-1;S I=-1;F K=0,N;S R(K)=K+1
12.14 S M=1E-6;F J=0,N;F K=0,N;D 13
12.18 S R(P)=0;F K=0,L;S A(P+L*K)=A(P+L*K)/M
12.20 F J=0,N;D 14
12.23 S I=I+1;I (I-N)12.14,12.26,12.14
12.26 F J=0,N;F K=0,N;D 15
12.28 F K=0,N;T !!!"A(",%,1,K,") ",%,B(K)

13.05 I (R(J))0,13.3,13.1
13.10 I (FABS(A(J+L*K))-FABS(M))13.3;S M=A(J+L*K);S P=J;S Q=K
13.30 R

14.10 I (J-P)14.2,14.4,14.2
14.20 S D=A(J+L*Q)
14.30 F K=0,L;S A(J+L*K)=A(J+L*K)-A(P+L*K)*D
14.40 R

15.10 I (1E-6-FABS(A(J+L*K)))15.20;R
15.20 S B(K)=A(J+L*L)
*
```

Figure 2.5. Program AD0007 - input and output.

```

*G
6
1.35 2.945
1.70 3.978
2.05 4.690
2.40 5.217
3.10 5.955
3.80 6.459

NO.= 1 W= 0.135000E+01 Y= 0.294500E+01 Z= 0.300105E+00
NO.= 2 W= 0.170000E+01 Y= 0.397800E+01 Z= 0.530628E+00
NO.= 3 W= 0.205000E+01 Y= 0.469000E+01 Z= 0.717840E+00
NO.= 4 W= 0.240000E+01 Y= 0.521700E+01 Z= 0.875469E+00
NO.= 5 W= 0.310000E+01 Y= 0.595500E+01 Z= 0.113140E+01
NO.= 6 W= 0.380000E+01 Y= 0.645900E+01 Z= 0.133500E+01

EQUATION : Y = A+B*LN(W) OR Y = A+B*Z
A(= 0) = 0.213373E+01
A(= 1) = 0.336200E+01
Y OBS.= 0.294500E+01 Y CALC.= 0.314268E+01 DIF.= -0.197674E+00
Y OBS.= 0.397800E+01 Y CALC.= 0.391770E+01 DIF.= 0.603061E-01
Y OBS.= 0.469000E+01 Y CALC.= 0.454710E+01 DIF.= 0.142902E+00
Y OBS.= 0.521700E+01 Y CALC.= 0.507705E+01 DIF.= 0.139954E+00
Y OBS.= 0.595500E+01 Y CALC.= 0.593749E+01 DIF.= 0.175076E-01
Y OBS.= 0.645900E+01 Y CALC.= 0.662199E+01 DIF.= -0.162991E+00
MEAN SQUARE DEVIATION= 0.165524E+00

EQUATION : Y = A+B*LN(W)+C/W OR Y = A+B*Z+C/W
A(= 0) = 0.669849E+01
A(= 1) = 0.890639E+00
A(= 2) = -0.542800E+01
Y OBS.= 0.294500E+01 Y CALC.= 0.294503E+01 DIF.= -0.281334E-04
Y OBS.= 0.397800E+01 Y CALC.= 0.397814E+01 DIF.= -0.143051E-03
Y OBS.= 0.469000E+01 Y CALC.= 0.469002E+01 DIF.= -0.152588E-04
Y OBS.= 0.521700E+01 Y CALC.= 0.521655E+01 DIF.= 0.454903E-03
Y OBS.= 0.595500E+01 Y CALC.= 0.595519E+01 DIF.= -0.188828E-03
Y OBS.= 0.645900E+01 Y CALC.= 0.645907E+01 DIF.= -0.686646E-04
MEAN SQUARE DEVIATION= 0.299330E-03*

```

Figure 2.6. Program AD0007 - listing.

```

*W
C-8K FOCAL @1969

01.05 E
01.09 A L1;F J1=1,L1;A W(J1),Y(J1);S X(J1)=1/W(J1);S Z(J1)=FLOG(W(J1))
01.12 F J1=1,L1;T !"NO.",%2,J1," W",%,W(J1)," Y",Y(J1)," Z",Z(J1)
01.15 S SX=0;S SY=0;S SZ=0;S XX=0;S XY=0;S XZ=0;S YZ=0;S ZZ=0
01.20 F J1=1,L1;D0 2
01.21 S L=2;T !!!"EQUATION : Y = A+B*LN(W) OR Y = A+B*Z"
01.22 S A(0)=L1;S A(1)=SZ;S A(2)=SZ;S A(3)=ZZ;S A(4)=SY;S A(5)=YZ
01.26 D 12;I (L-3)1.28,1.30,1.28
01.28 S B(2)=0
01.30 S SD=0;F J1=1,L1;D 3
01.35 S SD=FSQT(SD/(L1-L));T !"MEAN SQUARE DEVIATION",%,SD
01.38 I (2-L)1.50;
01.40 S L=3;T !!!"EQUATION : Y = A+B*LN(W)+C/W OR Y = A+B*Z+C/W"
01.42 S A(0)=L1;S A(1)=SZ;S A(2)=SX;S A(3)=SZ;S A(4)=ZZ;S A(5)=XZ
01.44 S A(6)=SX;S A(7)=XZ;S A(8)=XX;S A(9)=SY;S A(10)=YZ;S A(11)=XY
01.46
01.48 G 1.26
01.50 Q

02.10 S SX=SX+X(J1);S SY=SY+Y(J1);S SZ=SZ+Z(J1)
02.12 S XX=XX+X(J1)*X(J1);S XY=XY+X(J1)*Y(J1)
02.15 S XZ=XZ+X(J1)*Z(J1);S YZ=YZ+Y(J1)*Z(J1);S ZZ=ZZ+Z(J1)*Z(J1)

03.10 S YC=B(0)+B(1)*Z(J1)+B(2)*X(J1)
03.20 S DI=Y(J1)-YC;S SD=SD+DI*DI
03.30 T !"Y OBS.",%,Y(J1)," Y CALC.",%,YC," DIF.",%,DI

12.10 S N=L-1;S I=-1;F K=0,N;S R(K)=K+1
12.14 S M=1E-6;F J=0,N;F K=0,N;D 13
12.18 S R(P)=0;F K=0,L;S A(P+L*K)=A(P+L*K)/M
12.20 F J=0,N;D 14
12.23 S I=I+1;I (I-N)12.14,12.26,12.14
12.26 F J=0,N;F K=0,N;D 15
12.28 F K=0,N;T !"A(",%,1,K,") ",%,B(K)

13.05 I (R(J))0,13.3,13.1
13.10 I (FABS(A(J+L*K))-FABS(M))13.3;S M=A(J+L*K);S P=J;S Q=K
13.30 R

14.10 I (J-P)14.2,14.4,14.2
14.20 S D=A(J+L*Q)
14.30 F K=0,L;S A(J+L*K)=A(J+L*K)-A(P+L*K)*D
14.40 R

15.10 I (1E-6-FABS(A(J+L*K)))15.20;R
15.20 S B(K)=A(J+L*L)
*
```

3. SOLUTIONS OF A POLYNOMIAL EQUATION

3.1. Program AD0008

3.1.1. Abstract

This program finds the real and imaginary roots of a polynomial of the form:

$$B_0 + B_1X + B_2X^2 + \dots + B_{L2}X^{L2} = 0 \quad \dots (27)$$

where L2 can take any integer value except zero. Also, B0 cannot be zero.

3.1.2. Method

Baristow's method for finding the roots of polynomial is used (R.W. Hamming, 1962).

3.1.3. Input data

The input values consist of:

Symbol	Meaning
L2	The degree of the polynomial
B(J2); J2 = 0 ... L2	The coefficients of the polynomial

A set of input values are shown at the top of Figure 3.1. They correspond to the following equation:

$$6 - 5X + 4X^2 - 3X^3 - 2X^5 + X^7 = 0 \quad \dots (28)$$

L2 can take any integer value except zero. All B values, zero or non-zero, must be entered. The only restriction is that the equation should not have any zero roots. Thus, all zero roots of a polynomial must be factored out before entering the program.

The coefficients B are not destroyed during the computation. Thus, if this program is used as a subroutine in another program, these coefficients can be used again for other calculations.

3.1.4. Output data

A typical output is shown in Figure 3.1. It consists of the real (symbol RR) and imaginary (symbol RI) parts of the L2 roots.

3.1.5. The computer program

A listing of the program is reproduced in Figure 3.2. The program is written in FOCAL-69. It does not use any of the extended functions.

The group of statements number 1 contains the input and output operations, only. When this program is used as a subroutine, this group is not absolutely necessary.

The solution of equation (28) including input and output operations took approximately 100 seconds on a PDP-8/L.

3.1.6. References

1. Hamming, R.W. 1962. Numerical methods for Scientists and Engineers, McGraw Hill, p. 356.

Figure 3.1. Program AD0008 - input and output.

*G

SOLUTION OF AN EQUATION OF THE FORM :
 $B(0)+B(1)*X+B(2)*(X**2)+B(3)*(X**3)+\dots+B(L2)*(X**L2)=0$

DEGREE OF EQUATION-L2 = 7

COEFFICIENTS IN ORDER OF INCREASING POWER OF X :
(NOTE: B(0) CANNOT BE ZERO)

B(0) = 6
B(1) = -5
B(2) = 4
B(3) = -3
B(4) = 0
B(5) = -2
B(6) = 0
B(7) = 1

THE ROOTS ARE :

NO.	REAL PART	IMAGINARY PART
1	0.304607E+00	0.991915E+00
2	0.304607E+00	-0.991915E+00
3	0.110802E+01	0.000000E+00
4	-0.196249E+01	0.000000E+00
5	-0.646315E+00	0.111745E+01
6	-0.646315E+00	-0.111745E+01
7	0.153789E+01	0.000000E+00*

Figure 3.2. Program AD0008 - Listing.

```

*W
C-8K FOCAL 01969

01.10 E
01.15 T !!!"SOLUTION OF AN EQUATION OF THE FORM :!"!
01.16 T "B(0)+B(1)*X+B(2)*(X**2)+B(3)*(X**3)+...+B(L2)*(X**L2)=0"!!
01.17 T "DEGREE OF EQUATION-L2 ="3A L2
01.20 T !!!"COEFFICIENTS IN ORDER OF INCREASING POWER OF X :!"!
01.21 T "(NOTE: B(0) CANNOT BE ZERO)"!
01.25 F J2=0,L2;T !"B(",%2,J2,")" ="3A B(J2)
01.30 D 11
01.40 T !!!"THE ROOTS ARE :"!" NO. REAL PART IMAGINARY PART"
01.45 F J2=1,L2;T !,%2,J2," ",%,RR(J2)," ",RI(J2)
01.50 Q

11.03 F J2=0,L2;S MT=L2-J2;S C(J2+1)=B(MT)
11.05 S I=1;S P=1/C(1)
11.07 F J2=1,L2;S C(J2)=P*C(J2+1)
11.09 S IS=0
11.11 S P=C(L2-1)+1E-6;S Q=C(L2);I (I-L2+1)11.16,11.54,11.13
11.13 S RR(I)=-Q;S RI(I)=0;G 11.78
11.16 S IC=1;S B1=C(L2-2);I (B1)11.19,11.90,11.19
11.19 S B1=1/B1;S P=P*B1;S Q=Q*B1
11.21 S B1=1;S B3=1;S B2=0;S B4=0
11.24 F J2=1,L2;D 12
11.26 S RI(L2-1)=RI(L2-1)-RR(L2-1);S B2=1;S B3=RI(L2-1)
11.28 S B4=RI(L2-2);I (I-L2+2)11.30,11.32,11.30
11.30 S B2=RI(L2-3)
11.32 S B1=B4*B4-B3*B2;S B1=1/B1;S B3=(RR(L2-1)*B3-RR(L2)*B4)*B1
11.35 S B2=(RR(L2-1)*B4-RR(L2)*B2)*B1
11.38 I (FABS(B2)/(FABS(P)+1)-5E-6)11.40,11.40,11.42
11.40 I (FABS(B3)/(FABS(Q)+1)-5E-6)11.84,11.84,11.42
11.42 S P=P+B2;S Q=Q-B3;S IC=IC+1;I (IC-100)11.21,11.21,11.44
11.44 I (IS)11.46,11.78,11.78
11.46 S IS=1;S J3=L2;S L2=L2+1;S C(L2)=0
11.48 S C(J3+1)=C(J3+1)+C(J3);S J3=J3-1
11.50 I (J3)11.52,11.52,11.48
11.52 S C(1)=C(1)+1;G 11.11
11.54 I (P)11.56,11.61,11.56
11.56 S B4=4*Q/(P*P);I (FABS(B4)-1E-6)11.59,11.59,11.61
11.59 S RR(I)=-P;S RR(I+1)=-Q/P;G 11.69
11.61 S RR(I)=-.5*P;S RR(I+1)=RR(I);S B1=P*P-4*Q
11.63 I (B1)11.65,11.69,11.67
11.65 S RI(I)=-.5*FSQT(-B1);S RI(I+1)=-RI(I);G 11.70
11.67 S B1=-.5*FSQT(B1);S RR(I)=RR(I)+B1;S RR(I+1)=RR(I+1)-B1
11.69 S RI(I)=0;S RI(I+1)=0
11.70 S I=I+2;I (I-L2)11.11,11.11,11.78
11.78 R
11.80 F J2=J3,L2;S RR(J2)=RR(J2+1);S RI(J2)=RI(J2+1)
11.82 G 11.78
11.84 F J2=1,L2;S C(J2)=RR(J2-2)
11.86 G 11.54
11.90 S P=Q;G 11.21

12.05 S RR(J2)=C(J2)-P*B1-Q*B2;I (J2-L2)12.10,12.90,12.90
12.10 S RI(J2)=RR(J2)-P*B3-Q*B4;S B2=B1;S B4=B3
12.15 S B1=RR(J2);S B3=RI(J2)
12.90 R
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