POLYMATH

VERSION 3.0

USER-FRIENDLY
NUMERICAL ANALYSIS
PROGRAMS

- SIMULTANEOUS DIFFERENTIAL EQUATIONS
- SIMULTANEOUS ALGEBRAIC EQUATIONS
- POLYNOMIAL, MULTIPLE LINEAR AND NONLINEAR REGRESSION

for IBM and Compatible Personal Computers

TABLE OF CONTENTS - POLYMATH

INTRODUCTION

POLYMATH OVERVIEW

POLYMATH is an effective yet easy to use computational system which has been specifically created for professional or educational use. The various programs in the POLYMATH series allow the user to apply effective numerical analysis techniques during interactive problem solving on a personal computer. Whether you are student, engineer, mathematician, scientist, or anyone with a need to solve problems, you will appreciate the ease in which POLYMATH allows you to obtain solutions. Chances are very good that you will seldom need to refer to this manual beyond an initial reading because POLYMATH is so easy to use.

With POLYMATH, you are able to focus your attention on the problem at hand rather than spending your valuable time in learning how to use or reuse the program. You are encouraged to become familiar with the mathematical concepts being utilized in POLYMATH. These are discussed in most textbooks concerned with numerical analysis.

The available programs in POLYMATH include:

- ***SIMULTANEOUS DIFFERENTIAL EQUATION SOLVER***
- ***SIMULTANEOUS ALGEBRAIC EQUATION SOLVER***
- ***POLYNOMIAL, MULTIPLE LINEAR AND NONLINEAR REGRESSION***

Whether you are a novice computer user or one with considerable computer experience, you will be able to make full use of the programs in POLYMATH which allow numerical problems to be solved conveniently and interactively.

If you have limited computer experience, it will be helpful for you to read through this manual and try many of the QUICK TOUR problems. If you have considerable personal computer experience, you may only need to read the chapters at the back of this manual on the individual programs and try some of the QUICK TOUR problems.

This manual will be a convenient reference guide when using POLYMATH.

MANUAL OVERVIEW

This manual first provides general information on features which are common to all of the POLYMATH programs. Particular details of individual programs are then presented. Major chapter topics are outlined below:

INTRODUCTION

The introduction gives an overview of the POLYMATH computational system and gives general instructions for procedures to follow when using individual POLYMATH programs.

GETTING STARTED

This chapter prepares you for executing POLYMATH the first time, with information about turning on the computer, loading POLYMATH, and making choices from the various menu and option screens.

HELP

On-line access to a general help section is discussed.

SAVING INDIVIDUAL FILES AND PROBLEM LIBRARY:

This chapter discusses saving individual problems, data and/or result files on a floppy or hard disk. It also describes the use of the problem library for storing, retrieving and modifying problems on a disk.

UTILITIES

The access and use of a scientific calculator and a converter for units and dimensions is presented.

The remaining chapters of the manual present a QUICK TOUR of each individual POLYMATH program and are organized according to the following subsections:

1. **PROGRAM OVERVIEW**
   This subsection gives general details of the particular program.
2. **QUICK TOUR**
   You can use this subsection to see how easy it is to enter and solve a problem with a particular POLYMATH program.

DISPLAY PRESENTATION

Throughout this manual, a full screen is indicated by a total enclosure:

An upper part of screen is contained within a partial enclosure:

A lower part of screen is shown by a partial enclosure:

An intermediate part of a screen is given between vertical lines:

The option box is given by:

KEYBOARD INFORMATION

When using POLYMATH, it is not necessary to remember a complex series of keystrokes to respond to the menus, options, or prompts. The commands available to you are clearly labeled for easy use on each display. Normally the keystrokes which are available are given on the display as indicated on the PROBLEM OPTIONS display shown below.

```
                         PROBLEM OPTIONS
                     ⇧ F7 to solve this problem.
 ⇧↵ to alter the problem.            F6 for helpful information
 F9 for file and library options.    ⇧F10 for the MAIN MENU.
```

USING THE ↵ KEY

In this manual as in POLYMATH, the ↵ symbol is used to indicate the carriage return key which is also called the enter key. Usually when you are responding to a menu option, the enter key is not required. However, when data or mathematical functions are being entered, the enter key is used to indicate that the entry is complete.

SHIFTED KEYPRESSES

Some options require that several keys be pressed at the same time. This is indicated in POLYMATH and in this manual by a dash between the keys such as a ⇑ - F8 which means to press and hold the ⇑ key, then press the F8 function key and then release both keys.

THE EDITING KEYS

Use the left and right arrow keys to bring the cursor to the desired position, while editing an expression. Use the Del key to delete the character above the cursor or the ⟵ (Back Space) key to delete the first character to the left of the cursor. Typed in characters will be added to the existing expression in the first position left to the cursor.

BACKING UP KEYS

Press either the **F8** or the **Esc** key to have POLYMATH back up one program step.

ENTERING VARIABLE NAMES

A variable may be called by any alphanumeric combination of 10 characters or less, and the variable name MUST start with a lower or upper case letter. Blanks, punctuation marks and mathematical operators are not allowed.

Note that POLYMATH distinguishes between lower and upper case letters, so the variables 'MyVar2' and 'myVar2' are not the same.

ENTERING NUMBERS

All numbers should be entered with the upper row on the key board or with the numerical keypad activated. Remember that zero is a number from the top row and not the letter key from the second row. The number 1 is from the top row while letter l is from the third row.

The results of the internal calculations made by POLYMATH have at least a precision of eight digits of significance. Results are presented with at least four significant digits such as xxx.x or x.xxx . All mathematical operations are performed as floating point calculations, so it is not necessary to enter decimal points for real numbers.

MATHEMATICAL SYMBOLS

You can use familiar notation when indicating standard mathematical operations.

Operator	Meaning	Symbol	Entry
+	addition	+	+
-	subtraction	-	-
x	multiplication	*	*
÷	division	/	/
	power of 10	$x.x10^a$	x.xea
(x.x is numerical with a decimal and a is an integer)			
	exponentiation	r^s	r**s or r^s

MATHEMATICAL FUNCTIONS

Useful functions will be recognized by POLYMATH when entered as part of an expression. The underlined portion of the following functions is all that is required provided that all arguments are enclosed in parentheses:

<u>ln</u> ( ) = natural logarithm to the base e
<u>log</u> ( ) = logarithm to the base 10
<u>exp</u> ( ) =exponential
<u>abs</u> ( ) = absolute value
<u>sin</u> ( ) = trigonometric sine with argument in radians
<u>cos</u> ( ) = trigonometric cosine with argument in radians

POLYMATH MESSAGES

There are many POLYMATH messages which may provide assistance during problem solving. These messages will tell you what is incorrect and how to correct it. All user inputs, equations and data, are checked for format and syntax upon entry, and feedback is immediate. Correct input is required before proceeding to a problem solution.

HARD COPY

If there is a printer connected to the computer, hard copy of the problem statements, tabular and graphical results etc. can be made by pressing F7 key wherever this option is indicated on the screen. Screen copies can also be made if the DOS graphics command is used before entering POLYMATH and your printer accepts this graphics mode.

Problem statements and results can be also printed by saving them on a file and printing this file after leaving POLYMATH.

GRAPHICS

POLYMATH gives convenient displays during problem entry, modification and solution. Since the program always operates in a graphic mode, your computer must always have a color graphic adapter and a monochrome or color monitor.

GETTING STARTED

This chapter provides information on the hardware requirements and discusses the installation of POLYMATH.

HARDWARE REQUIREMENTS

POLYMATH runs on the IBM PC XT, AT, PS/2 and most compatibles. A variety of graphics boards are supported including CGA, EGA, Hercules, VGA and XGA. The minimum application memory requirement is 512Kb. POLYMATH works with PC and MS DOS 3.0 and above. POLYMATH can be a DOS application under Windows. Calculations are very fast since they utilize the floating point processor when it is available.

POLYMATH SOFTWARE

The complete set of POLYMATH application programs with a general selection menu is available on a single 3-1/2 inch 1.44 Mb floppy in compressed form. It is recommended that a backup disk be made before attempting to install POLYMATH onto a hard disk. Installation is available via an install program which is executed from any drive.

INSTALLATION TO INDIVIDUAL COMPUTERS AND NETWORKS

POLYMATH executes best when the software is installed on a hard disk or a network. There is a utility on the POLYMATH distribution disk which is called "install". Simply put the disk in a drive , typically A or B. Type "install" at the prompt, and press return. Follow the instructions on the screen to install POLYMATH on the particular drive and directory that you desire. Note that the default drive is "C:" and the default directory is called "POLYMAT3". Network installation will ask additional questions during installation.

Detailed installation instructions are found in the Appendix of this manual. The PRINTSET program which is automatically installed in the POLYMATH directory can be used to change the printer specifications without completely reinstalling POLYMATH. Latest detailed information can be found on the README.TXT file found on the installation disk and in the POLYMATH directory.

FIRST TIME EXECUTION OF POLYMATH

The execution of POLYMATH is started by first having your current directory set to the subdirectory of the hard disk where POLYMATH is stored or to the floppy disk where the program is stored.

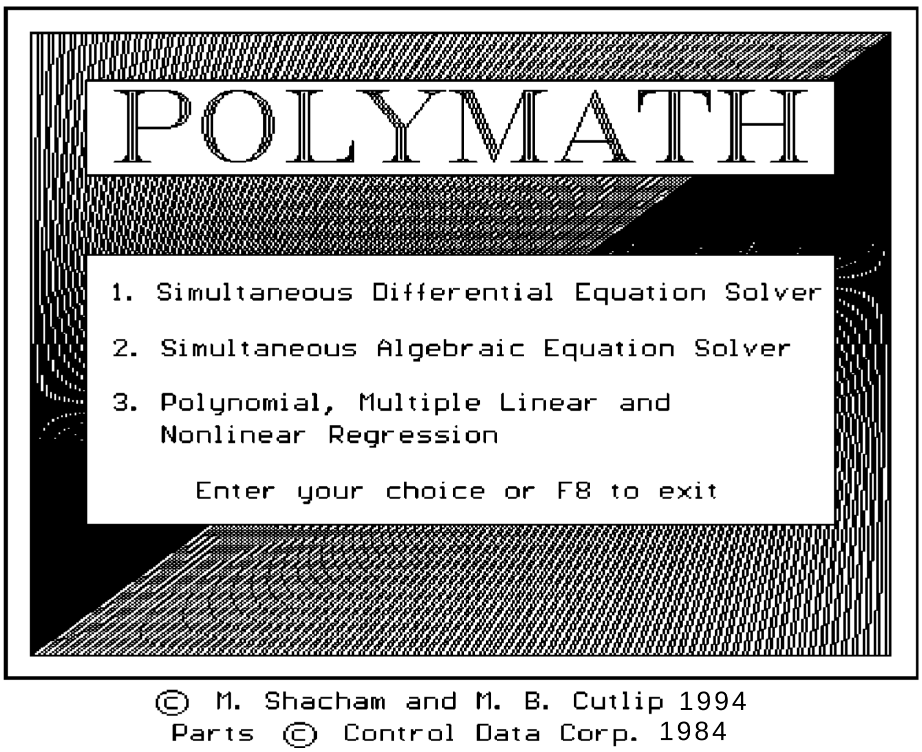
C >

Execution is started by entering POLYMATH at the cursor

C > polymath

and then press the Return (↵) key.

The Program Selection Menu should then appear:



The desired POLYMATH program is then selected by entering the appropriate letter. You will then taken to the Main Program Menu of that particular program. Individual programs are discussed in later chapters of this manual.

EXITING POLYMATH PROGRAM

The best way to exit POLYMATH is to follow the instructions on the program display. However, a ⇑ - F10 keypress will stop the execution of a particular POLYMATH program and return the user to the Polymath Program Selection Menu. *THIS ACTION WILL DELETE THE EXISTING PROBLEM* so be sure to store your problem in the library before exiting the program in this manner.

HELP

MAIN HELP MENU

Each individual POLYMATH program has a detailed help section which is available from many points in the program by pressing F6 when indicated. The Help Menu allows the selection of the topic area for specific help as shown below for the Differential Equation Solver:

```
                              HELP MENU

                     (Explanations and examples)

     The purpose of this POLYMATH program is to integrate a system
of up to 12 first-order, ordinary differential equations from initial
to final conditions.

     From the list below select a topic that you want to review about
this POLYMATH program.

                    a.  Entering the equations.
                    b.  Integration algorithms.
                    c.  Troubleshooting.
                    d.  The calculator.


                 ⇧ F8 to return to the program.
```

For example, pressing "a" gives a discussion on entering the equations.

```
                    ENTERING THE EQUATIONS

     The equations should be entered in the following form:

                d(x)/d(t)= an expression
       or,      d(x)= an expression.

     Here t is the independent variable and x is a dependent
variable.  Variable names must begin with a lower case alphabetic
character and can contain up to 10 lower-case alphabetic and
numeric characters.
```

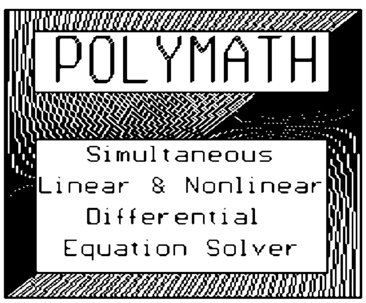
Once the current topic is completed, the Help Options Menu provides for additional options as shown below:

```
                         HELP OPTIONS
 ↵  to continue.                          F8 for the HELP MENU.
                 ⇑ F8 to return to the program.
```

The ⇑ - F8 option to return to the program will take you to the display where you originally requested HELP

ACCESSING HELP BEFORE PROBLEM ENTRY

The Main Help Menu is reached during the startup of your POLYMATH program from the Main Menu as shown below and from the Program Menu by pressing F6.




```
↵  to begin.
F6 for HELP menu.
F7 for sample problems.
F8 for POLYMATH menu.
F9 for file options.
⇑ F9 for the credits.
```

```
The following keys are
   always active:
-----------------------
⇑ F10 to return to
      this display
F4 for calculator
F5 for unit converter
```

ACCESSING HELP DURING PROBLEM ENTRY

When you are entering a problem, the HELP MENU is available from the displays entitled Introduction Options, Problem Options, Change Options, Equation Options and Results Options. This will allow you to obtain the necessary help and return to the same point where the HELP MENU was originally requested. As an example, this point is shown in the Change Options box in the next page.

```
                    CHANGE OPTIONS
          e. Enter/Change/Delete the equations.
 t.  Change the problem title.     i. Change the initial values.
              f.  Change the final value.
   F8 when done.                     F6 for helpful information.
```

<u>**CALCULATOR HELP**</u>

A detailed discussion of the POLYMATH Calculator is given in Chapter 4 of this manual. Two types of help are available:

1. The same page help can be accessed from the calculator utility which is reached by pressing F4 from any point in the program.

```
>_
CALCULATOR:   Enter an expression and press <ENTER> to evaluate it.
     Press <ESC> to leave or press F6 for information.
```

   F6 brings up the same page help which provides a brief instruction inside the calculator's window.

2. Extensive HELP for the Calculator is available from the Help Menu is discussed on page 3-1.

<u>**UNIT CONVERSION HELP**</u>

The Unit Conversion Utility is discussed in Chapter 4 of this manual. There is no on-line help.

UTILITIES

CALCULATOR

A sophisticated calculator is always available for use in a POLYMATH program. This calculator is accessed by pressing the F4 key . At this time a window will be open in the option box area which will give you access to the calculator.

```
≫_
CALCULATOR:  Enter an expression and press <ENTER> to evaluate it.
     Press <ESC> to leave or press F6 for information
```

The POLYMATH calculator allows you to enter an expression to be evaluated. After the expression is complete, press ↵ to have it calculated. You may then press ↵ again to clear the expression, or you may edit your expression using the standard editing functions. When you wish to leave the calculator, just press the F8 or Esc key.

CALCULATOR EXPONENTIATION

Numbers may also be entered in scientific notation. The calculator will recognize 'E' or 'e' as being equivalent to the notation '*10**'. For example, these three expressions are equivalent:

4.71*10**A = 4.71eA = 4.71*10^A

AVAILABLE FUNCTIONS

A number of standard functions are available for use in thecalculator. The underlined portion of the following functions is all that is required provided that all arguments are enclosed in parentheses. The arguments may themselves be expressions or other functions. The nesting of function is allowed.

ln ( ) or alog ( ) = natural logarithm to the base e
log ( ) or alog10 ( ) = logarithm to the base 10
exp ( ) = exponential (e^x)
exp2 ( ) = exponential of 2 (2^x)
exp10 ( ) = exponential of 10 (10^x)
sqrt ( ) = square root
abs ( ) = absolute value

int ( ) or ip ( ) = integer part
fract ( ) = or fp ( ) = fractional part
round ( ) = rounded value
sign ( ) = returns + 1 or 0 or -1
N! = factorial of integer part of number N (this only operates on a number)
sin ( ) = trigonometric sine with argument in radians
cos ( ) = trigonometric cosine with argument in radians
tan ( ) = trigonometric tangent with argument in radians
sec ( ) = trigonometric secant with argument in radians
csc ( ) = trigonometric cosecant with argument in radians
cot ( ) = trigonometric cotangent with argument in radians
arcsin ( ) = trigonometric inverse sine with result in radians, alternates arsin ( ) and asin ( )
arccos ( ) = trigonometric inverse cosine with result in radians, alternates arcos ( ) and acos ( )
arctan ( ) = trigonometric inverse tangent with result in radians, alternate atan ( )
arcsec ( ) = trigonometric inverse secant with result in radians
arccsc ( ) = trigonometric inverse cosecant with result in radians
arccot ( ) = trigonometric inverse cotangent with result in radians
sinh ( ) = hyperbolic sine
cosh ( ) = hyperbolic cosine
tanh ( ) = hyperbolic tangent
arcinh ( ) = inverse hyperbolic sine
arccosh ( ) = inverse hyperbolic cosine
arctanh ( ) = inverse hyperbolic tangent

You should note that the functions require that their arguments be enclosed in parentheses, but that the arguments do not have to be simple numbers. You may have a complicated expression as the argument for a function, and you may even nest the functions, using one function (or an expression including one or more functions) as the argument for another.

ASSIGNMENT FUNCTIONS

The assignment function is a way of storing your results. You may specify a variable name in which to store the results of a computation by first typing in the variable name, then an equals sign, then the expression you wish to store. For example, if you wish to store the value of sin $(4/3)^2$ in variable 'a', you would enter:

a = sin (4/3)**2

You can then use the variable 'a' in other calculations. These variables are stored as long, and only as long, as you are in the calculator.

Variable names must start with a letter, and can contain letters and digits. There is no limit on the length of the variable names, or on the number of variables you can use.

CALCULATOR EXAMPLES

Example 1. In this example the vapor pressure of water at temperatures of 50, 60 and 70 ^{o}C has to be calculated using the equation:

$$\log_{10} P = 8.10765 - \frac{1750.29}{235.0 + T}$$

For T = 50 the following expression should be typed into the calculator:

```
10^(8.10675 - 1750.29 / (235+50))

CALCULATOR: Enter an expression and press <ENTER> to evaluate it.
   Press <ESC> to leave or press F6 for information.
```

Pressing ↵ brings up the desired answer which is 92.5297905 mm Hg at 50 ^{o}C. To change the temperature use the left arrow to bring the cursor just right to the zero of the number 50, use the ← (BkSp) key to erase this number and type in the new temperature value.

Example 2. In this example the pressure of carbon dioxide at temperature of T = 400 K and molal volume of $\hat{V}$ = 0.8 liter is calculated using the following equations:

$$P = \frac{RT}{\hat{V} - b} - \frac{a}{\hat{V}^2}$$

Where $a = \frac{27}{64}\left(\frac{R^2 T_c^2}{P_c}\right)$ $b = \frac{RT_c}{8 P_c}$

$R = 0.08206$, $T_c = 304.2$ and $P_c = 72.9$.

One way to carry out this calculation is to store the numerical values in the named variables. First you can type in Pc = 72.9 and press ↵ to store this value as shown below.

```
» Pc=72.9
CALCULATOR: Enter an expression and press <ENTER> to evaluate it.
    =72.9.
```

After that you can type in Tc = 304.2 and R = 0.08206. To calculate b you type in the complete expression for it as follows:

```
» b=R*Tc/(8*Pc)
CALCULATOR: Enter an expression and press <ENTER> to evaluate it.
    =0.0428029012
```

a is calculated and stored the same way. Finally P can be calculated as shown:

```
» P=R*400/(0.8-b)-a/(0.8*0.8)
CALCULATOR: Enter an expression and press <ENTER> to evaluate it.
    =37.7148168
```

UNIT CONVERSION

A utility for unit conversion is always available for use within a POLYMATH program. Unit Conversion is accessed by pressing F5 wherever you desire. This will result in the following window in the option box area:

```
Type the letter of the physical quantity for conversion.
a) Energy     b)  Force     c) Length       d) Mass       e) Power
f) Pressure   g) Volume     h) Temperature     F8 or ESC to exit
```

The above listing indicates the various classes of Unit Conversion which are available in POLYMATH. A listing of the various units in each class is given below:

ENERGY UNITS: joule, erg, cal, Btu, hp hr, ft lb_f, (liter)(atm), kwh

FORCE UNITS: newton, dyne, kg, lb, poundal

LENGTH UNITS: meter, inch, foot, mile, angstrom, micron, yard

MASS UNITS: kilogram, pound, ton (metric)

POWER UNITS: watts, hp (metric), hp (British), cal/sec, Btu/sec, ft lb_f/sec

PRESSURE UNITS: pascal, atm, bar, mm Hg (torr), in Hg, psi [lb_f /sq in]

VOLUME UNITS: cu. meter, liter, cu. feet, Imperial gal, gal (U.S.), barrel (oil), cu. centimeter

TEMPERATURE UNITS: Celsius, Fahrenheit, Kelvin, Rankine

PREFIXES FOR UNITS

It is convenient to also specify prefixes for any units involved in a Unit Conversion. This feature provides the following prefixes:

deci 10^{-1}	centi 10^{-2}	milli 10^{-3}	micro 10^{-6}	deka 10
hecto 10^{2}	kilo 10^{3}	mega 10^{6}	giga 10^{9}	

UNIT CONVERSION EXAMPLE

Suppose you want to convert 100 BTU's to kilo-calories. First you should access the Unit Conversion Utility by pressing F5. This will bring up the following options

Type the letter of the physical quantity for conversion.				
a) Energy	b) Force	c) Length	d) Mass	e) Power
f) Pressure	g) Volume	h) Temperature	F8 or ESC to exit	

Press "a" to specify an Energy conversion:

From units: Type in a letter (F9 to set a prefix first)				
a. joule	b. erg	c. cal	d. Btu	e. hp hr
f. ft lb_f	g. (liter)(atm)	h. kwh		

Type a "d" to specify Btu:

From units : Btu		To units:	(F9 for a prefix)	
a. joule	b. erg	c. cal	d. Btu	e. hp hr
f. ft lb,	g. (liter)(atm)	h. kwm		

Use F9 to indicate a Prefix:

Press the number of the needed prefix or F9 for none.				
1) deci 10^{-1}	2) centi 10^{-2}	3) milli 10^{-3}	4) micro 10^{-6}	
5) deka 10	6) hecto 10^2	7) kilo 10^3	8) mega 10^6	9) giga 10^9

Please indicate kilo by pressing the number 7.

From units: Btu		To units: kilo -		
a. joule	b. erg	c. cal	d. Btu	e. hp hr
f. ft lb_f g. (liter)(atm)		h. kwh		

Complete the units by pressing "c" for calories. Indicate the numerical value to be 100:

From units: Btu	To units: kilo-cal
Numerical value: 100	
100.00 Btu = 25.216 kilo-cal	

DIFFERENTIAL EQUATIONS SOLVER

QUICK TOUR

This section is intended to give you a very quick indication of the operation of the POLYMATH Differential Equation Solver Program.

DIFFERENTIAL EQUATION SOLVER

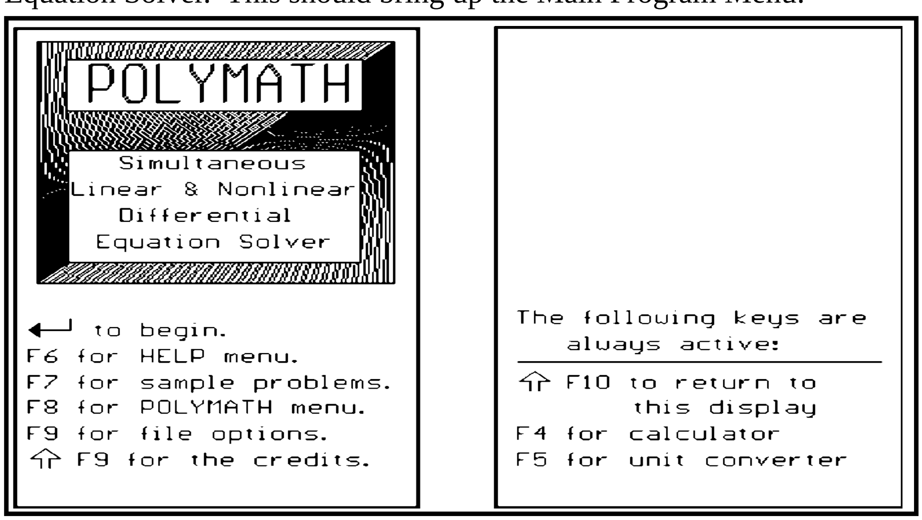
The program allows the numerical integration of up to twelve simultaneous nonlinear ordinary differential equations and explicit algebraic expressions. All equations are checked for syntax upon entry. Equations are easily modified. Initial values must be provided. Undefined variables are identified. The integration method and stepsize are automatically selected. Graphical output of problem variables is easily obtained with automatic scaling.

STARTING POLYMATH

To begin, please have POLYMATH loaded into your computer as detailed in Chapter 2. Here it is assumed that your computer is set to the hard disk subdirectory or floppy drive containing the POLYMATH package. At the prompt (assumed C: here), you should enter "polymath"

C > polymath

then press the Return (↵) key. The Program Selection Menu should then appear, and you should enter "1" on the keyboard to select the Differential Equation Solver. This should bring up the Main Program Menu:



Now that POLYMATH is loaded, please press the Return key. The Introductory Options Display for the Ordinary Differential Equation Solver should be on your screen as shown here:

```
                ORDINARY DIFFERENTIAL EQUATION SOLVER

     The purpose of this POLYMATH program is to solve systems of first-
order ordinary differential equations.  The system may contain up to 12
differential and auxiliary algebraic equations.  These equations may be
entered in one of the following forms:
                        d(x)/d(t)= an expression
or,                     d(x)= an expression
for a differential equation and the form:
                        x= an expression
for the supporting auxiliary equations.   In these equations 'x' is any
variable name 1 to 10 characters in length, and 't' is the independent
variable with the same rules.  Other information is contained in the
review material which can be obtained by pressing F6.

                         INTRODUCTION OPTIONS
 ←┘ to enter a problem.            F6 for helpful information.
F9 for library and file options    F7 to see the SAMPLE PROBLEMS MENU.
                        ⇧F10 for MAIN MENU.
```

SOLVING A SYSTEM OF DIFFERENTIAL EQUATIONS

Let us now enter and solve a system of three simultaneous differential equations:

$$d(A) / d(t) = k_A (A)$$
$$d(B) / d(t) = k_A (A) - k_B (B)$$
$$d(C) / d(t) = k_B (B)$$

In these equations, the parameter k_A is to be constant at a value of 1.0 and the parameter k_B is to be constant at the value of 2.0. The initial condition for dependent variable "A" is to be 1.0 when the initial value of the independent variable "t" is zero. The initial conditions for dependent variables "B" and "C" are both zero. The simultaneous solution for the three differential equations is desired for the independent variable "t" between zero and 3.0. Thus this problem will be entered by using the three differential equations as given above and using two expressions for the values for k_A and k_B given by:

$$k_A = 1.0; \qquad k_B = 2.0$$

Please press the Return key to enter a problem

```
     DIFF. EQN. :  0      AUX.  EQN. :  0     UNDEFINED VAR.  :  0

                       EQUATION OPTIONS
                     e.  Enter an equation
  F8  when done                       F6 for helpful information.
```

ENTERING THE EQUATIONS

The equations are entered into POLYMATH by first pressing the "e" option from the Equation Options Menu. The following display gives the first equation as it should be entered at the arrow. (Use the BackSpace key, to correct entry errors, and a Return key to indicate that the equation is to be entered). Please type the first equation and press (◄┘) to enter.

```
     DIFF. EQN. :  0      AUX.  EQN. :  0     UNDEFINED VAR.  :  0

 Please enter equation.     (◄┘ for EQUATION OPTIONS>)
 » d(A)/d(t)=-ka*A
```

The required format for the above differential equation is given by:

d(x)/d(t)=an expression

where the dependent variable name "x" and the independent variable name "t" must begin with an alphabetic character and can contain up to 10 alphabetic and numerical characters. In this Quick Tour problem, the dependent variables are A, B and C for the differential equations, and the independent variable is t. The constants k_A and k_B are considered to be variables which can be defined by auxiliary equations given by the format:

x=an expression

Thus in this problem, the variables for ka and kb will have constant values. Note that the subscript is not used in k_A and k_B as this is not allowed in POLYMATH.

Please continue to enter the equations until your display corresponds to the one in the next page. A useful feature here is that POLYMATH keeps track of the number of differential equations and auxiliary equations as they are entered. The listing of the names of the currently undefined variables is helpful in identifying input errors to the program. Syntax errors are checked prior to being accepted, and various messages are provided to help to identify input errors.

```
The equations:
      d(A)/d(t)=-ka*A                              **ENTER Mode**
      d(B)/d(t)=ka*A-kb*B
      d(C)/d(t)=kb*B
      ka=1
 →
      DIFF. EQN. :  3     AUX. EQN. :  1     UNDEFINED VAR. :  1
      Undefined variables:  kb

       Please enter the equation.      (↵   for EQUATIONS OPTIONS.)
      » kb=2
```

ALTERING THE EQUATIONS

After you have correctly entered the equations, please press ↵ with no equation at the arrow to go to the Equations Options display:

```
The equations:
      d(A)/d(t)=-ka*A                              **ENTER Mode**
      d(B)/d(t)=ka*A-kb*B
      d(C)/d(t)=kb*B
      ka=1
  →   kb=2

      DIFF. EQN.  :  3     AUX. EQN. :  2    UNDEFINED VAR.  :  0

                        EQUATION OPTIONS
              Use ↑  or ↓  to move the equation pointer
          e.  Enter an equation.        c.  Change an equation.
          u.  Duplicate an equation.    d.  Delete an equation.

          F8 when done.                 F6 for helpful information.
```

The Equation Options Menu allows you to make a number of alterations on the set of equations which has been entered. Please make sure that your equations all have been entered so that your display is identical to the one shown above. Remember to indicate the equation that needs altering by using the arrow keys on the numerical keypad before you select the desired Equation Option. Press F8 when you are ready to continue with the problem solution.

ENTERING THE BOUNDARY CONDITIONS

Once you have indicated that the equation has been entered properly, you will be asked to provide the initial values for all of the dependent variables used in the differential equations and for the independent variable.

Please enter the initial value. (↵ for 0.0)
t_0= »

Please indicate t_0 to be 0.0. Since zero is frequently used, this can be entered by just pressing ↵.

The next initial value request is for variable "A". Please enter it as shown below:

Please enter the initial value. (↵ for 0.0)
A_0= » 1

The initial values for B_0 and C_0 will be requested. Please enter these as zero by just pressing ↵ .

Next the final value for t, the independent variable, will be requested. Set this parameter at 3:

Please enter the initial value. (↵ for 0.0)
t_f=» 3

The final option during problem entry allows you to give a problem title:

Enter a title for this problem: (F8 or ↵ to omit.)
»

You can enter a title such as "Quick Tour Problem 1" or press F8 to omit a title. Press ⇑- ↵ for the Change Option display to make any needed corrections:

Quick Tour Problem 1

The equations:

d(A)/d(t)=-ka*A
d(B)/d(t)=ka*A-kb*B
d(C)/d(t)=kb*B
ka=1
kb=2

Initial values: t_o= 0.0, A_0=1. 0000, B_0=0.0, C_0=0.0
Final value: t_f = 3.0000

CHANGE OPTIONS

e. Enter/Change/Delete the equations.
t. Change the problem title. i. Change the initial values.
f. Change the final value.
F8 when done. F7 to print. F6 for help.

Press F8 when the problem is correctly entered.

The Problem Options Display for this Quick Tour problem should appear as follows:

Quick Tour Problem 1

The equations:

d(A)/d(t)=-ka*A
d(B)/d(t)=ka*A-kb*B
d(C)/d(t)=kb*B
ka=1
kb=2

Initial values: t_o= 0.0, A_0=1. 0000, B_0=0.0, C_0=0.0
Final value: t_f = 3.0000

PROBLEM OPTIONS

⇧ F7 to solve this problem. F7 to print the problem.
⇧↵ to alter the problem. F6 for helpful information
⇧ F8 for file and library options. ⇧F10 for the MAIN MENU.

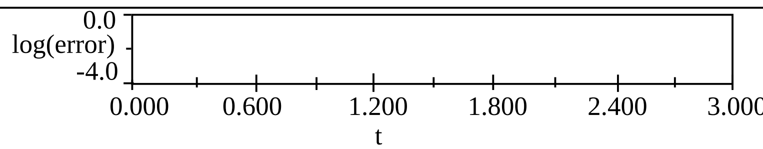
SOLVING THE PROBLEM

Lets solve this problem by pressing ⇑-F7. As the numerical integration is being done, you would see the log of the estimate of the local truncation error displayed as the independent variable proceeds from its initial condition to its final value, but it is very low in this problem. When the integration is complete, the Partial Results Display should appear as follows:

Quick Tour Problem 1

Partial results

Variable	Initial value	Max. value	Min.value	Final value
t	0.0	3.0000	0.0	0.0
A	1.0000	1.0000	0.0498	0.0498
B	0.0	0.2492	0.0	0.0473
C	0.0	0.9029	0.0	0.9029
ka	1.0000	1.0000	1.0000	1.0000
kb	2.0000	2.0000	2.0000	2.0000



F9 to display results. (g, t, d active)   F7 to print table.

⇑◄┘ to make changes. ⇑ F8 for new problem. F6 for help

The Partial Results display shown above provides a summary of the numerical simulation. To display or store the results you can press g (graphical display), t (tabular display) or d (storing the results on a DOS file). Press F9 and F9 again to see a more detailed Display Options Menu.

PLOTTING THE RESULTS

The Display Options Menu allows the results to be requested in either Tabular or Graphical form, or stored in a DOS file.

DISPLAY OPTIONS

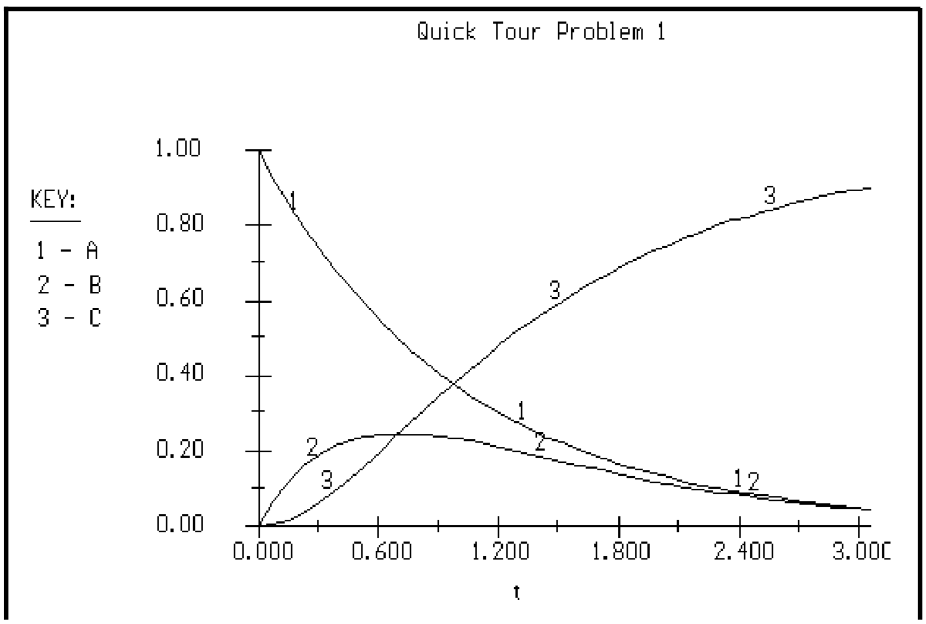
t. Results in TABULAR form   g. Results in GRAPHICAL form.
d. Output results to a DOS file   F7 to print Partial Results.
⇑ - F8 for new problem or library.   ⇑- ↵ to make changes.

Please enter a "g" for the graphical presentation. When asked to type in the variable for plotting, please enter the input indicated below at the arrow:

Type in the names of up to four (4) variables separated by commas (,)
and optionally one 'independent' variable preceded by a slash(/).
For example, myvar1, myvar2/timevar

» A, B, C _

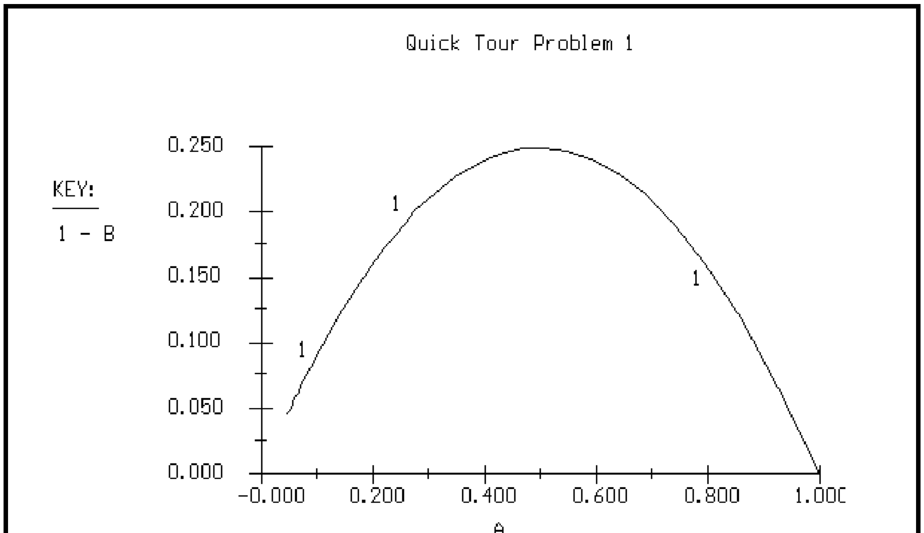
A Return key (↵) should generate the following graphical plot of the specified variables versus the independent variable which is t:



Suppose that you want to plot variable B versus variable A. Select the option "g" from the Display Options and enter B/A when asked for the variable names.

Type in the names of up to four (4) variables separated by commas (,)
and optionally one 'independent' variable preceded by a slash(/).
For example, myvar1, myvar2/timevar
» B/A

This will results in a scaled plot for only this variable:



DISPLAY OPTIONS

Results in: t. TABULAR form. g. GRAPHICAL form. d. DOS fiile.
p. Partial Results talbe F7 to print this graph.
⇑- F8 for new problem or library. ⇑- ↵ to make changes.

This concludes the Quick Tour problem using the Differential Equation Solver. If you wish to stop working on POLYMATH, please follow the exiting instructions in the next section.

EXITING OR RESTARTING POLYMATH

A ⇑ - F10 keypress will always stop the operation of POLYMATH and return you to the Program Selection Menu. THIS *ACTION WILL DELETE THE EXISTING PROBLEM.* The program can be exited or restarted from the Program Selection Menu.

INTEGRATION ALGORITHMS

The program alternates between three integration algorithms. It will first try to use the explicit Euler's method. If the estimated integration error is less then 0.01 times the error tolerance the integration will continue using this method. Otherwise the program will switch to the fourth order Runge-Kutta (RK) method. If the integration error too large when using RK method (greater than 0.1, relative error) the integration will be stopped and the user may select to restart it using the implicit Euler method.

Discussion of the Euler and Runge-Kutta methods can be found in: W. H. Press, B. P. Flannery, S. A. Teukolsky and W. T. Vetterling, *Numerical Recipes*, Cambridge University Press, Cambridge, 1986.

When using the RK method, the local truncation error of integration is estimated by comparing values of x(t) obtained using the third and fourth order RK methods. With the Euler methods, the integration error is estimated by repeating the same integration step and making two steps of h/2.

The integration error shown on the display during the time of the integration is the sum of the dependent variables. This error is displayed in the form of log (error) vs. time. If log (error) < -2, then the solution is correct at least up to 2 significant digits. If it is smaller than -3, then there are at least 3 correct digits. Error which are smaller than 10^{-4} are not shown.

The integration interval is divided at the beginning into 40 equal sections: hence, the initial stepsize is h = (integration interval)/40. The integration stepsize is changed automatically in order to get a solution accurate up to 3 significant digits using the Runge-Kutta method.

If the error is too large, the program halves and halves again the stepsize in order to reduce the error below the specified limit. The stepsize won't be reduced below the value h = (integration interval)/160. You can improve the accuracy of the results by separating the integration interval into smaller sections.

TROUBLE SHOOTING

If the correct solution cannot be obtained, the program will respond with either a specific error message, such as: "attempt to divide by zero", or a nonspecific message: "Integration error too large". Here are some of the steps that can be taken to correct the errors and find the solution.

1. SPECIFIC ERROR MESSAGE

A specific error message will most often result from functions which are undefined at certain points along the integration path. If the functions are undefined at t = 0 (the most common cause of difficulties), the problem can be often solved by starting the integration from $t = 0 + \varepsilon$, where ε is a very small number such as t =0.00000001.

The order in which the equations are calculated may be very important. The program first calculates the auxiliary equations in sequential order. It then evaluates the differential equations. If, for example, the auxiliary equations cannot be put in sequential (non-simultaneous) order, the message: "this program handles only sequential auxiliary equations" will appear and the execution will be stopped. The auxiliary equations can be often rearranged so that a simultaneous solution won't be required.

2. NON SPECIFIC ERROR MESSAGE: "TOO LARGE INTEGRATION ERROR"

There can be several reasons for obtaining such a message. In most cases the final value specified is too high, resulting in too large error even when using the smallest integration stepsize. In such a case, dividing the integration interval into smaller sections will usually solve the problem.

Sometimes the derivatives can approach infinity for a certain value of the independent variable. In such case the upper limit of the independent variable will have to be changed, so that the boundaries of definition of the functions are not approached too closely.

An additional cause for a large an integration error is the existence of a stiff system of equations. In such a system the response of some of the variables is much faster than that of the rest of them. In such case resolving the problem by using implicit Euler method option may be required for an accurate solution.

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ALGEBRAIC EQUATIONS SOLVER

QUICK TOUR

This section is intended to give a very brief discussion of the operation of the POLYMATH Algebraic Equation Solver.

ALGEBRAIC EQUATION SOLVER

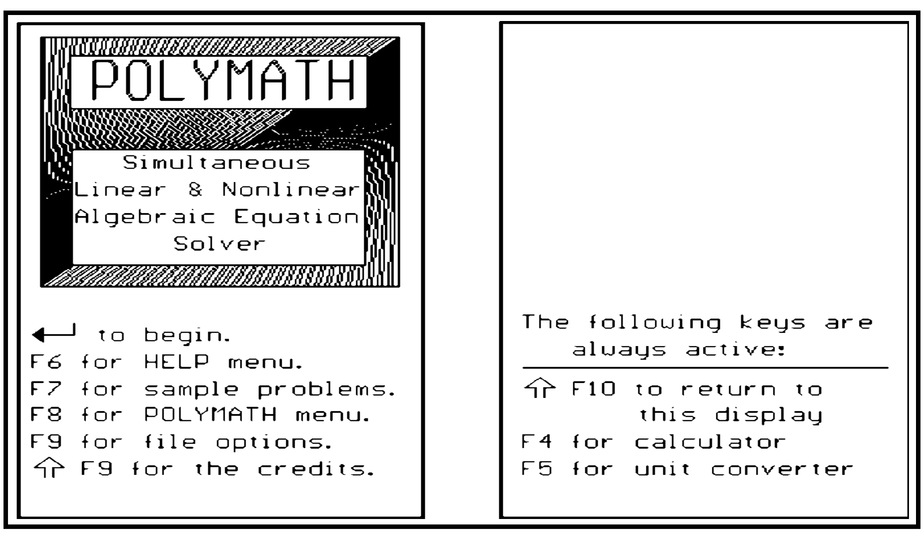
The user can solve up to a combination of 12 simultaneous equations and explicit algebraic expressions. All equations are checked for correct syntax and other errors upon entry. Equations can be easily be modified, added or deleted. Multiple roots are given for a single equation. A separate simple linear equation solver handles up to 6 simultaneous equations.

STARTING POLYMATH

To begin, please have POLYMATH loaded into your computer as detailed in Chapter 2. Here it is assumed that your computer is set to the hard disk subdirectory or floppy drive containing the POLYMATH package. At the prompt (assumed C: here), you should enter "polymath"

C>polymath

then press the Return (↵) key. The Program Selection Menu should then appear, and you should enter "b" on the keyboard to select the Algebraic Equation Solver. This should bring up the Main Program Menu as given below:



Now that POLYMATH is loaded, please press the Return (↵) key. The Program Menu Display should be on your screen as shown below:

```
                    PROGRAM  MENU

              Press a single letter to solve:

             a.  A system of linear equations
             b.  A system of nonlinear equations

  F6 for helpful information       ⇑ - F10 for the MAIN MENU.
```

SOLVING A SYSTEM OF LINEAR EQUATIONS

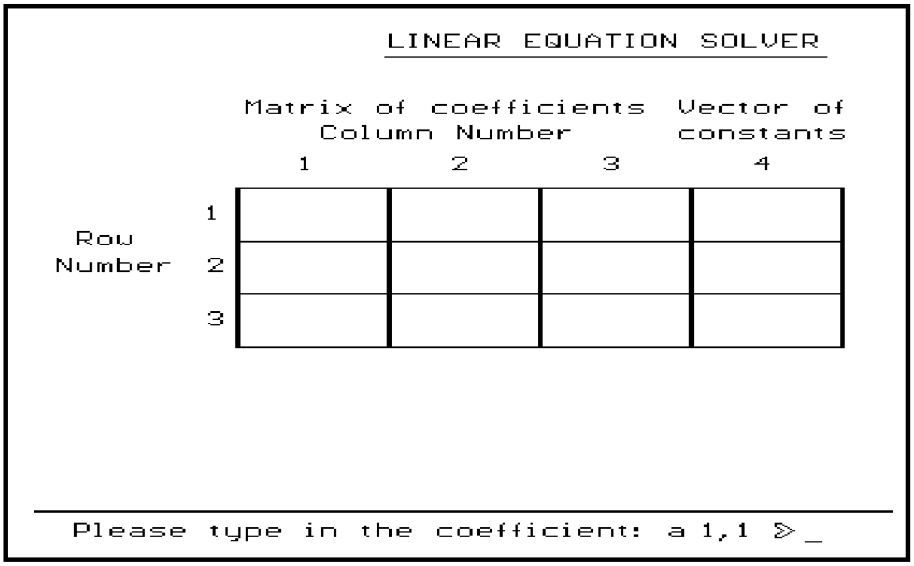
Let us first solve a system of linear equations. Please enter an "a" from keyboard while viewing the Problem Menu Display. This should bring you to the Introduction Options Display:

```
                 LINEAR EQUATION SOLVER

        The purpose of this program is to help you solve
    systems of linear equations.  The system may contain
    up to 6 linear equations.  The number of unknowns must
     be the same as the number of equations.
     You will be asked to enter the coefficients for
     each of the unknowns, one equation at a time.

                 INTRODUCTION OPTIONS
              ↵ to enter a problem
          F7   to see the SAMPLE  PROBLEMS  MENU
  F6  for helpful information      ⇑- F10  for the MAIN  MENU
```

Please press the Enter (↵) key to enter a problem.

```
  Enter the number of equations in your system  »
  ( ↵  for the MAIN MENU.)
```

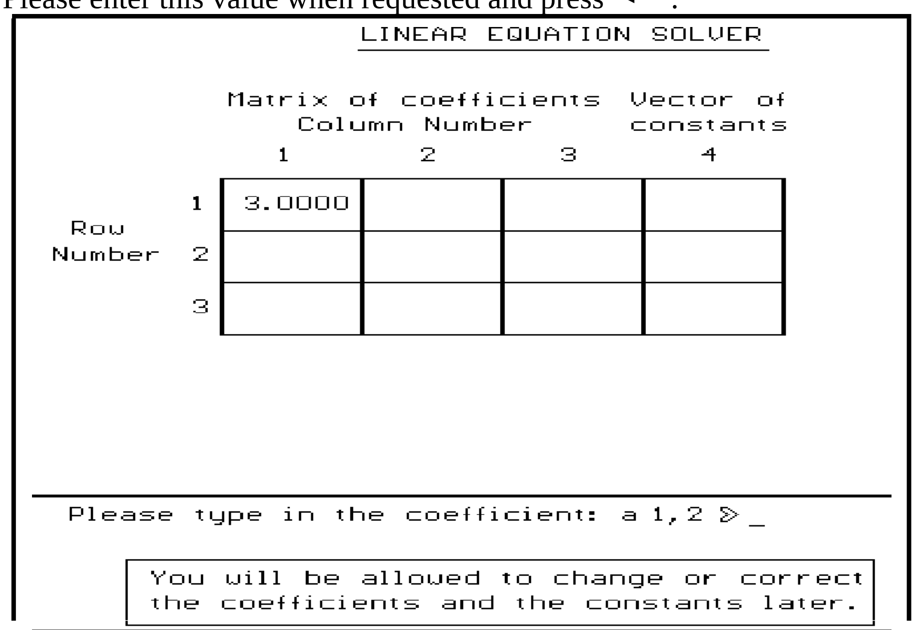
This problem will have three equations, so please enter "3" by using the numerical keys on the keyboard and press Enter (↵). The Backspace (←) key will erase one character at a time.



We will enter the following three equations in three unknowns:

$$\begin{array}{rrrcr} 3x & -y & +z & = & 2 \\ x & +2y & -z & = & -1 \\ 2x & +2y & +z & = & 4 \end{array}$$

The POLYMATH coefficient $a_{1,1}$ corresponds to "3" in the above equations. Please enter this value when requested and press ↵.



Coefficient $a_{1,2}$ should be given a value of "-1". Then please enter all of the other coefficients as given below. There will be an opportunity to correct any input errors at a later time.

LINEAR EQUATION SOLVER

Matrix of coefficients — Column Number; Vector of constants

Row Number	1	2	3	4
1	3.0000	-1.0000	1.0000	2.0000
2	1.0000	2.0000	-1.0000	-1.0000
3	2.0000	2.0000	1.0000	4.0000

Please enter a title for this problem

> _

A title such as "Quick Tour Problem 1" can be entered or you can press F8 to omit the title. The Problem Options box should then present several options:

PROBLEM OPTIONS

⇧ F7 to solve this problem. F7 to print the problem.
⇧↵ to alter the problem. F6 for helpful information
⇧ F8 for file and library options. ⇧F10 for the MAIN MENU.

To correct any entry errors, please press ⇑↵ to alter the problem.

To change a coefficient type the row and column number.
Row number >
F8 when done. F6 for helpful information.

This problem may be solved by pressing ⇑-F7 from the Problem Options Menu. Your solution should be as shown on the next page:

Quick Tour Problem 1

Solution

Variable	Value
1	0.0769
2	0.6923
3	2.4615

Please press ⇑-F10 to return to the Program Selection Menu and enter 'b" to work on a nonlinear equation example.

SOLVING ONE NONLINEAR EQUATION

The next problem to be solved is a nonlinear equation. Please press ⇑-F10 to return to the Main Program Menu. If you are just starting up POLYMATH, then follow the instructions on page 6-1 and the top of page 6-2. Enter a "b" from the keyboard when viewing the Program Menu box to solve a nonlinear equation.

You should now be viewing the Introduction Options Display for the Nonlinear Equation Solver. Press the Return (↵) key to see the screen below:

NONLINEAR EQUATION SOLVER

The purpose of this program is to help you to solve systems of nonlinear equations. The system may contain up to 12 nonlinear simultaneous and auxiliary equations. The equations should be entered in the following forms:

f(x)= an expression

for nonlinear functions which must be solved simultaneously, and:

x = an expression

for supporting auxiliary equations which are solved sequentially. In both of these forms, 'x' is any variable name 1 to 10 characters in length which must begin with an alphabetic character.

INTRODUCTION OPTIONS

↵ to enter a problem.

F7 to see the SAMPLE PROBLEM MENU.

F6 for helpful information. ⇧F10 for the MAIN MENU.

Please press the Return (↵) key again to enter a problem.

```
The equations:


 SIMUL. EQN.» 0    AUX. EQN. » 0  UNDEFINED VAR.» 0

                 EQUATION OPTIONS
              e.  Enter an equation
 F8  when done                  F6  for helpful information
```

The equation to be solved is a nonlinear equation:

$$x^2 -5x + 6 = 0$$

The solution is to be obtained over the range of x between 1 and 4. This equation is entered into POLYMATH by pressing the "e" option from the Equation Option Display. The following display gives the equation as it should be entered at the arrow: (use the ← key to erase entered characters).

```
The equations:                              ** ENTER MODE **


 SIMUL. EQN. »0    AUX. EQN.» 0  UNDEFINED VAR. »0
 Please enter the equation. ( ↵  for EQUATIONS OPTIONS.)
 » f(x)= x*x-5*x+6
```

The format for the above equation for f(x) is that the left side of the equation will be equal to zero when the solution has been obtained. The variable which is to be determined is set as an argument within the parentheses for the function f( ).

Thus in this case, the variable is x and the function to be solved as being zero is x^2-5x+6. Also note that in POLYMATH one way of entering x^2 is x*x. An alternative entry is x**2.

After you have correctly typed the equation at the arrow, please press ↵ to enter it. Then again press ↵ to go to the Equation Options Display:

```
The Equations:
  →f(x)= x*x-5*x+6

  SIMUL. EQN.≫1     AUX. EQN.≫0    UNDEFINED VAR.≫ 0

                    EQUATION OPTIONS

      e. Enter an equation.          c. Change an equation.
      u. Duplicate an equation.      d. Delete an equation.
   F8 when done.                      F6 for helpful information.
```

The Equation Options Menu indicates which options are now available for you to carry out a number of tasks. When the equation has been entered correctly, please press F8 from the above display.

Once you have indicated that the equation has been entered properly, you will be asked to provide the interval over which you wish to find solutions for the equation. This interval is only requested during the solution of a single nonlinear equation.

```
Please enter the limiting values of x.
xmin= ≫
```

Please indicate the x_{min} to be 1 and press (↵); then indicate x_{max} to be 4.

```
Please enter the limiting values of x.
xmin=       1   ok
xmax= ≫
```

Then press enter (↵). The entire problem is then displayed:

```
The equations:
   f(x)=x*x-5*x+6
Search range:  xmin=1.0000,  xmax=4.0000

  Enter a title for this problem:          (F8 or ↵ to omit)
  ≫
```

You can enter a title such as "Quick Tour Problem 2" or press F8 to omit the title. The Problem Options Menu box then allows you a number of options:

PROBLEM OPTIONS

⇑-F7 to solve this problem.

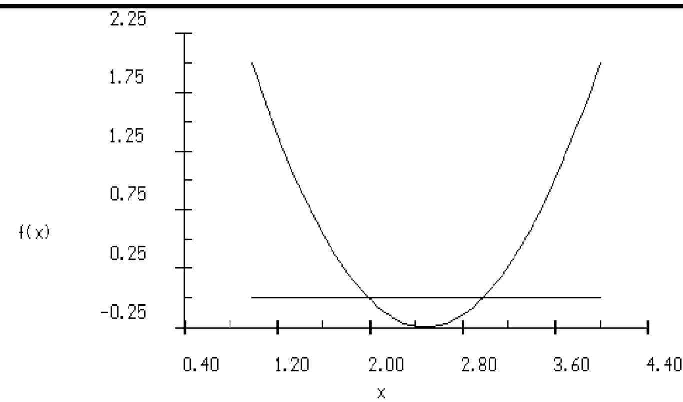
⇑ ↵ to alter the problem — ⇑ -F8 new problem or library

⇑- F10 for the MAIN MENU — F6 for helpful information

Lets solve this problem by pressing ⇑ F7. the solution requires a number of calculations, and while this is occurring you will see the message:

Solving....please wait.

For this single equation, the solution is presented graphically over the search range which you indicated. The solution is where the function f(x) is equal to zero. POLYMATH has the ability to determine multiple solutions to a single equation problem.



Solution 1 is:

x = 2.0000

f(x) = $-0.973*10^{-6}$

↵ for root number 2 — F7 to print this solution.

Press enter (↵) for the second solution.

Solution 2 is:

x = 3.0000

f(x) = $0.430*10^{-6}$

↵ for other options — F7 to print this solution.

Any keypress will return you to the Problem Options Display.

SOLVING A SYSTEM OF NONLINEAR EQUATIONS

Next, you will solve two nonlinear equations with two unknowns. To enter this new set of equation press ⇑-F8 for a new problem, then press ↵ to enter a new problem and finally select "b" for a system of nonlinear equations.

The equations that will be solved are:

$$k\,C_{A1}^2 = \frac{v\,(C_{A0} - C_{A1})}{V} \quad \text{and} \quad k\,C_{A2}^2 = \frac{v\,(C_{A1} - C_{A2})}{V}$$

where k = 0.075; v = 30; C_{A0} = 1.6 and C_{A2}/C_{A0} = 0.2 .
Thus there are two unknowns: C_{A1} and V.

To solve this system the equations must be rewritten in the form f(x) = (an expression that is to have the value of zero at the solution). An appropriate form for these equations is:

$$f\,(C_{A1}) = kC_{A1}^2 - \frac{v\,(C_{A0} - C_{A1})}{V}$$

and

$$f\,(V) = kC_{A2}^2 - \frac{v\,(C_{A1} - C_{A2})}{V}$$

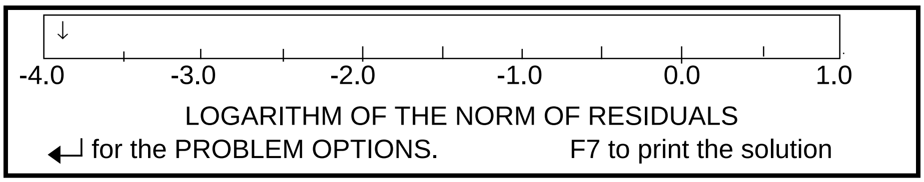
These equations can be entered into POLYMATH as shown below. Note that each of the problem unknowns (C_{A1} and V) should appear once and only once inside the brackets in the left of the equal sign. The variable need not be in that particular equation. POLYMATH just needs to know the variable names that you are using.

```
                    Quick Tour Problem 3
The equations:
        f(Ca1)=k*Ca1*Ca1-v*(Ca0-Ca1)/V
        f(V)=k*Ca2*Ca2-v*(Ca1-Ca2)/V
        k=0.075
        Ca0=1.6
        v=30
        Ca2=Ca0*0.2
Initial values:   Ca1_0=1.0000,   V_0=300.00
```

Note that the numerical values of the constants are specified using auxiliary equations. Also since POLYMATH won't accept subscripts, some of the variable names have been changed.

If there are several equations with several unknowns, one initial estimate has to be specified for each unknown. While the solution method used is very robust, it often will not be able to find the solution if unreasonable initial estimated are entered. In this example, physical considerations dictate that C_{A1} must be smaller than C_{A0} and bigger than C_{A2}. So the initial estimate C_{A1}=1.0 was selected. As for V, any positive value up to about V=5000 can be a reasonable estimate. Try to use V_0=300 for example.

After entering the equations, initial values and title press ⇑-F7 to solve the problem. The solution process will start and its progress will be indicated on the screen by a needle moving along a ruler scale as shown below:



The arrow indicates how far from zero the function values are at a particular stage of the solution. For example, when the logarithm of the norm of residuals is 1.0, the square root of the sum of squares of the function values is 10.0. When the arrow stands at the value of -4.0, the error is at or less than 10^{-4}. At this point the final solution is displayed:

Quick Tour Problem 3

Solution

Variable	Value
Ca1	0.6020
V	1101.5
k	0.0750
Ca0	1.6000
v	30.000
Ca2	0.3200

Any keypress will return you to the Problem Options Display.

EXITING OR RESTARTING POLYMATH

A ⇑-F10 keypress will always stop the operation of POLYMATH and Return you to the Program Selection Menu. *THIS ACTION WILL DELETE THE EXISTING PROBLEM.* The program can be exited or restarted from the Program Selection Menu.

METHOD OF SOLUTION

For systems that contain more than one equation, the program uses the continuation method*. The original system of equations $\mathbf{f}(\mathbf{x})=0$ is transformed into a sequence of problems:

$$\mathbf{G}(\mathbf{x}, \theta_j) = \mathbf{f}(\mathbf{x}_j) - \theta_j \mathbf{Y}_0 = 0 \qquad j = 1, 2,.....,19$$

where $\mathbf{Y}_0 = \mathbf{f}(\mathbf{X}_0)$ is the value of the vector of residuals at the starting point; j is the sequence number; and θ_1, θ_2, ... are constants with the values $\theta_1 = 0.96$, $\theta_{j+1} = \theta_j - 0.04$, and $\theta_{25} = 0$.

For $\theta = 0$, the roots of the modified equations are identical to those of the original system. Each problem in the sequence is solved by applying a single iteration of the Newton-Raphson method in which the solution of the previous problem is used as initial estimate for the current one. In the final stage, when $\theta = 0$, five Newton-Raphson iterations are made. This method has proven to be quite stable and reliable even when started from an initial point far from the solution.

During the solution process, the logarithm of the Euclidean norm of the function residuals will appear. This norm is defined as

$$||\mathbf{f}(\mathbf{x})|| = \left[\sum_i \mathbf{f}_i(\mathbf{x})^2\right]^{1/2}$$

If, for example, $\log ||\mathbf{f}(\mathbf{x})|| < -3$, then the largest component of the vector $\mathbf{f}(\mathbf{x})$ is below 10^{-3}. Norm values below 10^{-4} are not shown.

TROUBLE SHOOTING

Here are some of the most common difficulties that arise when using this program, together with the steps you should take to avoid them.

1. THE SOLUTION PROCESS DOES NOT START.

(nothing is plotted on the screen before an error message appears)

* For more detailed explanation of this method, see SHACHAM, M., *Computers and Chemical Engineering*, Vol. 2, pp. 228-229, 1980.

In this case, either the equations are incorrect, or some of the functions are undefined at the starting point. For example, if $x1_0 = 0$ and log(x1) is to be evaluated, then an error message will be generated.

The order in which functions and expressions are calculated should be kept in mind too. The program first calculates the auxiliary equations in sequential order and then it calculates the functions. If the auxiliary equations cannot be ordered sequentially, an error message will indicate that the solution accuracy is unpredictable.

2. THERE IS NO CONVERGENCE.

(The Euclidean norm is larger than 10^{-3} when all the iterations are done, or the error message "Unable to solve this problem" appears after solution has started.) There may be three different reasons for nonconvergence:

a. The initial estimate is too far from the solution.

If the norm shows a tendency to decrease during the solution but does not decrease enough, use the current solution values as new initial estimates. If no tendency to converge is seen (the norm oscillates or increases), you should try to find a better initial estimate.

b. Poor scaling of the equations

A difference of several orders of magnitude between the residuals of the different equations at the starting point may prevent convergence.

For example, one of the equations may represent a mole fraction balance where the residual seldom exceeds 1 in absolute value, and the other equation may be an enthalpy balance with residuals values in the millions. In cases such as this, you should divide the equations by appropriate constants in order to make the residuals the same order of magnitude.

c. The system has no solution

If a system with proper scaling does not converge from several starting points, it probably has no solution. This can be due to errors in the problem setup. Check the basic equation set, its corresponding POLYMATH equations, and the numerical values and units of the constants.

REGRESSION

QUICK TOUR

This chapter is intended to give a very brief overview of the operation of the POLYMATH Polynomial, Multiple Linear and Nonlinear Regression program.

REGRESSION PROGRAM

This program allows you to input numerical data into up to 30 columns, with up to 100 data points in each column. The data can be manipulated by defining expressions containing the names of previously defined columns. Relationships between different variables (columns of data) can be found using polynomial, multiple linear and nonlinear regression as well as cubic spline interpolation. Fitted curves can be interpolated, differentiated and integrated. Graphical output of the fitted curves and expressions is presented, and a statistical analysis of the parameters found during the regressions is given.

STARTING POLYMATH

To begin, please have POLYMATH loaded into your computer as detailed in Chapter 2. Here it is assumed that your computer is set to the hard disk subdirectory or floppy drive containing the POLYMATH package. At the prompt (assumed C: here), you should enter "polymath"

```
C > polymath
```

then press the Enter (↵) key. The Program Selection Menu should then appear, and you should enter "3" on the keyboard to select the Polynomial Curve Fitting Program. This should bring up the Main Program Menu as given in the next page.

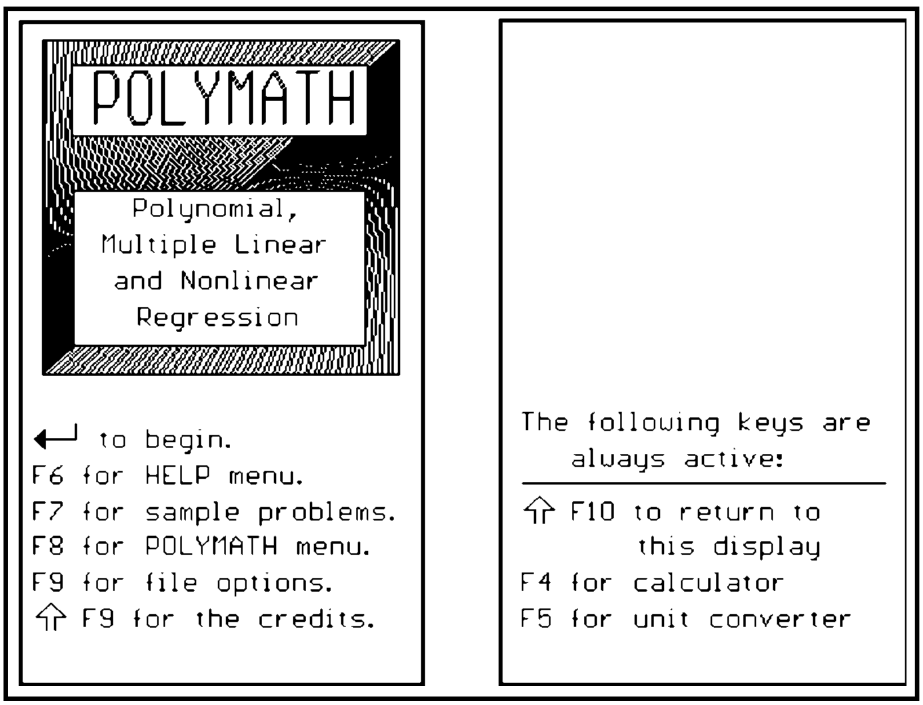
In order to save time in entering data points during this quick tour, we will use sample problems which have been stored in POLYMATH. Press F7 to access the Sample Problems Menu from the Main Program Menu.

QUICK TOUR PROBLEM 1

Let us consider a fairly typical application of the Regression Program in which some data are available. When these data are fitted to a polynomial within POLYMATH, the polynomial expression has the form:

$$P(x) = a_0 + a_1x + a_2x^2 + ... + a_nx^n$$

where y is the dependent variable, x is the independent variable, and the parameters are a_0 ...a_n. Variable "n" here represents the degree of the polynomial. In POLYMATH, the maximum degree which is shown is 5. The above polynomial expression gives a relationship between the dependent variable and the independent variable which is obtained by determining the parameters according to a least squares objective function. Data points are usually available which give x and y values from which the parameters a_0... a_n can be determined.



RECALLING SAMPLE PROBLEM 3

After pressing F7 at the Main Program Menu, the Sample Problems Menu should appear on your screen as shown on the next page.. The sample problem to be discussed should be retrieved by pressing "3" on the keyboard. This will result in the Problem Options Display which includes 10 data points of x and y as shown on the next page.

SAMPLE PROBLEMS MENU

1 One independent variable fitted to an equation of the form

$Y = a_0 X^{a_1}$ linearized to:

$\ln(Y) = a_0 + a_1 X$

---

2 One independent variable fitted to a nonlinear equation:

$Y = 10^{\{ a_0 + a_1/(X+z) \}}$

---

3 One independent variable fitted to a polynomial.

---

4 Two independent variables fitted to a linear equation:

$Y = a_0 + a_1 X_1 + a_2 X_2$

---

5 Two independent variables fitted to an equation of the form:

$Y = a_0 X_1^{a_1} X_2^{a_2}$ linearized to:

$\ln(Y) = a_0 + a_1 * \ln(x_1) + a_2 * \ln(x_2)$

---

6 Three independent variables fitted to an equation of the form:

$Y = 1000 [x_1/(a_0 + a_1 x_1 + a_2 x_2 + a_3 x_3)]$

linearized to:

$1000/y = a_0 + (a_1 + a_2 x_2 + a_3 x_3) / x_1$

F8 to return

Sample Problem 3

Name	X	Y					
1	0.23	5.64					
2	1.01	7.83					
3	2.29	17.04					
4	2.87	21.38					
5	4.15	24.56					
6	5.36	16.21					
7	5.51	14.57					
8	6.36	0.78					
9	6.84	-7.64					
10	7	-12.52					
11							
12							
13							
14							
15							
16							
17							
18							

PROBLEM OPTIONS

↵ to edit current box. ↑,↓,→,←, PgUp, PgDn, Home, End to move pointer.
⇧ ↵ for row/column options. T. to change title.
⇧ F7 to fit a curve or do regression. F6 for helpful information.
⇧ F8 for file and library options. F7 to print problem.

FITTING A POLYNOMIAL

The Problem Options Menu includes problem editing, library, printing, help and solution options. To fit a polynomial to the data of Y versus X you should select the: "⥣ F7 to fit a curve or do regression" option. After pressing ⥣ F7 the following "Solution Options" menu appears:

SOLUTION OPTIONS

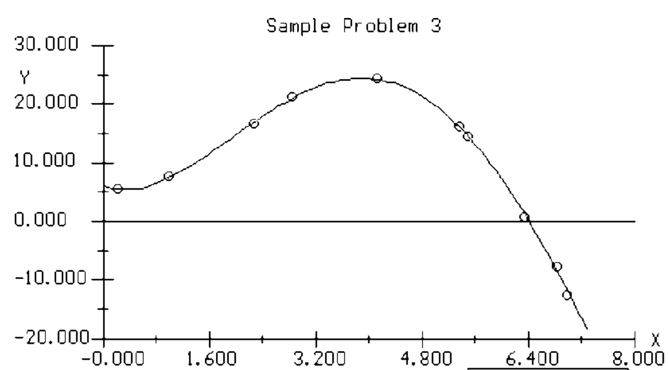
l. Do Linear regression.	L. Linear regression without free parameter.
p. Fit a polynomial.	P. Polynomial passing through origin.
s. Fit a cubic spline.	R. Do nonlinear regression.

⥣↵ or F8 for problem options

After pressing "p" (lower case), you should be asked for the name of the independent variable's column, as shown below:

Enter independent column name (↵ to cancel):
≫_

You should enter a capital "X" (upper case) as name of the independent variable and press ↵. The same question regarding the dependent variable will be presented. Please enter a capital "Y" (upper case) at the arrow. The following display should appear:

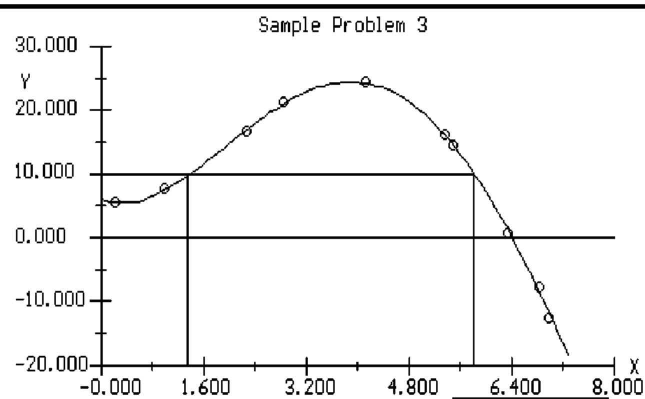


Deg.	1	2	3	4	5
a0	18.2007	-2.41992	3.68736	6.31569	6.21607
a1	-2.2623	15.8712	4.23908	-4.23011	-3.78885
a2		-2.41526	1.63518	6.95477	6.52291
a3			-0.368083	-1.49302	-1.33232
a4				0.0760754	0.0508872
a5					0.00140166
var.	135.88	12.263	1.49732	0.257127	0.319264

DISPLAY OPTIONS

s. Save results to a file — 1, 2, 3, 4, 5 to choose a polynomial
x. Y value for specific X — y. X value for specific Y
i. Integrate polynomial — d. differentiate polynomial
F9 for statistical analysis. F7 to edit graph F8 for problem options

On this display the coefficients of the polynomial P(x), up to the fifth order are shown together with the value of the variance. One of the polynomials is highlighted by drawing a box around it. This is the lowest order polynomial, such that higher order polynomial does not give significantly better fit. The same polynomial is also plotted versus the experimental data. Other polynomials can be highlighted and plotted by pressing a number between 1 and 5. There are many additional calculations and other operations that can be carried out using the selected polynomial. Let us find the value of X for Y = 10. To do that you should press "y" and enter after the prompt regarding the value of Y: "10". The following display results:



Deg.	1	2	3	4	5
a0	18.2007	-2.41992	3.68736	6.31569	6.21607
a1	-2.2623	15.8712	4.23908	-4.23011	-3.78885
a2		-2.41526	1.63518	6.95477	6.52291
a3			-0.368083	-1.49302	-1.33232
a4				0.0760754	0.0508872
a5					0.00140166
var.	135.88	12.263	1.49732	0.257127	0.319264

DISPLAY OPTIONS

Y = 10

X = 1.36962, 5.83496

Press any key to continue.

F9 for statistical analysis F7 to edit graph F8 for problem options

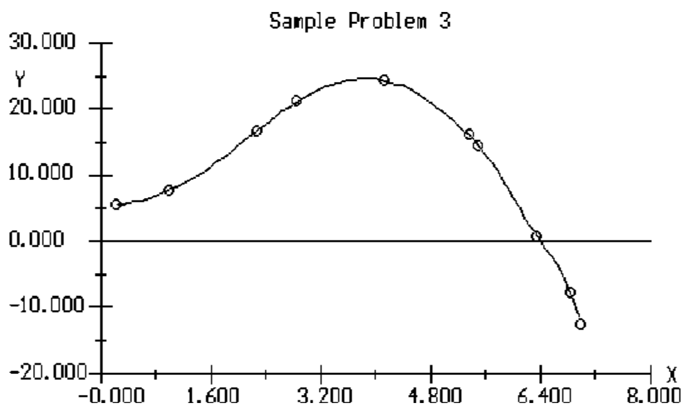
The resultant X values are shown both graphically and numerically. For Y = 10 there are two X values, X = 1.36962 and X = 5.83496.

FITTING A CUBIC SPLINE

We will now fit a cubic spline to these data of Sample Problem 3. Please press F8 to return to the Solutions Options Menu as shown on the next page, and press ⇑ F7 to indicate the next regression.

SOLUTION OPTIONS	
l. Do linear regression.	L. Linear regression without free parameter.
p. Fit a polynomial.	P. Polynomial passing through origin.
s. Fit a cubic spline.	R. Do nonlinear regression.
	⇑↵ or F8 for problem options

Enter "s" (lower case) for a cubic spline followed by "X" and then "Y". The following display should present the results:



DISPLAY OPTIONS		
x. Y value for specific X		y. X value for specific Y
i. Integrate spline.		d. differentiate spline.
F6 for HELP	F7 to edit graph	⇑↵ or F8 for problem options

EVALUATION OF AN INTEGRAL WITH THE CUBIC SPLINE

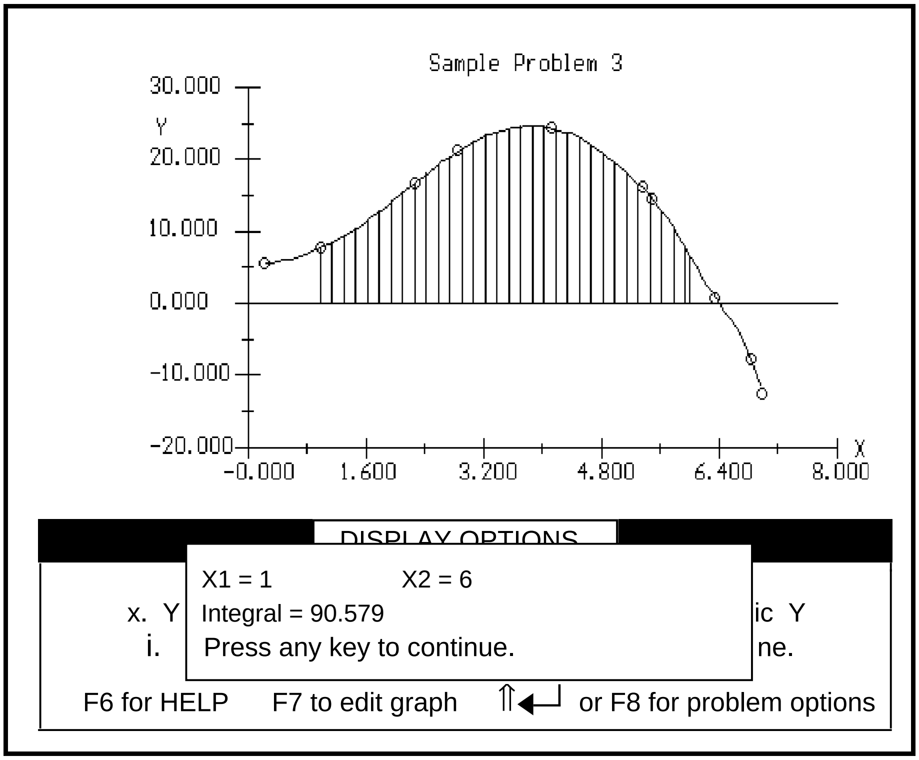
Please take options "i" and request the initial value for the integration to be "1" at the arrow:

```
Enter first value for X : » 1_
```

Press ↵ and then enter "6" at the arrow for the find value of the integration.

```
Enter second value for X : » 6_
```

Press ↵ to have the resulting integration shown on the next display with both graphical and numerical results:



MULTIPLE LINEAR REGRESSION

It will often be useful to fit a linear function of the form:

$$y(\underline{x}) = a_0 + a_1 x_1 + a_2 x_2 + \ldots + a_n x_n$$

where x_1, x_2, ..., x_n are n independent variables and y is the dependent variable, to a set of N tabulated values of $x_{1,i}$, $x_{2,i}$, ... and y ($\underline{x}_i$). We will examine this option using Sample Problem 4.

RECALLING SAMPLE PROBLEM 4

First exit to the main title page by pressing ⇑ F10. Press F7 to access the Sample Problems Menu, and select problem number 4 by pressing "4". (The problem display is shown on the next page).

Sample Problem 4

Name	X1	X2	Y				
1	78	1	1.5				
2	113.5	3.2	6				
3	130	4.8	10				
4	154	8.4	20				
5	169	12	30				
6	187	18.5	50				
7	206	27.5	80				
8	214	32	100				
9							
10							
11							
12							
13							
14							
15							
16							
17							
18							

PROBLEM OPTIONS

↵ to edit current box. ↑,↓,→,←, PgUp, PgDn, Home, End to move pointer.
⇧ ↵ for row/column options. T. to change title.
⇧F7 to fit a curve or do regression. F6 for helpful information.
⇧F8 for file and library options. F7 to print problem.

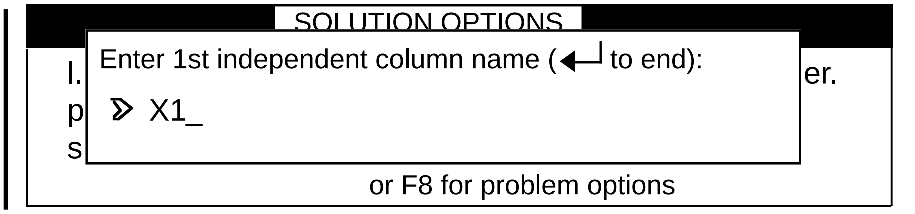
SOLVING SAMPLE PROBLEM 4

After you press ⇑ F7 to "do regression" the following Solution Options Menu should appear.

SOLUTION OPTIONS

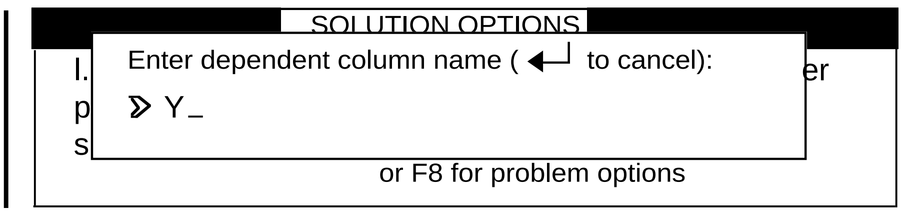
l. Do linear regression. L. Linear regression without free parameter.
p. Fit a polynomial. P. Polynomial passing through origin.
s. Fit a cubic spline. R. Do nonlinear regression.
⇑↵ or F8 for problem options

This time press "l" (lower case letter "l") to do "linear regression". You will be prompted for the first independent variable (column) name as shown on the next page.

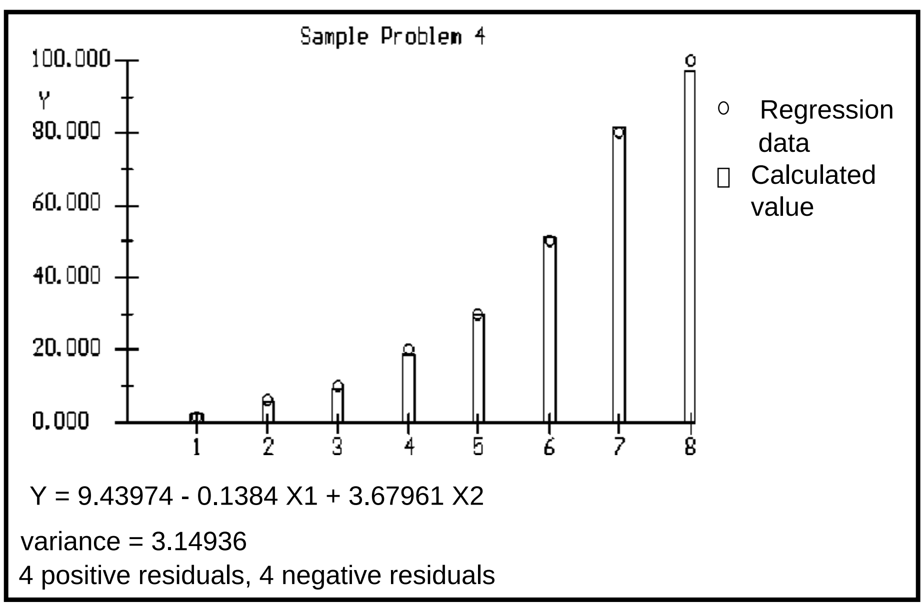


Please type in "X1" at the arrow and press ↵. You will be prompted for the 2nd independent variable. Enter "X2" as the second independent variable name and press ↵ once again. A prompt for the 3rd independent variable will appear. You should press ↵ here without typing in anything else, since there are no additional independent variables.

At the prompt for the dependent variable (column) name shown below



you should type "Y" and press ↵. Once the calculations are completed, the linear regression (or correlation) is presented in numerical and graphical form.



DISPLAY OPTIONS	
s. To save results on a file.	
F7 to edit the graph.	
F9 for statistical analysis	F8 for problem options.

Please note that the above correlation the equation for variable "Y" has the form of the linear expression: $Y = a_0 + a_1X_1 + a_2X_2$ where a_0 = 9.43974, a_1 = -0.1384 and a_2 = 3.67961. The plot of the results of the regression data versus the calculated value, the numerical value of the variance and the number of the positive and negative residuals give an indication regarding the validity of the assumption that Y can be represented as linear function of X1 and X2. The results in this case indicate a good fit between the observed data and the correlation function.

TRANSFORMATION OF VARIABLES

A nonlinear correlation equation can be often brought into a linear form by a transformation of the data. For example, the nonlinear equation:

$$Y = a_0 X_1^{a_1} X_2^{a_2}$$

can be linearized by taking logarithm of both sides of the equation:

$$\ln Y = \ln a_0 + a_1 \ln X_1 + a_2 \ln X_2.$$

To demonstrate this option please recall Sample Problem 5. To do this, please press ⇑ F10 to get to the title screen, F7 to access the Sample Problems Menu and select Sample Problem number 5. This should result in the Problem Option Display shown on the next page.

In this display X1, X2 and Y represent the original data, the variables (columns) lnX1, lnX2 and lnY represent the transformed data. You can see the definition of ln X1 , for example, by moving the cursor (the highlighted box), which located in row number 1 of the first column, into the box containing "lnX1" (using the arrow keys) and press ↵ . The following window is brought up:

```
Enter column definition:
» lnX1=ln(X1)_
```

Note that the expression in the right hand side of the column definition equation must be a valid algebraic expression, and any function arguments used in the expression should be enclosed within parentheses.

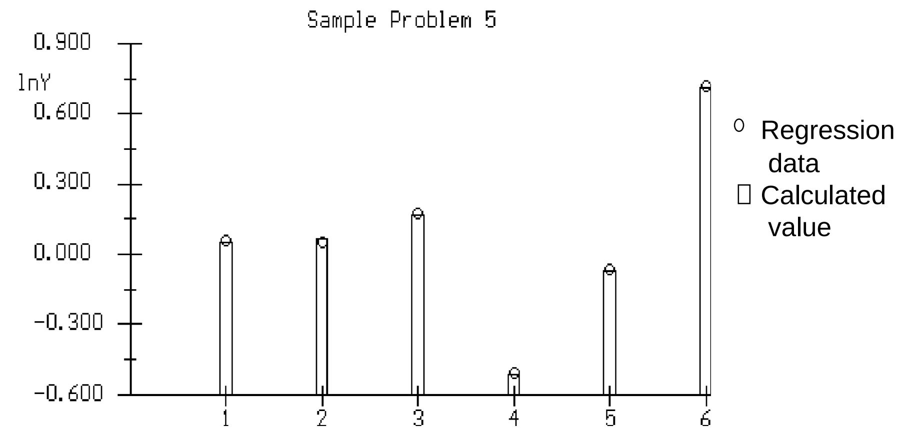
Sample Problem 5

Name	X1	X2	Y	lnX1	lnX2	lnY	
1	0.475	0.475	1.063	-0.74444	-0.74444	0.0610951	
2	0.465	0.465	1.05	-0.765718	-0.765718	0.0487902	
3	0.421	0.42	1.2	-0.865122	-0.867501	0.182322	
4	0.32	0.52	0.6	-1.13943	-0.653926	-0.510826	
5	0.54	0.54	0.9375	-0.616186	-0.616186	-0.06454	
6	0.57	0.37	2.063	-0.562119	-0.994252	0.724161	
7							
8							
9							
10							
11							
12							
13							
14							
15							
16							
17							
18							

PROBLEM OPTIONS

↵ to edit current box. ↑,↓,→,←, PgUp, PgDn, Home, End to move pointer.
⇧ ↵ for row/column options. T. to change title.
⇧F7 to fit a curve or do regression. F6 for helpful information.
⇧F8 for file and library options. F7 to print problem.

Since we do not want to change this expression, please press ↵ to close the window. Now press ⇑ F7 to do regression, then "l" to do linear regression. Type in "lnX1" as the name of the first independent variable, "lnX2" as the name of the second independent variable and "lnY" as the name of the dependent variable. The results should be displayed as shown on the next page:



ln Y = -0.666796 + 0.986683 ln X1 - 1.95438 ln X2

variance = 0.000266993
5 positive residuals, 1 negative residual

Please note that the results indicate that the equation for variable "Y" can be written as: $Y = a_0 X_1^{a_1} X_2^{a_2}$ where $a_0 = \exp(-0.666796) = 0.5133$, $a_1 = 0.986683$ and $a_2 = -1.95438$.

NONLINEAR REGRESSION

It is often desirable to fit a general nonlinear function model to the independent variables as indicated below:

$$y(\underline{x}) = f(x_1, x_2, ..., x_n; a_0, a_1, ..., a_m)$$

In the above expression, $x_1, x_2, ..., x_n$ are n independent variables, y is the dependent variable, and $a_0, a_1, ..., a_m$ are the model parameters. The data are represented by a set of N tabulated values of $x_{1,i}$, $x_{2,i}$, ... and $y(\underline{x}_i)$. The regression adjusts the values of the model parameters to minimize the sum of squares of the deviations between the calculated $y(\underline{x})$ and the data $y(\underline{x}_i)$.

In the previous example, the nonlinear regression capability of POLYMATH allows the model function to be treated directly without any transformation. Thus consider the model equation to be

$$Y = a_0 X_1^{a_1} X_2^{a_2} \quad .$$

Please recall Sample Problem 5. From the Problem Options Display press ⇑ F7 and then enter "R" for nonlinear regression.

Enter the model equation using the defined variables and any parameters (maximum of six) which are needed. For this example

≫Y = a0*X1**a1*X2**a2

Then enter all initial guesses for the parameters as unity "1", and then solve this example problem. You will then see the search progress to a solution where the final results are given as shown below. Note that additional graphical and statistical results are provided. It is good practice to provide realistic initial estimates which can come from a linear regression of the linearized model for challenging problems.

Sample Problem 5

Nonlinear regression model equation:

Y=a0*X1**a1*X2**a2

Initial estimates:	Current values:
a0 = 1	a0 = 0.509711
a1 = 1	a1 = 0.987817
a2 = 1	a2 = -1.96425

This concludes the Quick Tour section for the Polynomial, Multiple Linear and Nonlinear Regression Program. When you wish to stop POLYMATH, please follow the exiting instructions given below.

EXITING OR RESTARTING POLYMATH

A ⇑ F10 keypress will always stop the operation of POLYMATH and return you to the Program Selection Menu. *THIS ACTION WILL DELETE THE EXISTING PROBLEM.* The program can be exited or restarted from the Program Selection Menu.

SOLUTION METHODS

When fitting a polynomial of the form

$$P(x) = a_0 + a_1x + a_2x^2 + ... + a_nx^n$$

to N points of observed data, the minimum sum of square error correlation of the coefficients $a_0, a_1, a_2 ... a_n$ can be found by solving the system of linear equation (often called normal equations):

$$\mathbf{X}^T \mathbf{X} \mathbf{A} = \mathbf{X}^T \mathbf{Y}$$

where

$$\mathbf{Y} = \begin{bmatrix} y_1 \\ y_2 \\ \cdot \\ \cdot \\ \cdot \\ y_N \end{bmatrix} \quad \mathbf{A} = \begin{bmatrix} a_o \\ a_1 \\ \cdot \\ \cdot \\ \cdot \\ a_n \end{bmatrix} \quad \mathbf{X} = \begin{bmatrix} x_1^0 & x_1^1 & \cdot & \cdot & \cdot & \cdot & x_1^n \\ x_2^0 & x_2^1 & \cdot & \cdot & \cdot & \cdot & x_2^n \\ x_N^0 & x_N^1 & \cdot & \cdot & \cdot & \cdot & x_N^n \end{bmatrix}$$

and where y_1, y_2...y_N are N observed values of dependent variable, and x_1, x_2...x_N are N observed values of the independent variable.

Multiple linear regression can also be expressed in the same form except that the matrix **X** is redefined as follows:

$$\mathbf{X} = \begin{bmatrix} 1 & x_{1,1} & x_{2,1} & \cdot & \cdot & \cdot & x_{n,1} \\ 1 & x_{1,2} & x_{2,2} & \cdot & \cdot & \cdot & x_{n,2} \\ 1 & x_{1,N} & x_{2,N} & \cdot & \cdot & \cdot & x_{n,N} \end{bmatrix}$$

where $x_{i,j}$ is the j-th observed value of the i-th independent variable.

When polynomial or multiple linear regression are carried out without the free parameter (a_0), the first element in vector **A** and the first column in matrix **X** must be removed.

In POLYMATH the normal equations are solved using the Gauss-Jordan elimination. It is indicated in the literature that direct solution of normal equations is rather susceptible to round off errors. Practical experience has should this method to sufficiently accurate for most practical problems.

The nonlinear regression problems in POLYMATH are solved using the Levenberg-Marquardt method. A detailed description of this method can be found, for example, in the book by Press et al.*

*Press, W. H., Flannery, B. D., Teukolsky, S. A. and Vetterling, W. T., *Numerical Recipes*, Cambridge Univ. Press, Cambridge, 1986, pp 523-527.

SAVING INDIVIDUAL FILES AND USING THE PROBLEM LIBRARY

INTRODUCTION

POLYMATH allows you to save and retrieve problem files on any hard or floppy disks. All the problems and data are stored as DOS ASCII files that can be accessed, edited or used by various text editors, spreadsheet or graphic programs.

Problems can be stored as individual DOS files or in a convenient Problem Library. Results can be stored only as individual DOS files. The various options for storing and retrieving files will be discussed separately.

USING THE PROBLEM LIBRARY

After entering a particular problem, it is good practice to store it. Such situation is shown in the next display for the Quick Tour Problem 1 from the Differential Equations Solver Program:

```
                         Quick Tour Problem 1
The equations:
    d(A)/d(t)=-ka*A
    d(B)/d(t)=ka*A-kb*B
    d(C)/d(t)=kb*B
    ka=1
    kb=2
Initial values:  t0=0.0,   A0=1.0000,  B0=0.0,    C0=0.0
Final value:      tf=3.0000

                         PROBLEM OPTIONS
⇑-F7  to solve the problem.              F7  to print the problem.
⇑ ↵  to alter the problem.               F6  for helpful information.
⇑ F8  for file and library options.      ⇑ F10  for the MAIN MENU.
```

Quick Tour Problem 1 from the Differential Equations Solver has been entered into POLYMATH. As an example, this problem is to be stored for future use or modification. Press ⇑F8 from the Problem Options Display to access the file and library options. The Task Menu should result as shown on the next page:

TASK MENU

Current problem: Quick Tour Problem 1

⇑↵ to continue to work on your current problem.
↵ to enter a new problem.
F7 for SAMPLE PROBLEMS MENU.
F9 for LIBRARY OPTIONS.

DOS file options:
L. Load problem from DOS file.
S. Save problem on DOS file.

⇑F10 for the MAIN MENU.

Press F9 for library options. The following screen should appear:

Differential Eqs. Library directory: C:\

No library in this directory

LIBRARY OPTIONS

s. Store current problem. c. Change library directory

F8 to return

Please note that the name of the currently active directory is indicated at the top of the screen. (C:\ is the root directory in drive C for this example.) There is a message saying that in this particular directory there is no POLYMATH library associated with this particular POLYMATH program. To create the library and store the current problem, press "s". The following prompt appears:

Enter DOS filename to write to: Directory: C:\

» _

Press F6 for directory listing, F8 to return.

You must specify a filename in which the problem will be stored. The name should be set according to the file naming rules of DOS. This example will use the name "quictr1.dat". After typing it in and pressing enter, the following should be displayed on the screen:

```
Enter DOS filename to write to:          Directory:  C:\
» quictr1.dat
Done saving problem to file quictr1.dat.
Press any key to continue
```

You can press any key now. The list of the problems stored in the library (containing only one problem at this moment) together with the available options will appear

```
                    Library directory:  C:\

      File name          Problem title
→ 1)  quictr1.  dat      Quick Tour Problem 1

                     LIBRARY OPTIONS
    s.  Store current problem.      c.  Change library directory.

    L.  Load problem.      d.   Delete problem.         F8 to return.
```

Once a problem has been stored in the Library, that problem and any other problems for only the current POLYMATH Program will be conveniently displayed. Options permit you to change the library directory or to return to the application program. Other options refer to the particular problem in the Library list (only one is indicated above) which you indicate by the arrow. If there are several problems in the library, the arrow can be moved up and down by using the appropriate arrow keys on the keyboard. Once the desired problem has been located, it must be loaded in order to be used, modified and solved by the application program or deleted from the library and the disk.

OUTPUTTING RESULTS TO A DOS FILE

After the solution has been reached, the results can be saved on a DOS file in tabular form. The following screen shows the typical options available from the Display Options Menu:

Quick Tour Problem 1

Partial results

Variable	Initial value	Max. value	Min. value	Final value
t	0.0	3.0000	0.0	3.000
A	1.0000	1.0000	0.0498	0.0498
B	0.0	0.2499	0.0	0.0473
C	0.0	0.9029	0.0	0.9029
ka	1.0000	1.0000	1.0000	1.0000
kb	2.0000	2.0000	2.0000	2.0000

DISPLAY OPTIONS

t. Results in TABULAR form. g. Results in GRAPHICAL form.
d. Output results to a DOS file.
⇑-F8 for new problem or library. ⇑↵ to make changes.

You should press "d" from this display to output the results to a DOS file. After pressing "d", you will be asked for the names of the variables, the values of which you want to store. Let say that you want to store variables A, B and C versus the independent variable t. You should type in: A, B, C/ t as shown below and press ↵ .

Type in the names of up to four (4) variables separated by commas (,)
and optionally one 'independent' variable preceded by a slash (/).
For example, myvar1,myvar2/timevar
» **A,B,C/t**

After pressing Return you will be asked for a DOS filename to write to. Let us save the results in a file named "quictr1.res" Please type in this

Enter DOS filename to write to: Directory: C:\POLYMAT3

» **quictr1.res**

Press F6 for directory listing, F9 to change directory, F8 to return

Note that the name of the default directory is indicated in the previous display. In this case it is C:\POLYMAT3 . If you want to store the results in a different directory, you should specify a path using the regular DOS convention.

After typing in the file name and pressing Return, the response "Dump of results to file quictr1.res done" is obtained. Now the results are stored and they can be accessed after quitting POLYMATH, by text editors, spreadsheets or other applications.

For example, printing the file quictr1.res using the DOS print utility gives the following (only the first few lines are shown):

Quick Tour Problem 1

t	A	B	C
0	1	0	0
0.075	0.92774351	0.067034912	0.005221582
0.15	0.86070801	0.11988873	0.019403258
0.225	0.79851627	0.16088675	0.040596985
0.3	0.74081828	0.19200507	0.067176644
.	.	.	.
.	.	.	.
.	.	.	.

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APPENDIX

This Appendix provides complete instructions for the installation of POLYMATH and detailed information for advanced users. Most users will not need to refer to the information contained here.

INSTALLATION - INDIVIDUAL COMPUTER OR NETWORK

Place the distribution disk in an appropriate diskette drive. This is usually drive A or drive B. This drive must be capable of reading a 3.5 inch double sided, high density diskette. First set your current disk to the drive the diskette to be used. For example, if the drive to be used is A, then insert "A:" at the cursor and press Enter.

POLYMATH installation is initiated by typing "install" at the cursor. The installation program will ask the following questions:

1. Enter drive and directory for POLYMATH [C:\POLYMAT3].
   ==>

The default response is indicated by the contents of the brackets [...] which is given by pressing Enter key. The full path (drive and directory) where you wish the POLYMATH program files to be stored must be provided here. If the directory does not exist, then the installation procedure will automatically create it.

NOTE: Network clients will need read and execute permission for this directory and its subdirectories. This procedure does not provide the needed permissions.

2. Is this a network installation? [N] _

If you are installing POLYMATH on a stand-alone computer, take the default or enter "N" for no and **GO TO 5. on the next page of this manual.** If you are installing on any kind of network server, answer "Y" and continue with the installation.

3. What will network clients call <POLYdir> [POLYdir]?
===> _

This question will only appear if you answered "Y" to question 2 to indicate a Network installation. Here "POLYdir" is what was provided in question 1. On some networks, the clients "see" server directories under a different name, or as a different disk, than the way the server sees them. This question enables POLYMATH to print by indicating where the printer-driver files are located. They are always placed in subdirectory BGI of the POLYMATH directory by the installation procedure. During run time, they must be accessed by the client machines, thus POLYMATH must know what the client's name is for the directory.

4. Enter drive and directory for temporary print files [C:\TMP]:
===> _

This question will only appear if you answered "Y" to question 2 to indicate a Network installation. Depending on the amount of extended memory available, and the type of printer is use, POLYMATH may need disk workspace in order to print. Since client machines are not normally permitted to write on the server disk, you are requested to enter a directory where files may be written. The temporary print files are automatically deleted when a print is completed or cancelled.

5. The POLYMATH installation program now copies all of the needed files according to your previous instructions. This may take some time as the needed files are compressed on the installation diskette.

6. Please select the type of output device you prefer [1]: _

1. Printer
2. Plotter

===> _

Your answer here will take you to an appropriate selection menu.

7 A. POLYMATH INSTALLATION - printer selection

Please select the type of printer you have:

1. Epson 9-pin Dot Matrix Printer
2. Epson 24-pin Dot Matrix Printer
3. Epson 9-pin Dot Matrix Printer (color)
4. Epson 24-pin Dot Matrix Printer (color)
5. HP LaserJet II
6. HP LaserJet III or IV
7. HP DeskJet (Black & White)
8. HP DeskJet (Color)
9. HP PaintJet
10. IBM Proprinter
11. IBM Proprinter X24
12. IBM Quietwriter
13. OkiData Dot Matrix Printer (native mode)
14. PostScript printer
15. Toshiba 24-pin Dot Matrix Printer (native mode)

===> _

Type in the number of your printer (or a type of printer that your printer can emulate) and press Enter.

7 B. POLYMATH INSTALLATION - plotter selection

Please select the type of plotter you have:

1. HP 7090 Plotter
2. HP 7470 Plotter
3. HP 7475 Plotter
4. HP 7550 Plotter
5. HP 7585 Plotter
6. HP 7595 Plotter

===> _

Type in the number of your plotter (or a type of plotter that your plotter can emulate) and press Enter.

Once you have selected either a printer or a plotter, you will be asked to select the mode for your output.

8. POLYMATH INSTALLATION - printer/ plotter mode selection

Please select the mode you want for output [1]:

1. Half Page, Low Resolution
2. Half Page, Medium Resolution
3. Half Page, High Resolution
4. Landscape, Low Resolution
5. Landscape, Medium Resolution
6. Landscape, High Resolution
7. Portrait, Low Resolution
8. Portrait, Medium Resolution
9. Portrait, High Resolution

===> _

Generally, the fastest printing with adequate resolution is option (1), which is also the default. This choice is recommended. It is easy to change your printer/plotter selection and mode by using the PRINTSET program which is installed in the POLYMATH directory.

9. POLYMATH INSTALLATION - printer/ plotter port selection

Please select the port for your printer/plotter [1]:

1. LPT1
2. LPT2
3. COM1
4. COM2
5. LPT3

===> _

The default port, LPT1, is the first parallel port on most personal computers and usually is connected to the printer. For network installations, these are usually "logical" printer names, but they work just as well. If your network uses other printer logical names, please read the Appendix section on "POLYMATH Printing for Advanced Users" on the next page of this manual.

10. POLYMATH Execution

The POLYMATH program can now be executed by first changing the directory of your personal computer to the one where the program has been installed. Then you should enter "polymath" at the cursor as shown below and press Enter:

> polymath

Windows users must use POLYMATH as a DOS program. Advanced users may wish to place the polymath program in the "path" statement of the autoexec.bat file so that POLYMATH is more easily available from any cursor.

CHANGING PRINTER SELECTION

The printer selection may be changed without a complete reinstallation of POLYMATH by using the PRINTSET utility program which is stored on the directory containing POLYMATH. This program is executed by entering "printset" while in the POLYMATH directory. If there are several printers to be used with POLYMATH, then different POLYMATH.BAT files can be created for each printer. The batch file for printers is discussed in the following section.

PRINTING FOR ADVANCED USERS

POLYMATH printing is accomplished using GRAF/DRIVE PLUS which is a trademark for copyrighted software from Fleming Software. The printer setup is controlled by three environmental variables which are set in the POLYMATH.BAT file. This file is created by the INSTALL procedure, and it can be subsequently be modified by the PRINTSET utility or with an editor. CAUTION: This file should only be altered with an editor by advanced users.

A typical POLYMATH.BAT file is shown below:

```
echo off
set BGIPATH=c:\POLYMAT3\BGI
set PM_WORKPATH=c:\POLYMAT3
set PM_PRINTER=$LJ3R,0,LPT1
polymenu
cls
```

In the above file, the three environmental variables are:

BGIPATH - This is the directory in which the printer driver "BGI" files for POLYMATH reside. It is usually the BGI subdirectory of the POLYMATH directory. This variable is not normally changed.

PM_WORKPATH - This is the directory in which temporary print files are stored.

PM_PRINTER - This variable has the following form:

<printer_type>,<page_format>,<printer_port>

This variable in the previous POLYMATH.BAT file is defined as:

PM_PRINTER=$LJ3R,0,LPT1

where $LJ3R indicates the **printer_type** as HP LaserJet III, 0 (the number zero) indicates the **page_format** as half page with low density print, and LPT1 indicates the **printer_port** as LPT1.

PM_PRINTER Options for <printer_type> and <page_format>

A detailed listing of the <printer-type> and <page_format> options is given in Table 1 at the end of this appendix.

PM_PRINTER Options for <printer_port>

The <printer_port> may be any of the following: LPT1, LPT2, LPT3, COM1, COM2 or other physical/logical device names.

PRINTING TO STANDARD GRAPHICS FILES

It is possible to have all output which is "printed" by POLYMATH to be saved as various graphics files for use in word processing, desktop publishing, etc. This involves specialized use of the PM_PRINTER variable which is not available during the INSTALL procedure or the PRINTSET program for printer modification. **All printing to graphics files requires the creation of a special batch file for this purpose.**

A typical file for this purpose which is arbitrarily called POLYGRAP.BAT is shown below:

```
echo off
set BGIPATH=c:\POLYMAT3\BGI
set PM_WORKPATH=c:\POLYMAT3
set PM_PRINTER=$TIF,0,FILE:C:\GRAPHS\PMOUT+++.TIF
polymenu
cls
```

In the above file, the PM_PRINTER variable $TIF indicates the **printer_type** as a Tagged Image Format (TIFF), 0 indicates low resolution with two colors, and FILE:C:\GRAPHS\PMOUT+++.TIF indicates the location and name of the resulting graphics file.

PM_PRINTER Options for <printer_type> and <page_format> for Graphics Files

A detailed listing of the <printer-type> and <page_format> options for graphics file output is given in Table 2 at the end of this appendix

PM_PRINTER Options for <printer_port> for Graphics Files

This variable can be defined as FILE:<filename> when the output is to be to a file and not a port. (Note that if <filename> is a logical device name, such as LPT3, the output will be printed.) <filename> may be a particular filename or a general template, including '+' signs where a sequence number is to be written. The above example will create a sequence of files named PMOUT001.TIF, PMOUT002.TIF, etc., stored in directory C:\GRAPHS .

Table 1.1 - PM_PRINTER OPTIONS

<printer_ type>	<page_format>	Output Page /Resolution /Color	<page_format>	Output Page /Resolution /Color
Epson-compatible 9-pin Dot Matrix, and IBM Proprinter				
$FX	0	HalfLo	5	LandHi
	1	HalfMed	6	FullLo
	2	HalfHi	7	FullMed
	3	LandLo	8	FullHi
	4	LandMed		
Epson-compatible 24-pin Dot Matrix				
$LQ	0	HalfLo	5	LandHi
	1	HalfMed	6	FullLo
	2	HalfHi	7	FullMed
	3	LandLo	8	FullHi
	4	LandMed		
Epson-compatible 9-pin Dot Matrix Printer (color)				
$CFX	0	HalfLoC	3	LandMedC
	1	HalfMedC	4	FullLoC
	2	LandLoC	5	FullMedC
Epson-compatible 24-pin Dot Matrix Printer (color)				
$CLQ	0	HalfLoC	3	LandMedC
	1	HalfMedC	4	FullLoC
	2	LandLoC	5	FullMedC

Table 1.2 - PM_PRINTER OPTIONS

<printer_ type>	<page_format>	Output Page /Resolution /Color	<page_format>	Output Page /Resolution /Color
IBM Proprinter X24				
$PP24	0	HalfLo	5	LandHi
	1	HalfMed	6	FullLo
	2	HalfHi	7	FullMed
	3	LandLo	8	FullHi
	4	LandMed		
IBM Quietwriter				
$IBMQ	0	HalfLo	5	LandHi
	1	HalfMed	6	FullLo
	2	HalfHi	7	FullMed
	3	LandLo	8	FullHi
	4	LandMed		
OkiData Dot Matrix Printer (native mode)				
$OKI92	0	Half	2	Full
	1	Land		
Toshiba 24-pin Dot Matrix Printer (native mode)				
$TSH	0	Half	2	Full
	1	Land		

Table 1.3 - PM_PRINTER OPTIONS

<printer_ type>	<page_format>	Output Page /Resolution /Color	<page_format>	Output Page /Resolution /Color
LaserJet II, LaserJet III & IV, DeskJet (black cartridge)				
$LJ $LJ3R $DJ	0	HalfLo	5	LandHi
	1	HalfMed	6	FullLo
	2	HalfHi	7	FullMed
	3	LandLo	8	FullHi
	4	LandMed		
DeskJet (color cartridge)				
$DJC	0	HalfLo	5	LandHi
	1	HalfMed	6	FullLo
	2	HalfHi	7	FullMed
	3	LandLo	8	FullHi
	4	LandMed		
PaintJet				
$PJ	0	HalfLoC2	8	FullLoC8
	1	LandLoC2	9	HalfHiC8
	2	FullLoC2	10	LandHiC8
	3	HalfHiC2	11	FullHiC8
	4	LandHiC2	12	HalfLoC16
	5	FullHiC2	13	LandLoC16
	6	HalfLoC8	14	FullLoC16
	7	LandLoC8		

Table 1.4 - PM_PRINTER OPTIONS

<printer_ type>	<page_format>	Output Page /Resolution /Color	<page_format>	Output Page /Resolution /Color
PostScript Printers				
$PS	0	Half	6	HalfC16
	1	Land	7	LandC16
	2	Full	8	FullC16
	3	HalfGR	9	HalfC256
	4	LandGR	10	LandC256
	5	FullGR	11	FullC256
Hewlett-Packard Plotters				
$HP7090	0	DraftPL	2	DraftPLB
	1	LQPL	3	LQPLB
$HP7470	0	DraftPL	1	LQPL
$HP7475 $HP7550	0	DraftPL	4	DraftPLr
	1	LQPL	5	LQPLr
	2	DraftPLB	6	DraftPLBr
	3	LQPLB	7	LQPLBr
$HP7585 $HP7595	0	DraftPL	5	LQPLC
	1	LQPL	6	DraftPLD
	2	DraftPLB	7	LQPLD
	3	LQPLB	8	DraftPLE
	4	DraftPLC	9	LQPLE

Table 2 - PM_PRINTER OPTIONS

<printer_ type>	<page_format>	Output Page /Resolution /Color	<page_format>	Output Page /Resolution /Color
Zsoft PCX and Windows 3 BMP				
$PCX $BMP	0	ColorMode	1	MonoMode
GEM IMG				
$IMG	0	LoRes	2	HiRes
	1	MedRes		
Tagged Image Format (TIFF) compressed and uncompressed				
$TIF $UTIF	0	LoRes	2	HiRes
	1	MedRes		
ANSI CGM				
$CGM	0	ColorMode	1	ColorMode
AutoCad DXF				
$DXF	0	ColorMode		
Video Show (ANSI NAPLPS)				
$VSHO	0	ColorMode		
Word Perfect Graphics				
$WPG	0	ColorMode	1	MonoMode