Appendix 1: Mathcad Overview

This appendix is provided as a mini tutorial for readers who wish to learn Mathcad and use the available worksheets. The basic operations needed to create or edit Mathcad worksheets are covered, including the most important keyboard data entry operations. With the instructions below, the new user should be able to make changes to the example worksheets to perform the exercises. For more extensive training and help, the tutorials in Mathcad (click on Help) are very good. The author learned Mathcad through use of those resources alone.

The Mathcad reader is encouraged to copy this file and then edit and try the operations as you read. Because some of the later operations depend on earlier definitions, please use new variable names, such as names that include one of your initials.

For those reading the pdf version of the book, this appendix explains some of the syntax (e.g. the different kinds of equals signs) in Mathcad. That information may be helpful while reading the book.

Entering expressions and equations

$X := 2$ $Y := 15$

$Z := X \cdot Y^2$

Define variables and functions with the colon (:). Mathcad displays :=
This definition symbol may be changed in "Tools>Worksheet Options > Display" if desired for reports.

Q

When typing begins in a new area, Mathcad assumes it is a math region unless a space is entered. Entering a space converts the entry to a text region such as this and the first Q on the left.

Q

The second Q on the left was created by typing the letter, then by left clicking on empty white space away from the entry. At this point, the variable has been created but not assigned a value. Placing the cursor back on the variable and clicking will allow further definition, including the addition of subscripts and superscripts discussed later.

Two more kinds of "equals" symbols

$Z = 450$

Use the normal keyboard = to obtain a numerical result

$a = y^3 \cdot x + sin(z)$

Use the Boolean equal sign from toolbar or Ctrl = for symbolic math or defining a system of equations

Editing expressions and formulas

Define the constants, *a*, *b*, *c*, and *d*.

$a := 1$ $b := 3$ $c := 2$ $d := 6$

$xn := \frac{a+b}{c+d}$

Clicking inside a math region produces a blue cursor for editing. The space bar may be used to increase the span of the cursor in a cyclic manner from small to large span. The left and right arrow keys will change the operating direction of the cursor. In the example on the left, using the Backspace key would delete $a + b$. Using the Delete key would remove the division operator because Delete acts on characters to the right of the cursor. In Mathcad syntax, the divisor is "to the right" of the cursor in this example.

The following are basic keyboard operations. They all start with the blue cursor behind a variable name, pointing left. If the variable has just been created, that will be the position of the cursor.

$a^{\blacksquare}$

^ (shift 6) creates an exponent placeholder

$a_{\blacksquare}$

The subscript placeholder is inserted with left square bracket, [

$a_{i,\blacksquare}$	A comma after the first subscript will insert a placeholder for another subscript
b_Q	A period after a variable allows the insertion of a literal, non-mathematical subscript, (e.g. "Q") which can be used to provide additional variable naming options
$M^{\langle \blacksquare \rangle}$	Ctrl ^ creates a placeholder for specifying a column in a matrix, e.g. $M^{\langle 2 \rangle}$ identifies the third column of M (when "ORIGIN = 0")

Most other operators can be obtained from the toolbars. The creation of range variables and vectors is described next.

Using range variables and subscripts

$ORIGIN = 0$	Array indexes start with 0 by default, unless the variable "ORIGIN" has been changed by the user with "Tools>Worksheet Options> Built-in Variables"
$NR := 5$	Define a variable for the index maximum value of a vector or array.

Range variables are most often used as subscripts for vectors and matrices.

$i := 0 .. NR$	Define the range variable i
$a := 2$	.
$x_i := a \cdot i^2$	Defining the elements of a vector, x, using a formula.

$$x = \begin{pmatrix} 0 \\ 2 \\ 8 \\ 18 \\ 32 \\ 50 \end{pmatrix}$$ result (A1.1)

Caution: Operations using range variables are "single pass", not loops. In the example below, each operation (definition) is performed for each value of i before moving on to the next operation. In the typical loop programming structure, all of the operations would be performed for a given i before moving to $i + 1$. If a loop construct is needed, Mathcad has a "programming" option.

$i := 0 .. 4$ The index variable is defined

$xp_i := i + 4$ The *xp* vector is defined

$y_i := xp_i + if\left(i \le 3, xp_{i+1}, xp_i\right)$ The y vector is defined using i and *xp*

The last statement would not be valid in Fortran because xp_{i+1} would not be available in the loop construct, with i as the loop index.

$$xp = \begin{pmatrix} 4 \\ 5 \\ 6 \\ 7 \\ 8 \end{pmatrix} \qquad y = \begin{pmatrix} 9 \\ 11 \\ 13 \\ 15 \\ 16 \end{pmatrix}$$ The *xp* and y vectors created above.

Vectors are the appropriate form for non index variables.

$xvector_i := i \cdot 2 + 2$ This vector, *xvector* , is preferred to ..

$xrange := 2, 4 .. 10$ ... this range variable, *xrange* , if the intent is to create a variable that has addressable elements.

Compare vector result to a range variable result.

$$xvector = \begin{pmatrix} 2 \\ 4 \\ 6 \\ 8 \\ 10 \end{pmatrix}$$

$xrange =$

2
4
6
8
10

$xrange_2 = \blacksquare$

An error (indicated by red) results when attempting to address an element of a range variable,

$xvector_2 = 6$

whereas elements of vectors may be addressed.

The "units advantage" in Mathcad

$T_{sp} := 300$ $\quad T := 310 \cdot K$

Variable definitions

$difference := T - T_{sp}$

Units checking catches problems as you code.

$T_{sp} := 300 \cdot K$

Corrected a variable.

$difference := T - T_{sp}$

Now no error indication.

$difference = 10\,K$

$bbl := 42 \cdot gal$

Define new units in terms of existing units.

$Vol := 20 \cdot bbl$ $Vol = 20 \cdot bbl$ Now the variable *Vol* is defined using the new unit.

$Vol = 3.18 \times 10^3 \, L$ Results initially use the default units

$Vol = 112.292 \cdot ft^3$ but they can easily changed to any appropriate unit.

$Vol = 840 \cdot gal$

$Vol = 20 \cdot bbl$

To change, click in the result and then type the desired unit in the placeholder on the right. Once a result has a non-default unit, just click in the result and edit the unit by deleting and typing the new unit.

Functions

$cot(d) = -3.436$

$tan(d) = -0.291$

Built-in functions may be inserted with the f(x) button on the toolbar or typed directly.

$f(h, m1, c1) := c1 \cdot h + m1^2$ User created functions are extremely useful.

$(g(h, ml) := ek + h \cdot ml)$

This variable is undefined.

Undefined variables must appear as an argument in a function definition.

$g2(h, ml) := d + h \cdot ml$

A previously defined variable (e.g. d) will be treated as a constant, using the value at the time the function was defined.

$g2(1, 2) = 8$ $g2$ with $d = 6$ from above

$d := 10$ redefining d ...

$g2(1, 2) = 8$ ... doesn't change definition of $g2$

Calculus Operations

Derivatives or integral of a function or expression may be solved symbolically. The Antoine relationship for the vapor pressure of a liquid will be used as an example.

$$ANT := \begin{pmatrix} 18.3036 & 3816.44 & -46.13 \\ 18.0994 & 4055.45 & -76.49 \\ 16.8641 & 3558.18 & -47.86 \end{pmatrix}$$

Antoine constants for three compounds, with water in first row, row 0 (A1.2)

$$P_w(t) := exp\left(ANT_{0,0} - \frac{ANT_{0,1}}{\frac{t}{K} + ANT_{0,2}}\right) \cdot \frac{atm}{760}$$

Vapor pressure of water as a function of temperature, *t*. The coefficients in row 0 have been used. (A1.3)

$$\frac{d}{dt}P_w(t) \rightarrow \frac{5.0216315789473684211 \cdot atm \cdot e^{18.3036 - \frac{3816.44}{\frac{t}{K} - 46.13}}}{K \cdot \left(\frac{t}{K} - 46.13\right)^2}$$

The derivative operator may be used with a function. Use Ctrl . (Ctrl period) and then Enter to obtain the symbolic result. (A1.4)

$$\nabla_t P_w(t) \rightarrow \frac{5.0216315789473684211 \cdot atm \cdot e^{18.3036 - \frac{3816.44}{\frac{t}{K} - 46.13}}}{K \cdot \left(\frac{t}{K} - 46.13\right)^2}$$

The gradient operator may also be used to obtain the symbolic derivative. (A1.5)

$$\int_0^1 f\,(h, m, c1)\; dh \rightarrow m^2 + \frac{c1}{2}$$

A symbolic definite integral. (A1.6)

If the derivative or integral is needed repeatedly, say in solving a differential equation, the symbolic result can be used to create a new function so that the symbolic calculus operation doesn't need to be solved repeatedly.

First, define the new function leaving the value on the right side of the definition blank.

$$dPwdt(t) := \blacksquare$$

Copy and paste the symbolic result from Eq (A1.4) into the placeholder.

$$dPwdt(t) := \frac{5.0216315789473684211 \cdot atm \cdot e^{18.3036 - \frac{3816.44}{\frac{t}{K} - 46.13}}}{K \cdot \left(\frac{t}{K} - 46.13\right)^2} \qquad \text{(A1.7)}$$

The derivative or integral of a function or expression may be numerically determined if all variables are defined.

$t := 300 \cdot K$ $\qquad \frac{d}{dt}P_w(t) = 2.051 \times 10^{-3} \cdot \frac{atm}{K}$

The gradient operator may also be used with more than one independent variable

$$g(x1, y1) := 2 \cdot x1 + sin(y1)$$

$$\nabla_{x1, y1}\, g(x1, y1) \rightarrow \begin{pmatrix} 2 \\ cos(y1) \end{pmatrix}$$

The Jacobian of a vector

If a vector, f, has n elements and there are m elements in the independent variable vector, X, then the Jacobian will be an (n x m) matrix.

$$Jacobian = \begin{pmatrix} \frac{d}{dX_0} f_0 & \frac{d}{dX_1} f_0 & \frac{d}{dX_2} f_0 \\ \frac{d}{dX_0} f_1 & \frac{d}{dX_1} f_1 & \frac{d}{dX_2} f_1 \end{pmatrix}$$ definition of Jacobian

$$f2(xx) := \begin{bmatrix} xx_0 + 3 \cdot xx_1 \\ sin(xx_2) + (xx_0)^2 + (xx_1)^3 \end{bmatrix}$$

definition of *f2* with 2 elements.
the *xx* vector has 3 elements (implied from the *f2* definition) (A1.8)

The symbolic Jacobian of f2:

$$Jacob(f2(x2), x2) \rightarrow \begin{bmatrix} 1 & 3 & 0 \\ 2 \cdot x2_0 & 3 \cdot (x2_1)^2 & cos(x2_2) \end{bmatrix}$$ Jacobian has 2 rows and 3 columns (A1.9)

The dependent variable may use any name as shown above (*x2* replaced *xx*), but the result may be un-intended if the variable has been previously defined for another purpose. For example, the vector *x* has been previously defined, Eq (A1.1), with six elements, each with a numerical value. If *x* is used as the argument in the Jacobian function, the following result is obtained:

$$Jacob(f2(x), x) \rightarrow \begin{pmatrix} 1 & 3 & 0 & 0 & 0 & 0 \\ 0 & 12 & cos(8) & 0 & 0 & 0 \end{pmatrix}$$ (A1.10)

The Jacobian now has six columns, the dimension of *x*, and the result is numeric instead of symbolic.

Solving for a variable in an equation

Often, nonlinear equations need to be solved for one of the variables. For example, the Antoine relationship is used to calculate vapor pressure as a function of temperature, t, but the user desires the temperature as a function of pressure.

$$Pw = exp\left(ANT_{0,0} - \frac{ANT_{0,1}}{\frac{t}{K} + ANT_{0,2}}\right) \cdot \frac{atm}{760} \qquad \text{(A1.11)}$$

Pw and *t* both unknown, with coefficients for water selected by row index 0 in *ANT*.

Note that Eq (A1.11) has been written using the symbolic equal sign from the Boolean toolbar.

To create a function for the temperature with vapor pressure as the argument, use the cursor to select "*t*", and then "Symbolics>variable>Solve" on the toolbar. The result will be printed below the original equation. Set the symbolic result as the right hand side of the definition for the temperature function.

$$t\_vap(Pw) := -K \cdot \left(\frac{ANT_{0,1}}{ln\left(\frac{760 \cdot Pw}{atm}\right) - ANT_{0,0}} + ANT_{0,2}\right) \qquad \text{(A1.12)}$$

$$t\_vap(1 \cdot atm) = 373.152\,K$$

Plots: seeing results as you develop the model

Plots are very easy to create in Mathcad and thus they can be used as a means of checking intermediate results while a worksheet is being written. There are numerous plot formats: the most commonly used are shown below.

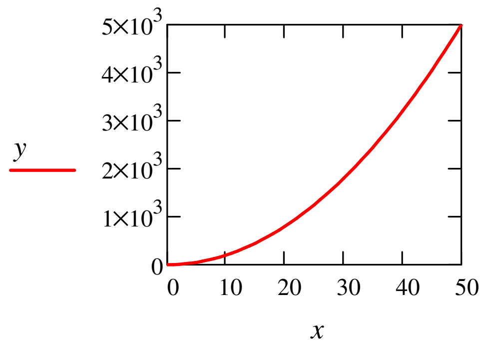
2D plots

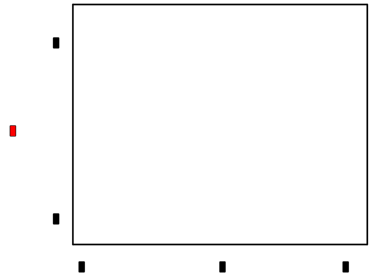
of vectors

$i := 0..50$

$x_i := i$

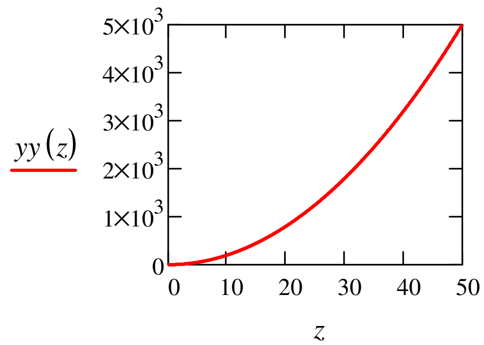
$y_i := 2 \cdot (x_i)^2$





of functions

$yy(z) := 2 \cdot z^2$

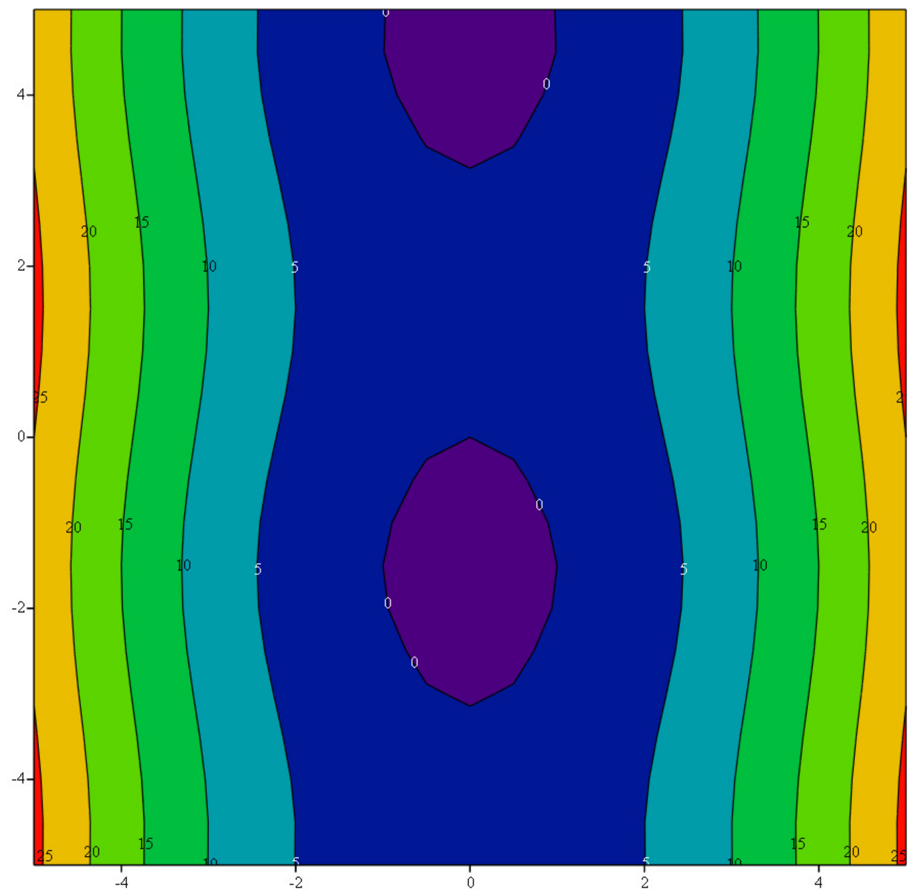


To insert a plot go to toolbar, "Insert>graph>" and choose the type of plot. Alternatively, the keystroke @ may be used to insert an xy plot like the one on the left.

Type the variables in the placeholders and the axis limits if needed and you have a plot. Right clicking on the plot shows a menu with Format as an option. Labels, colors, etc. can be set with the Format option.

3D contour plot

$f3D(x, y) := x^2 + sin(y)$



f3D

Other features of Mathcad

- Methods for solving ordinary and partial differential equations
- Programming capability to extend Mathcad's functionality (e.g.. loops are not allowed in normal Mathcad but they can be used in the programming construct)
- Data can be read and written to text files, Excel, MATLAB, other formats
- Solving systems of nonlinear equations
- Parameter estimation, optimization methods
- Animated videos can be created from graphs and saved to a file for playback