Appendix 2: Linear Algebra

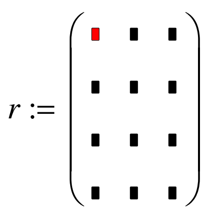
This appendix provides a brief overview of operations using linear algebra, and how they are implemented in Mathcad. This overview should provide readers with the ability to understand the mathematical operations in the worksheets. New users of Mathcad may consult the Mathcad tutorials and help files for further information regarding the user interface and the creation of worksheets. As was recommended for Appendix 1, the Mathcad reader is encouraged to make a copy of this file, and then editing and trying the operations as you read.

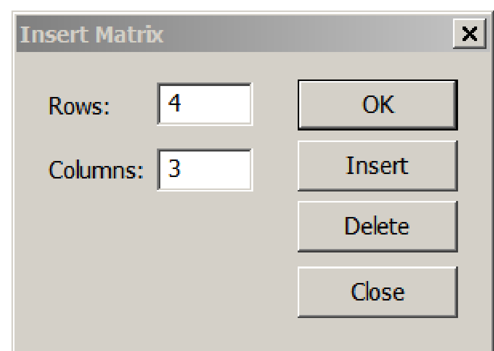
The basic operations covered below include the following:

- matrix creation
- selection of rows or columns for use in a formula or graph
- transpose
- inverse of square matrix
- vector sum (summation of elements in a vector)
- multiplication of vectors and matrices (dot product)
- vectorization of mathematical expression
- solution of linear equations.

Direct entry of vectors and matrices

Use the matrix toolbar to create an empty matrix of the size needed:





Enter the numbers for each element using the cursor. The "Tab" key may be used to move to the next empty cell.

$$r := \begin{pmatrix} 1 & 0 & 0 \\ 2 & 2 & 7 \\ 9 & 8 & 8 \\ 3 & 8 & 5 \end{pmatrix} \cdot m$$

A unit, m, has been supplied.

$$rv := \begin{pmatrix} 3 \\ 5 \\ 1 \end{pmatrix}$$

The creation of vectors and matrices by use of variables was previously demonstrated in Appendix 1.

The matrix tool bar may be used to perform the operations below. Alternatively, shortcut keys may be used. The shortcuts are shown when the cursor is placed over the toolbar item.

Rows and Columns

Elements in an array (vector or matrix) can be referenced using subscripts with the array name.

$$r_{2,0} = 9m$$

The element's row is indicated by the first subscript, columns by the second. The origin (first row or column) is 0 by default but can be changed for each worksheet (not recommended). Thus, in the example given on the left, the element is in the third row, first column.

General matrix operations

transpose of matrix or vector

$$r^T = \begin{pmatrix} 1 & 2 & 9 & 3 \\ 0 & 2 & 8 & 8 \\ 0 & 7 & 8 & 5 \end{pmatrix} m$$

rows become columns and columns become rows

selection of a particular column

$$r^{\langle 2 \rangle} = \begin{pmatrix} 0 \\ 7 \\ 8 \\ 5 \end{pmatrix} m$$

selection of a particular row

$$\left(r^{T}\right)^{\langle 3 \rangle^{T}} = \begin{pmatrix} 3 & 8 & 5 \end{pmatrix} m$$

Only columns can be selected in their entirety. Thus, the array is transposed, the column (previously a row) is indicated, and then the result is transposed back. Row 3 is the fourth row of *r*.

matrix dot product

Two matrices, one with k columns and one with k rows may be multiplied using the dot product operation. The formula for dot product of two matrices is

$$result_{i,j} = \sum_{n=0}^{k-1} \left(M_{i,n} \cdot N_{n,j}\right)$$

For example, let

$$M := \begin{pmatrix} 2 & 3 \\ 5 & 2 \\ 1 & 9 \end{pmatrix} \qquad N := \begin{pmatrix} 1 & 3 & 5 & 7 \\ 2 & 6 & 4 & 8 \end{pmatrix}$$

3x2 2x4

"Interior" dimensions must be same. For (3x2)x(2x4) matrices, the "2" is the "interior" dimension

$i := 0..2$ $j := 0..3$ $k := cols(M) = 2$

$$result_{i,j} := \sum_{n=0}^{k-1} \left(M_{i,n} \cdot N_{n,j}\right)$$

note that the sum is over the "interior dimension"

$$result = \begin{pmatrix} 8 & 24 & 22 & 38 \\ 9 & 27 & 33 & 51 \\ 19 & 57 & 41 & 79 \end{pmatrix}$$

3x4

result matrix has the "exterior" dimensions, i.e. the number of rows in left matrix x number of columns right matrix

The Mathcad way is easier to code, and it reads like a textbook written in vector/matrix notation:

$result := M \cdot N$

The Mathcad operation.

$$result = \begin{pmatrix} 8 & 24 & 22 & 38 \\ 9 & 27 & 33 & 51 \\ 19 & 57 & 41 & 79 \end{pmatrix}$$

The solution.

Vector operations

vector sum

$$rv = \begin{pmatrix} 3 \\ 5 \\ 1 \end{pmatrix}$$

$$\sum rv = 9$$

Mathcad determines the summation limits based on the vector.

vector dot product

$$M1 := \begin{pmatrix} 2 \\ 4 \\ 7 \end{pmatrix} \qquad N1 := \begin{pmatrix} 8 \\ 10 \\ 6 \end{pmatrix}$$

The vectors *M1* and *N1* will be used to demonstrate this operation.

The dot product is defined according to the formula below:

$$product = \sum_{n=0}^{last\_n} \left(M1_n \cdot N1_n \right)$$

For the example,

$$\sum_{n=0}^{2} \left(M1_n \cdot N1_n \right) = 98$$

In Mathcad, the dot product may be obtain using the multiplication of the transpose of *M1* by *N1* :

$$M1^T \cdot N1 = 98$$

Mathcad also allows the following form,

$$M1 \cdot N1 = 98$$

when it recognizes the multiplication of two vectors of equal length.

vectorization of operations

$$Mw := \begin{pmatrix} 2 \\ 18 \\ 44 \end{pmatrix} \cdot \frac{gm}{mol} \qquad X := \begin{pmatrix} .25 \\ .30 \\ .45 \end{pmatrix}$$

molecular weight mole fraction

Convert mol fraction, X, to mass fraction, Y, using vectorized multiplication.

$$Y := \frac{\overrightarrow{(X \cdot Mw)}}{X \cdot Mw} \qquad Y = \begin{pmatrix} 0.019 \\ 0.21 \\ 0.77 \end{pmatrix}$$

The vectorization operation acts like a "For Loop" for vectors, performing an operation using the same element (index) of the vectors involved. The above operation would have been something like the following in Fortran:

$wt\_total = 0$

For i=0,2

$wt_i = X_i \cdot Mw_i$

$wt\_total = wt\_total + wt_i$

End

For i=0,2

$$Y_i = \frac{wt_i}{wt\_total}$$

End

Vectorization is not restricted to operations with only two vectors. All vectors must have the same number of elements. Operations other than multiplication may be included.

$$\overrightarrow{\left(X \cdot Mw \cdot \sqrt{rv}\right)} = \begin{pmatrix} 8.66 \times 10^{-4} \\ 0.012 \\ 0.02 \end{pmatrix} \frac{kg}{mol}$$

Square matrix operations

inverse of matrix

$$S := \begin{pmatrix} 2 & 1 & .5 \\ .3 & 3 & 4 \\ 1 & 2 & 2 \end{pmatrix} \qquad S^{-1} = \begin{pmatrix} 1.111 & 0.556 & -1.389 \\ -1.889 & -1.944 & 4.361 \\ 1.333 & 1.667 & -3.167 \end{pmatrix}$$

$$S^{-1} \cdot S = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Multiplying the two results in the diagonal identity matrix, *I*. The identity matrix is the matrix equivalent of the scalar "1" and thus can be eliminated from expressions.

If the operation is reversed,

$$S \cdot S^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & -1.776 \times 10^{-15} \\ 0 & 0 & 1 \end{pmatrix}$$

the result is still *I* within the tolerance.

linear equations

If $S \cdot x = Y$

and Y is given,

$$Y = \begin{pmatrix} 0.019 \\ 0.21 \\ 0.77 \end{pmatrix}$$

then to find x , multiply both sides of equation with inverse of S to eliminate S from the left side.

To illustrate,

$$S^{-1} \cdot S \cdot x = S^{-1} \cdot Y$$

but $S^{-1} \cdot S = I$

thus $I \cdot x = S^{-1} \cdot Y$ or $x = S^{-1} \cdot Y$

The actual "live" Mathcad operation:

$$x := S^{-1} \cdot Y$$

$$x = \begin{pmatrix} -0.932 \\ 2.915 \\ -2.064 \end{pmatrix}$$ the solution

When performing multiplication operations on an equation, the operation must be performed on both sides of the equation in the same manner. For the above example, the following would be incorrect because the left side has been pre-multiplied and the right side has be post-multiplied by S^{-1}.

$$S^{-1} \cdot S \cdot x = Y \cdot S^{-1}$$

$$x = Y \cdot S^{-1}$$

The above operation $x := Y \cdot S^{-1}$

results in an error because the dimensions of Y (3x1) and S^{-1} (3x3) are not compatible for a dot product operation, i.e. the interior dimension are not equal.

The above information should be sufficient to continue with the book. If the reader would like further information on linear algebra and matrices, a paperback introductory outline can be used for self study.