UNIVERSITY OF EDINBURGH
Edinburgh Regional Computing Centre

# User Note 11

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Title:

**CURVEFIT on EMAS-3**

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Software Support Category: See Note 15

## Synopsis

User Note 13 describes curve-fitting in general and refers to several other curve-fitting packages. This note describes CURVEFIT, a package on EMAS for automatic curve-fitting with special emphasis on splines.

## Keywords

CURVEFIT, Curveplot, Cuspline, exponential function, least squares approximation, polynomial, rational function, spline fit, spline interpolation

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## 1.0 CURVEFIT - A curve-fitting program for least squares approximation to data

### 1.1.0 Description

From discrete non-overlapping data points, this program computes the coefficients for three different choices of least squares approximation. The following choices have been built into the program:

1) polynomials of the form: $\sum_{i=0}^{n} a_i x^i$

2) rational functions of the form: $\dfrac{\sum_{i=0}^{n} a_i x^i}{\sum_{i=0}^{n} b_i x^i}$

3) sum of exponential functions: $\sum_{i=0}^{n} a_i e^{b_i x}$

   The constants a(I) and b(I) may be complex, in which case the terms will appear in pairs, the constants in the second member being conjugate to the constants in the first member. Such a pair of terms thus combine to give a real contribution. The data for this fit must be evenly spaced. Users requiring in general a non-complex fit to the exponential function should use an alternative package.

4) cubic splines: computation of a least squares approximation to an arbitrary set of data points by a cubic spline with knots prescribed by the user.

   Cubic spline interpolation can also be carried out.

   An extra facility, mainly for curve plotting purposes, for the determination of a cubic spline function which is either interpolative or a fit with a specified degree of smoothness is also provided. In this particular case the output includes the coefficients A(I), B(I), C(I) and D(I) of the spline function as described under 'Method' for routine CUSPLINE (see Appendix 1).

An option for automatic plotting of graphical output on the graph plotter forms an integral part of the program.

Graphical output on the plotter with more comprehensive facilities may be obtained by use of certain Control words within CURVEFIT which gives access to the EASYGRAPH package. (See Example 2 in Section 1.3.1)

### 1.2.0 Access

The program is accessed on EMAS-A via

*Command:* SEARCHDIR ERCLIB:GRAPHICS

whether the standard graph plotting or the EASYGRAPH option is used.

Before running the program streams 1 and 2 require definition for input and output respectively. This is achieved by typing

*Command:* DEFINE 1,*filename1*
*Command:* DEFINE 2,*filename2*

where *filename1* is the file containing the data and CURVEFIT instructions and *filename2* is the file which will contain the results.

If the option for graph plotter output but not for EASYGRAPH is to be invoked, the following file definition is also required:

*Command:* DEFINE 50,*filename3*

*filename3* is the name of a plotter file. We note here that graph plotter output files are IMP sequential files, and their structure is fixed 80-byte records i.e. card images. Once the program has run, the user must issue an EMAS command to direct the plotter file to a graph plotter viz.

*Command:* GPLIST *filename3*,.GP*xx* — where *xx* indicates the actual plotter (use Help Plottertypes or see ERCC User Note 17). For example .GP15 is the A3/A4 plotter in Room 3210, JCMB.

The program is run by issuing the command

*Command:* CURVEFIT

**Example**

| | |
|---|---|
| *Command:* SEARCHDIR ERCLIB:GRAPHICS | : to access curve-fitting program. This command need only be issued once. |
| *Command:* DEFINE 1,DATA | : to define input file containing program instructions and data. |
| *Command:* DEFINE 2,LPOUT | : to define output file or device. |
| *Command:* DEFINE 50,GRAFOUT | : to define plotter file if graph plotter output option used: not required if EASYGRAPH is invoked. |
| *Command:* CURVEFIT | : to run the curve-fitting program. |
| *Command:* GPLIST GRAFOUT,.GP*xx* | : if required, where *xx* specifies the plotter to be used. |
| *Command:* LIST LPOUT,.LP*nn* | : if required, where *nn* is a 2-digit number specifying line printer to be used. |

### 1.3.0 Input

The input file is read in free format, and uses the following 17 Control words to control the curve-fitting:

(a) GRAPH

(b) PLOT

(c) POLYNOMIAL

(d) EXPONENTIAL

(e) RATIONAL

(f) SPLINE FIT

(g) SPLINE INTERPOLATION

(h) CURVEPLOT

(i) SELECT

(j) DATA or UNSORTED DATA

(k) END

(l) REPEAT

(m) STOP

(n) EASYGRAPH

(p) EASYPLOT

(s) .END

(t) RAW

These must be edited into the file one to a line. If the user wishes he can build his own control phrases using one Control word per phrase. Each phrase must be typed on a new line.

The user can build up the input file by working through the following list.
The Control words and data must appear in the given order:

1. Control word GRAPH is mandatory if any graph plotting is required subsequently: the Control word GRAPH appears only once. Delivery information within quotes must be input next on a new line so that graph plotter output may be directed to the user by staff at Job Reception.

   Note that if the graph plotting option has *not* been selected then no delivery information should be supplied.

2. Control word POLYNOMIAL or EXPONENTIAL or RATIONAL or SPLINE FIT or SPLINE INTERPOLATION or CURVEPLOT which specifies the choice of approximation.

3. Single number which specifies the degree of the approximation in POLYNOMIAL or EXPONENTIAL cases.

   In RATIONAL case two numbers: the degree of the numerator followed by the degree of the denominator.

   In SPLINE FIT, SPLINE INTERPOLATION and CURVEPLOT cases a number for plotting purposes which indicates the number of sub-divisions between successive abscissae where the spline is additionally evaluated: for example if the number chosen is 5, then the spline is evaluated at 4 intermediate points between X(I), X(I+1), I = 1(1)M-1 where M is the number of data points.
   The choice of 5 is recommended.

   In SPLINE FIT case the number of knots followed by the position of the knots themselves.

   In SPLINE INTERPOLATION case no information is required.

   In CURVEPLOT case the smoothing factor. Note that a smoothing factor of zero is equivalent to spline interpolation.

4. Control word DATA or UNSORTED DATA

5. Next comes the input data, specified as X and Y coordinate pairs, one pair per line. If DATA is specified the values must appear in numerical order sorted by the x variate in the form

   x1 y1
   x2 y2
   etc.

   An important restriction in that the number of pairs (X,Y) must be less than 500. This limit has been found to be adequate in most cases, but if you need more please contact your Support Team.

   The curve-fitting routines all deal with SINGLE-VALUED functions. Multi-valued functions are not catered for - hence the user must only provide one y-value for each x-value.

   Note also that for exponential fit, data must be equally spaced.

6. Control word END to terminate the list of data points.

7. For approximations POLYNOMIAL, SPLINE FIT, SPLINE INTERPOLATION and CURVEPLOT, the Control word SELECT may optionally appear here. When this option is used in conjunction with splines, it imparts more information about their first three derivatives.

   On subsequent lines the following items of data are needed:

   (i) number of user-selected points where the y-values are required.
   (ii) the x-coordinate values of the user-selected points. This option allows the user to select intermediate x-points where he requires the corresponding y-values.

8. Control word PLOT if results are to be plotted on the graph plotter.

9. If PLOT is used then two numbers are required; these give the dimensions of the window size in inches within which all the drawing will be imprisoned until the next window is defined. If the A3/A4 plotter is required, then 3.5 5 might be specified as the plotting dimensions. Note that it would be unwise to plot more than 6 drawings in one job when using the A3/A4 plotter.

   If you wish to obtain full-size A3/A4 output, then by all means use 7 10 after the Control word PLOT but restrict yourself to just one plot at a time.

10. Now the user has three choices of continuation:

10.1 Control word STOP which terminates program execution.

10.2 If the user wants to re-use the same X and Y coordinates as listed in 5 then Control word REPEAT must appear. This is followed by items 2 and 3.

10.3 If the user wants to use a different set of X and Y coordinates, the complete block of items 2 to 6 must be typed in.

   Thus the user can perform any number of tasks until STOP is chosen.

11. The user may alternatively use Control words EASYGRAPH and EASYPLOT for better graphical output rather than use Control words GRAPH and PLOT which provide for the default settings for graphical output if required. Note that if the Control word EASYPLOT is used then the Control word .END must also be

used as a delimiter (see Example 2).

The 'better' facilities include labelling axes, drawing different symbols, providing own titles, scaling the output as required, drawing diagrams with different coloured pens etc. The EASYGRAPH package has many more facilities than are mentioned here. There is no reason why the full facilities of EASYGRAPH should not be independently exploited by the user. Indeed one can generate appropriate output from CURVEFIT, edit it suitably and input it to EASYGRAPH as a separate exercise. Full information about this package may be obtained by reading User Note 12, EASYGRAPH, or using the EMAS command HELP EASYGRAPH.

The control phrases recognized by the EASYGRAPH package such as PEN RED etc. must be presented to the CURVEFIT package as PEN=RED etc.

### 1.3.1 EXAMPLES

**Example 1 a**

Example of definitions and valid input:

*Command:* DEFINE 1,INP
*Command:* DEFINE 2,OUT
*Command:* DEFINE 50,GRAF
*Command:* CURVEFIT

where file INP contains:

```
GRAPH
'N MOOLJEE JCMB'
POLYNOMIAL
3
DATA
        0.00000      -3.11000
        0.40000      -3.06000
        0.80000      -2.32000
        1.20000      -2.40000
        1.60000      -2.29000
        2.00000      -1.88000
        2.40000      -1.65000
        2.80000      -2.44000
        3.20000      -2.45000
        3.60000      -2.81000
        4.00000      -3.64000
        4.40000      -3.15000
        4.80000      -3.01000
        5.20000      -3.53000
        5.60000      -3.84000
        6.00000      -3.28000
        6.40000      -3.02000
        6.80000      -2.19000
        7.20000      -3.81000
        7.60000      -4.16000
        8.00000      -2.91000
        8.40000       0.63000
        8.80000       0.91000
        9.20000       5.03000
END
SELECT
```

```
3 0.5 2.6 7.5
PLOT
3.5 5
STOP
```

**Note**

The user may, for example, subsequently wish to issue the EMAS commands

*Command:* LIST OUT,.LP15
*Command:* GPLIST GRAF,.GP15

to display the results.

Graphical output from Example 1 a

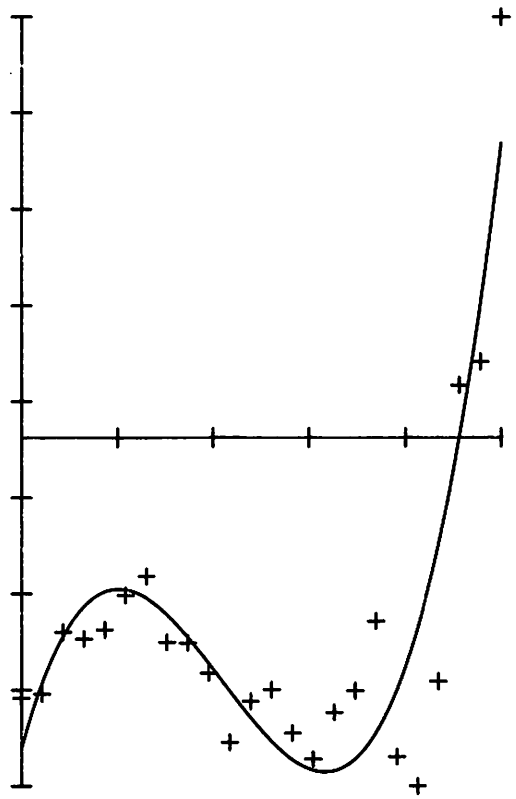


**Fig 1 a: Polynomial fit of degree 3**

**Example 1 b**

Example of definitions and valid input:

*Command:* DEFINE 1,INP
*Command:* DEFINE 2,OUT
*Command:* CURVEFIT

where file INP contains:

```
EXPONENTIAL
3
DATA
        0.00000        -3.11000
        0.40000        -3.06000
        0.80000        -2.32000
        1.20000        -2.40000
        1.60000        -2.29000
        2.00000        -1.88000
        2.40000        -1.65000
        2.80000        -2.44000
        3.20000        -2.45000
        3.60000        -2.81000
        4.00000        -3.64000
        4.40000        -3.15000
        4.80000        -3.01000
        5.20000        -3.53000
        5.60000        -3.84000
        6.00000        -3.28000
        6.40000        -3.02000
        6.80000        -2.19000
        7.20000        -3.81000
        7.60000        -4.16000
        8.00000        -2.91000
        8.40000         0.63000
        8.80000         0.91000
        9.20000         5.03000
END
STOP
```

**Notes**

(1) The Control word GRAPH is not used since there is no graphical output.

(2) The given data are evenly spaced as is necessary for the algorithm for fitting exponential functions.

**Output obtained from CURVEFIT (with data as supplied in Example 1 b)**

```
EDINBURGH REGIONAL COMPUTING CENTRE - CURVE FITTING PROGRAM CURVEFIT


EXPONENTIAL
          3

        0.0000000@-99          -3.1100000@  0
        4.0000000@ -1          -3.0600000@  0
        8.0000000@ -1          -2.3200000@  0
        1.2000000@  0          -2.4000000@  0
        1.6000000@  0          -2.2900000@  0
        2.0000000@  0          -1.8800000@  0
```

```
      2.4000000@  0          -1.6500000@  0
      2.8000000@  0          -2.4400000@  0
      3.2000000@  0          -2.4500000@  0
      3.6000000@  0          -2.8100000@  0
      4.0000000@  0          -3.6400000@  0
      4.4000000@  0          -3.1500000@  0
      4.8000000@  0          -3.0100000@  0
      5.2000000@  0          -3.5300000@  0
      5.6000000@  0          -3.8400000@  0
      6.0000000@  0          -3.2800000@  0
      6.4000000@  0          -3.0200000@  0
      6.8000000@  0          -2.1900000@  0
      7.2000000@  0          -3.8100000@  0
      7.6000000@  0          -4.1600000@  0
      8.0000000@  0          -2.9100000@  0
      8.4000000@  0           6.3000000@ -1
      8.8000000@  0           9.1000000@ -1
      9.2000000@  0           5.0300000@  0
END


CLASS=       3

APPROXIMATION OF DISCRETE FUNCTIONS BY A SUM OF 3 EXPONENTIAL TERMS


   COEFFICIENTS
                        CR                          CI
TERM 1 =  2.726177906189@ -1          3.011654195770@  0
TERM 2 =  2.726177906189@ -1         -3.011654195770@  0
TERM 3 = -1.375544152229@  0          0.000000000000@-99


   EXPONENTS
                        TR                          TI
TERM 1 = -2.913724699864@ -1          5.444200057489@ -1
TERM 2 = -2.913724699864@ -1         -5.444200057489@ -1
TERM 3 = -1.098929005392@  0          7.853981633975@  0


THE TERMS (1,2) MAY BE COMBINED TO GIVE 1 TERM OF THIS FORM:
      2*EXP(TR)*(CR*COS(TI*X)-CI*SIN(TI*X))
WHERE CR,CI AND TR,TI ASSUME THE VALUES IN TERM 1.

THE REMAINING TERMS ARE OF THE FORM: CR*EXP(TR)

STANDARD DEVIATION: 2.5466@  0

24 DATA POINTS USED IN ABOVE CALCULATION

**********

END OF INPUT DATA
```

**Example 2**

This example demonstrates the use of the EASYGRAPH package for the same data as above.

*Command:* DEFINE 1,INP
*Command:* DEFINE 2,OUT
*Command:* CURVEFIT

where file INP contains:

```
EASYGRAPH
"N MOOLJEE JCMB"
POLYNOMIAL
3
DATA
        0.00000        -3.11000
        0.40000        -3.06000
        0.80000        -2.32000
        1.20000        -2.40000
        1.60000        -2.29000
        2.00000        -1.88000
        2.40000        -1.65000
        2.80000        -2.44000
        3.20000        -2.45000
        3.60000        -2.81000
        4.00000        -3.64000
        4.40000        -3.15000
        4.80000        -3.01000
        5.20000        -3.53000
        5.60000        -3.84000
        6.00000        -3.28000
        6.40000        -3.02000
        6.80000        -2.19000
        7.20000        -3.81000
        7.60000        -4.16000
        8.00000        -2.91000
        8.40000         0.63000
        8.80000         0.91000
        9.20000         5.03000
END



SELECT
3 0.5 2.6 7.5
-------------------------------------------
EASYPLOT                                   !
PLOTTER=.GP15                              !
PEN=BLUE                                   !
FILE=G1OUT                                 !
SYMBOL=1                                   !
LINETYPE=CURVE                             !----REQUIRED FOR EASYGRAPH
TITLE="GRAPH 1"                            !
XAXIS=10,"Any suitable text for xaxis"     !
YAXIS=10,"Any suitable text for yaxis"     !
ANNOTATE="GRAPH1 OUTPUT"                   !
.END                                       !
-------------------------------------------
```

```
REPEAT
EASYGRAPH RAW
SPLINE FIT
5
13 1.4 2.0 2.5 3.0 4.0 4.5 5.0 5.5 6.0 6.5 7.0 7.5 8.0
-------------------------------------------
EASYPLOT                                    !
PLOTTER=.GP15                               !
PEN=GREEN                                   !
FILE=G2OUT                                  !
SYMBOL=2                                    !
LINETYPE=LINE                               !
FLATNUMBER                                  !----REQUIRED FOR EASYGRAPH
XFORMAT=2,0                                 !
YFORMAT=1,0                                 !
TITLE="GRAPH 2"                             !
XAXIS=10,"Any suitable text for xaxis"      !
YAXIS=10,"Any suitable text for yaxis"      !
ANNOTATE="GRAPH2 OUTPUT"                    !
.END                                        !
-------------------------------------------
REPEAT
EASYGRAPH RAW
SPLINE INTERPOLATION
2
-------------------------------------------
EASYPLOT                                    !
PLOTTER=.GP15                               !
PEN=BLACK                                   !
FILE=G3OUT                                  !
SYMBOL=3                                    !
LINETYPE=LINE                               !
FLATNUMBER                                  !----REQUIRED FOR EASYGRAPH
TICKOUT                                     !
XFORMAT=2,0                                 !
YFORMAT=1,0                                 !
TITLE="GRAPH 3"                             !
XAXIS=10,"Any suitable text for xaxis"      !
YAXIS=10,"Any suitable text for yaxis"      !
ANNOTATE="GRAPH3 OUTPUT"                    !
.END                                        !
-------------------------------------------
STOP
```

**Notes**

(1) Channel 50 does not require definition if all plotting is done by EASYGRAPH.

(2) The Control word EASYGRAPH appears each time this option is used.

(3) The user may additionally obtain a point plot of the raw data superimposed in the main plot by planting the Control word RAW after EASYGRAPH. This facility has been incorporated to make the graphical output similar to that obtainable if GRAPH had been used.

(4) With EASYGRAPH the package produces only one drawing at a time in the file

specified via the FILE = phrase.

e.g. FILE=G1OUT
FILE=G2OUT etc.

Each file so produced may be listed out to a plotter via the EMAS command GPLIST, e.g. if PLOTTER=.GP15 had been set then GPLIST G1OUT,.GP15

(5) With spline fits and interpolation the option in EASYGRAPH LINETYPE=CURVE is not advised; instead use LINETYPE=LINE.

### 1.3.2 Output Obtained From CURVEFIT (with data as supplied in Example 2)

```
EDINBURGH REGIONAL COMPUTING CENTRE - CURVE FITTING PROGRAM CURVEFIT


EASYGRAPH

POLYNOMIAL
      3

      0.0000000@-99          -3.1100000@  0
      4.0000000@ -1          -3.0600000@  0
      8.0000000@ -1          -2.3200000@  0
      1.2000000@  0          -2.4000000@  0
      1.6000000@  0          -2.2900000@  0
      2.0000000@  0          -1.8800000@  0
      2.4000000@  0          -1.6500000@  0
      2.8000000@  0          -2.4400000@  0
      3.2000000@  0          -2.4500000@  0
      3.6000000@  0          -2.8100000@  0
      4.0000000@  0          -3.6400000@  0
      4.4000000@  0          -3.1500000@  0
      4.8000000@  0          -3.0100000@  0
      5.2000000@  0          -3.5300000@  0
      5.6000000@  0          -3.8400000@  0
      6.0000000@  0          -3.2800000@  0
      6.4000000@  0          -3.0200000@  0
      6.8000000@  0          -2.1900000@  0
      7.2000000@  0          -3.8100000@  0
      7.6000000@  0          -4.1600000@  0
      8.0000000@  0          -2.9100000@  0
      8.4000000@  0           6.3000000@ -1
      8.8000000@  0           9.1000000@ -1
      9.2000000@  0           5.0300000@  0
END


CLASS=       1

LEAST SQUARES APPROXIMATION OF DISCRETE FUNCTIONS BY A POLYNOMIAL OF
DEGREE 3


COEFFICIENTS        (IN ASCENDING ORDER)
```

A( 0) = -3.71280626780571@ 0
A( 1) = 2.293080939457@ 0
A( 2) = -8.12782155445021@ -1
A( 3) = 7.05369844862476@ -2

STANDARD DEVIATION: 7.8653@ -1

24 DATA POINTS USED IN ABOVE CALCULATION

**********

| User-Selected X | Y(FIT) | DER1 |
|---|---|---|
| 5.00000000@ -1 | -2.76064421@ 0 | 1.53320152@ 0 |
| 2.60000000@ 0 | -2.00544516@ 0 | -5.02896223@ -1 |
| 7.50000000@ 0 | -2.47590514@ 0 | 2.00446474@ 0 |

**********

REPEAT

EASYGRAPH RAW

SPLINE FIT

ABOVE DATA POINTS BEING REUSED IN THE FOLLOWING COMPUTATION.

CLASS= 6 SPLINE FIT

| X | Y(FIT) |
|---|---|
| 0.00000000@-99 | -3.90722854@ 0 |
| 4.00000000@ -1 | -2.94795217@ 0 |
| 8.00000000@ -1 | -2.33756315@ 0 |
| 1.20000000@ 0 | -2.04403591@ 0 |
| 1.60000000@ 0 | -2.02666085@ 0 |
| 2.00000000@ 0 | -2.04499561@ 0 |
| 2.40000000@ 0 | -1.87548907@ 0 |
| 2.80000000@ 0 | -2.06086962@ 0 |
| 3.20000000@ 0 | -2.56869578@ 0 |
| 3.60000000@ 0 | -3.06849231@ 0 |
| 4.00000000@ 0 | -3.33856077@ 0 |
| 4.40000000@ 0 | -3.24632276@ 0 |
| 4.80000000@ 0 | -3.04856065@ 0 |
| 5.20000000@ 0 | -3.47179910@ 0 |
| 5.60000000@ 0 | -3.86765634@ 0 |
| 6.00000000@ 0 | -3.31269549@ 0 |

| | |
|---|---|
| 6.40000000@ 0 | -2.91095768@ 0 |
| 6.80000000@ 0 | -2.36146135@ 0 |
| 7.20000000@ 0 | -3.59288687@ 0 |
| 7.60000000@ 0 | -4.55721920@ 0 |
| 8.00000000@ 0 | -2.13526523@ 0 |
| 8.40000000@ 0 | -2.85169466@ -1 |
| 8.80000000@ 0 | 1.45524347@ 0 |
| 9.20000000@ 0 | 4.90234154@ 0 |

VALUE OF INTEGRAL BETWEEN LIMITS 0.0000@-99 AND 9.2000@ 0 IS -2.218314@ 1

24 DATA POINTS USED IN ABOVE CALCULATION

**********

REPEAT

EASYGRAPH RAW

SPLINE INTERPOLATION

ABOVE DATA POINTS BEING REUSED IN THE FOLLOWING COMPUTATION.

CLASS= 4 SPLINE INTERPOLATION

| X | Y(FIT) |
|---|---|
| 0.00000000@-99 | -3.11000000@ 0 |
| 4.00000000@ -1 | -3.06000000@ 0 |
| 8.00000000@ -1 | -2.32000000@ 0 |
| 1.20000000@ 0 | -2.40000000@ 0 |
| 1.60000000@ 0 | -2.29000000@ 0 |
| 2.00000000@ 0 | -1.88000000@ 0 |
| 2.40000000@ 0 | -1.65000000@ 0 |
| 2.80000000@ 0 | -2.44000000@ 0 |
| 3.20000000@ 0 | -2.45000000@ 0 |
| 3.60000000@ 0 | -2.81000000@ 0 |
| 4.00000000@ 0 | -3.64000000@ 0 |
| 4.40000000@ 0 | -3.15000000@ 0 |
| 4.80000000@ 0 | -3.01000000@ 0 |
| 5.20000000@ 0 | -3.53000000@ 0 |
| 5.60000000@ 0 | -3.84000000@ 0 |
| 6.00000000@ 0 | -3.28000000@ 0 |
| 6.40000000@ 0 | -3.02000000@ 0 |
| 6.80000000@ 0 | -2.19000000@ 0 |
| 7.20000000@ 0 | -3.81000000@ 0 |
| 7.60000000@ 0 | -4.16000000@ 0 |

```
8.00000000@  0          -2.91000000@  0
8.40000000@  0           6.30000000@ -1
8.80000000@  0           9.10000000@ -1
9.20000000@  0           5.03000000@  0
```

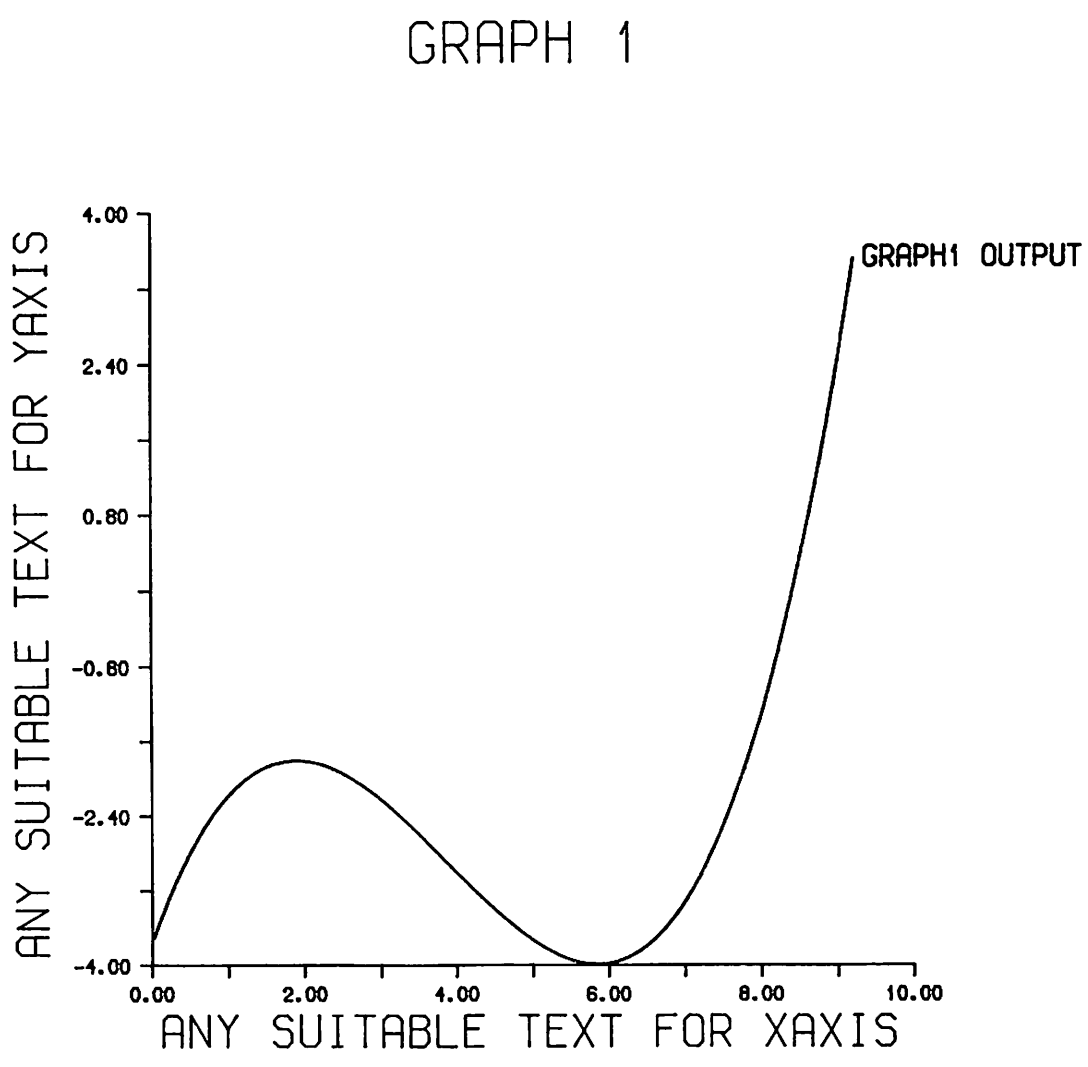
VALUE OF INTEGRAL BETWEEN LIMITS 0.0000@-99 AND 9.4000@  0 IS -2.249403@ 1

24 DATA POINTS USED IN ABOVE CALCULATION

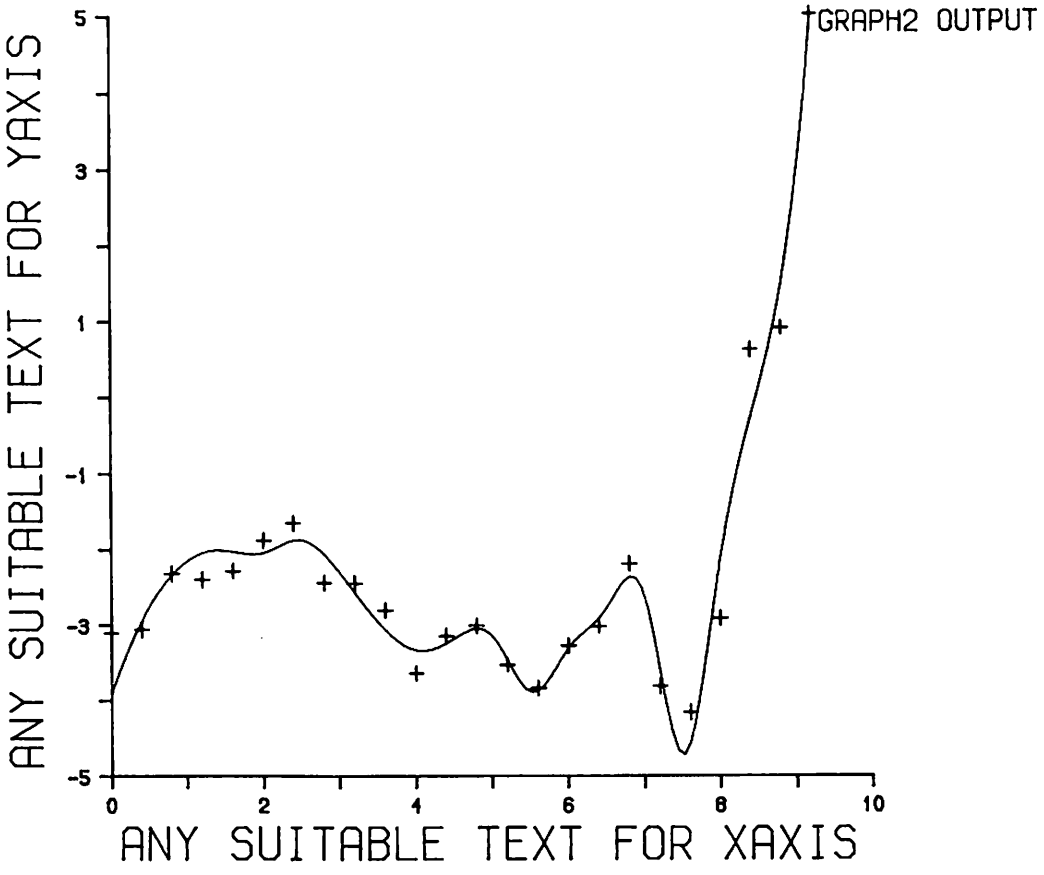
**********

END OF INPUT DATA

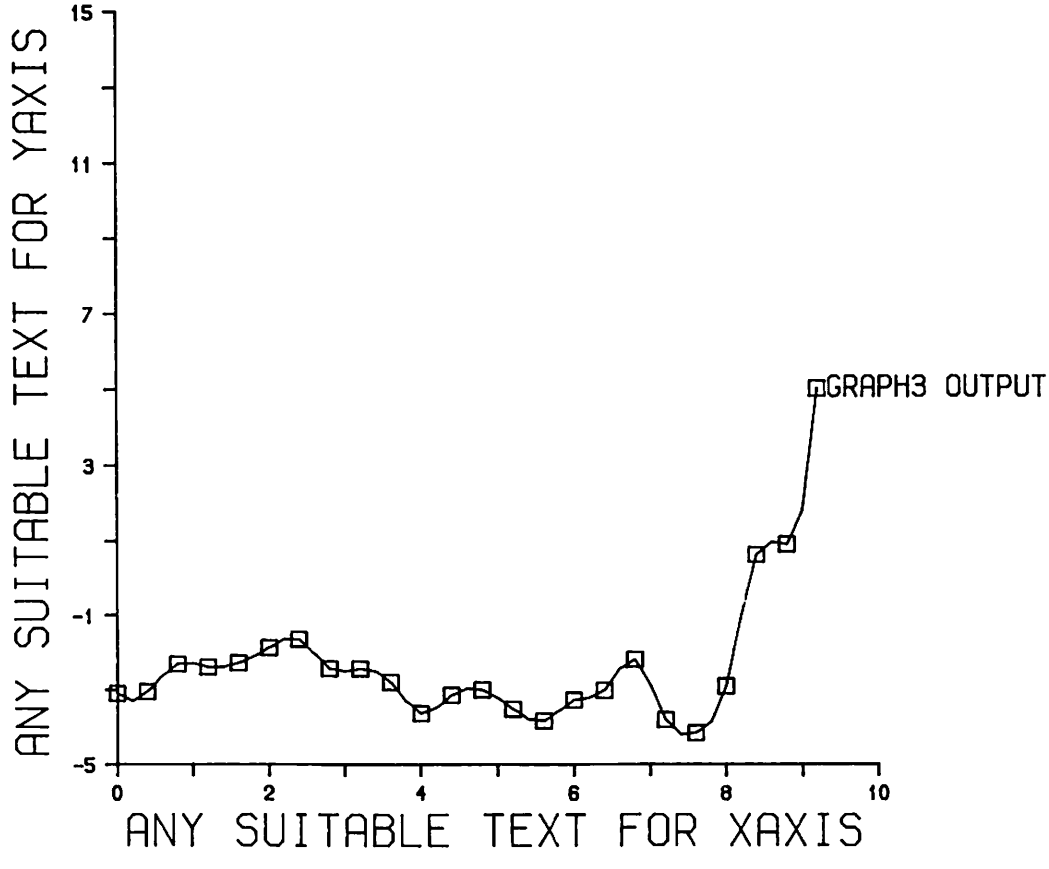
**Graphical output from Example 2**



# GRAPH 2




# GRAPH 3



### 1.4.0 Error messages

If an error occurs during the computation of the desired coefficients an appropriate error message is printed out.

1. If an invalid Control word or a control phrase without a Control word is input, a message to that effect is printed out, and the program goes on to the next calculation, or stops if that was the last.

2. If the Control word DATA is not read in where expected, then the message '***ERROR IN DATA***' is output and the program stops.

3. Any alphabetical characters read in during the reading of data causes the data input to be terminated. An 'ERROR IN DATA' message is printed out if the string of letters does not contain the word 'END'.

4. If an attempt is made to input more than 500 data points, the program stops with the message '***TOO MANY DATA POINTS***'.

5. If the number of data points input is insufficient to enable the type of approximation requested to be carried out, a message to that effect is output, and the program goes onto the next calculation, or stops if that was the last.

6. The message '***ORDER TOO LARGE***' is output if

   a) the requested degree of the polynomial in a polynomial approximation is > 11.

   b) the sum of degrees of the 2 polynomials in a rational approximation is > 12.

   c) the number of terms requested in an exponential approximation is > 7.

7. If any of the algorithms used by the program fails, the message is:

   '***ALGORITHM FAILED; PROBABLY THIS CLASS OF APPROXIMATION IS NOT SUITABLE FOR THE GIVEN DATA***'

   Further, if graph plotting had been requested in this case the message is:

   'NO GRAPH OUTPUT FOR THE ABOVE CASE IS PRODUCED AS A CONSEQUENCE OF PROGRAM FAILURE'

### 1.5.0 Methods used

The techniques used are polynomial and rational least squares approximation [2], and Prony's method for exponential approximation.

For spline interpolation and spline fits, NAG library routines, E02BAF and E02BBF (originally NPL routines [3]) are used.

For derivative evaluation of splines NAG routine E02BCF is invoked. Finally smoothing by spline functions was carried out by employing the algorithm described fully by Rheinsch [1].

## 2.0 References


[1] RHEINSCH, C.H. Smoothing by Spline functions, *Numerische Mathematik* 10, pp 134-149, 1972.

[2] MARQUARDT, D.W. An algorithm for least squares estimation of nonlinear parameters, *SIAM Journal* 2, pp 431-441, 1963.

[3] COX, M.G. *A data fitting package for the non-specialist user, Report NAC 40,* National Physical Laboratory, Teddington, Middlesex, July 1973.


## 2.1 Further Reading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ROUTINE:CUSPLINE

**Description**

Given pairs of data

X(I), Y(I), I = N1,....., N2

this routine determines a cubic spline function f(x) with knots at X(I) which is either interpolative or a fit with a specified degree of smoothness. The spline f(x) is such that it minimizes the functional integral

(G"(T)**2*DT) , integrated from

t = X(N1) to t = X(N2) .

The routine also produces a smooth fit in the least-squares sense:

$$\sum_{i=N1}^{i=N2} W_i(F(X_i) - Y_i)^2 <= SF .$$

The parameter SF controls the extent of smoothing. If SF = 0 is chosen, a spline interpolation is computed i.e. $F(X_i) = Y_i$ will hold.

**Method**

By application of the calculus of variation it can be shown that the minimizing function is composed of cubic parabolae:

F(X) = ((D(I)*H + C(I))*H + B(I))*H + A(I)

with

H = X - X(I) for I = N1,....., N2-1

and

X(I) <= H <= X(I+1) .

The transition from one cubic parabola to the next is such that they agree in value, 1st and 2nd derivative at the knot X(I).