Matrices

Introduction to Matrices

There are two primary data structures in Origin: worksheets and matrices. Data stored in worksheets can be used to create any 2D graph and some 3D graphs, but in order to create a 3D surface graph or a 3D contour graph you must have your data stored in a matrix. Origin provides methods for converting worksheets to matrices, and for converting matrices to worksheets.

Matrices have numbered columns which are mapped to linearly spaced X values and numbered rows which are mapped to linearly spaced Y values. You can view the X and Y values in the matrix column and row headings by selecting **View:Show X/Y**. Each cell value in a matrix represents a Z value which is located in the XY plane by the cell's X value (determined by its column) and by the cell's Y value (determined by its row).

Opening a Matrix Window

The matrix window is similar to a worksheet in that it is used to store and manipulate data. However, in the matrix window, there is an underlying X, Y, Z relationship for each cell. Each column is associated with an X value, and each row is associated with a Y value (though you can reverse these relationships). Thus, each cell thus has three values: one associated with the row, one associated with the column, and the actual value that appears in the cell, which is the Z value.

To open a new matrix, select **File:New**. This menu command opens the New dialog box. Select Matrix from the Window Type list box. Select Origin from the Template drop-down list. Click OK to open a matrix window based on the ORIGIN.OTM template. Shortcut: Click the New Matrix button  on the Standard toolbar.

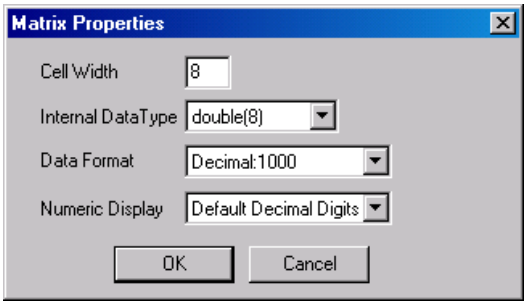
To open a previously saved matrix window, select **File:Open**. Select 'Matrix (*.OGM)' from the Files of Type drop-down list. Select the desired file and click Open.

Shortcut: Click the Open button  on the Standard toolbar.

Setting the Matrix Data Properties

Origin provides controls to set the internal data type, data format, and data display for a matrix. To customize these properties, select **Matrix:Set Properties** when the matrix is active. This menu command opens the Matrix Properties dialog box.

The Matrix Properties Dialog Box



The Cell Width Text Box

Type the desired cell width in this text box. This text box value is in units of characters.

The Internal Data Type Drop-down List

This drop-down list sets the maximum size for each matrix cell value, in bytes. The default data type is Double, which allocates eight bytes of storage space to each value. Double is the only data type that supports missing values. The Float data type allocates four bytes of storage space per value. The Int data type allocates four bytes of storage space per value. The Short data type allocates two bytes of storage space per value. The Char data type allocates 1 byte of storage space per value.

The Data Format Drop-down List

Use the Data Format drop-down list to select between the decimal, engineering, and scientific display formats. In the matrix, the display formats differ as follows:

Data Format Types

Format	Matrix Display
Decimal:	1000 (1, 1000, 1E6, 1E9) The threshold for conversion to scientific notation is controlled on the Numeric Format tab of the Options dialog box (**Tools:Options**).
Scientific:	1E3 (1E0, 1E3, 1E6, 1E9)
Engineering*:	1k (1.0, 1.0k, 1.0M, 1.0G)
Decimal:	1,000 (1, 1,000, 1E6, 1E9) The threshold for conversion to scientific notation is controlled on the Numeric Format tab of the Options dialog box (**Tools:Options**).

*Origin supports the following Engineering data suffixes:

k - kilo, 10^3
M - mega, 10^6
G - giga, 10^9

T - tera, 10^12
P - peta, 10^15
m - milli, 10^-3
u - micro, 10^-6
n - nano, 10^-9
p - pico, 10^-12
f - femto, 10^-15

Note that "u" is Origin's universal notation for micron. The only exception is graph axes tick labels, which support "mu". Note also that Origin 7 does not support "E" and "a" as suffixes.

The Numeric Display Drop-down List

Select Default Decimal Digits to display all digits in a matrix cell as determined by the Number of Decimal Digits combination box value on the Numeric Format tab of the Options dialog box.

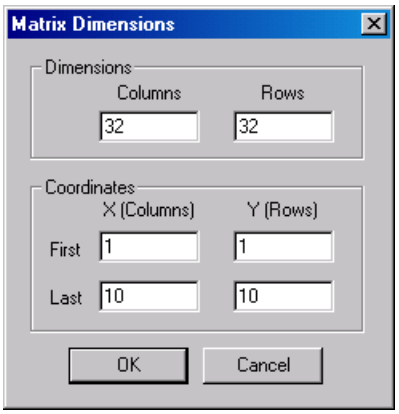
Select Set Decimal Places = to control the display of the number of digits after the decimal place (supersedes the Number of Decimal Digits setting on the Numeric Format tab of the Options dialog box). Type the desired decimal place value (*n*) in the associated text box. This value determines the maximum number of digits displayed after the decimal point. If the field is blank, the default value is used, which is 5 (for Double (8) internal data types).

Select Significant Digits = to control the number of digits displayed. Type the desired significant digit value in the associated text box.

Setting the Matrix Dimensions and XY Coordinates

To set the matrix dimensions and the XY mapping relationship, select **Matrix:Set Dimensions**. This menu command opens the Matrix Dimensions dialog box.

The Matrix Dimensions Dialog Box



The Dimensions Group

Type the desired number of columns and rows in the associated text boxes.

The Coordinates Group

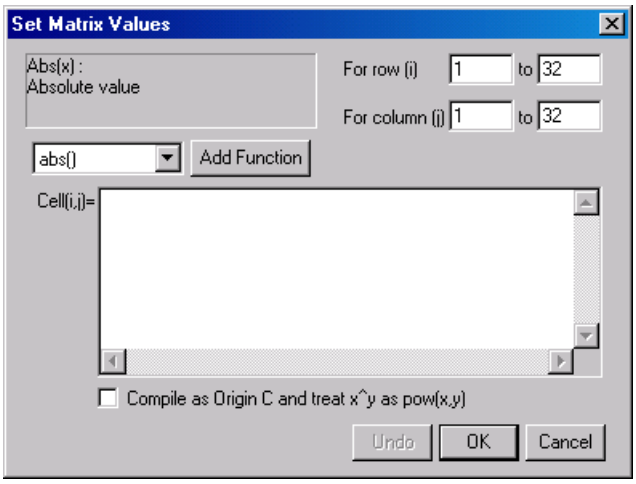
Type the first and last X and Y values in the associated text boxes.

After clicking OK, Origin will linearly map the matrix in X by columns based on the First and Last X (Columns) values and the number of columns (set in the Dimensions group). Origin will linearly map the matrix in Y by rows based on the First and Last Y (Rows) values and the number of rows (set in the Dimensions group).

Setting the Matrix Values

To fill the matrix with Z values, select **Matrix:Set Values**. This menu command opens the Set Matrix Values dialog box.

The Set Matrix Values Dialog Box



Select the Matrix Column and Row Range

The initial and final cells in the selection range are indicated by column number (*j*) and row number (*i*) in the associated 'from' and 'to' text boxes. Enter new values to change the selection range. Matrix values are only entered in the cells that fall within the selection range.

Select a Function

The Add Function drop-down list and button are provided to help you build the desired expression in the Cell(i,j)= text box. Instead of typing the proper function syntax directly in the Cell(i,j)= text box, you can select a function (or functions) from the drop-down list.

The Add Function drop-down list includes Origin's built-in mathematical and statistical distribution functions. To view the details of a function, select the function from the drop-down list. A function summary including a description of the function arguments displays in the upper view box. To select a function so that it displays in the Cell(i,j)= text box, click the Add Function button after selecting it from the drop-down list. How the function displays in the Cell(i,j)= text box depends on whether any text was highlighted in the text box prior to selecting the function. If text was highlighted in the text box, then that text becomes the (last) argument for the selected function. If no text was highlighted, then the function displays at the last active cursor location in the text box.

Complete the Expression in the Cell(i,j)= Text Box

The expression you type in this text box is used to fill the selected matrix cells with values. The expression can include any of Origin's built-in functions. The Add Function controls provide an easy method for adding mathematical and statistical distribution functions to the expression. However, you can use any of Origin's built-in functions following the syntax described in the *LabTalk Manual*. In addition to functions, you can use any operators recognized by Origin, as well as any defined variables.

Note 1: Do not include a semicolon after the expression entered in the Cell(i,j)= text box.

Note 2: You can reference a single cell in a matrix by using the following syntax:

MatrixName[*N**(*i*-1)+*j*]

where:

N = the number of columns in the matrix.

i = the row number in the matrix.

j = the column number in the matrix.

The "Compile as Origin C and Treat x^y as pow(x,y)" Check Box

You can define and compile an expression using Origin C in this dialog box. After you enter an Origin C expression, select this check box, and then click OK, if any compiler errors are encountered they are output to the Script window. To learn more about Origin C, see the Programming Guide Help file.

The OK Button

Click this button to close the dialog box and set the values for the selected cells according to the specified expression in the Cell(i,j)= text box.

The Undo/Redo Button

Click this button to undo/redo the last change made to the expression in the Cell(i,j)= text box.

Viewing the Matrix Values

Use the scroll bars on the right and bottom edges of the matrix window to view the desired cells. Alternatively, select **View:Go to Row** to view a specific matrix row. This menu command opens the Go to Row dialog box. Type the desired row number in the associated text box.

Customizing the Display Properties of a Matrix

To customize the text color, style, and heading and grid options of a matrix, double-click in the upper-left corner of the matrix window. This action opens the Matrix Display Control dialog box.

For a complete description of this dialog box, see Worksheets.

Importing Data into a Matrix

To import ASCII data into a matrix, select **File:Import ASCII**. This menu command opens the Import ASCII dialog box. Select the desired data file and click Open to import the file into the matrix.

The values imported into the matrix are assumed to be Z values. Set the matrix XY mapping relationship in the Matrix Dimensions dialog box after reading in the Z data (**Matrix:Set Dimensions**).

Matrix Operations

Transposing

To transpose the active matrix, select **Matrix:Transpose**. This menu command exchanges the matrix columns with rows, and rows with columns.

Inverting

To invert the active matrix, select **Matrix:Invert**. This menu command transposes the matrix, and then divides the matrix by its determinant.

Flipping and Rotating

To flip the active matrix horizontally (first column becomes last, etc.), select **Matrix:Flip H**.

To flip each column vertically (last cell becomes first, etc.), select **Matrix:Flip V**.

To rotate the matrix so that the columns become rows and the previously first value in the column becomes the last value in the row, select **Matrix:Rotate90**.

Shrinking

Matrix shrinking is a simple averaging of grid points. To shrink the active matrix, select **Matrix:Shrink**. This menu command opens the Shrink into 1x1 for Every dialog box. Type the column and row shrinkage factors. For example, if the original matrix is 100 columns by 20 rows, and you type 2 in the Columns and Rows text box, the matrix dimensions after shrinking will be 50 columns by 10 rows.

Expanding

Matrix expansion uses a bilinear interpolation method to add the inserted points. To expand the active matrix, select **Matrix:Expand**. This menu command opens the Expand for Every Cell dialog box. Type the column and row expansion factors. For example, if the original matrix is 100 columns by 20 rows, and you type 2 in the Columns and Rows text box, the matrix dimensions after expanding will be 200 columns by 40 rows.

Smoothing

To smooth the active matrix, select **Matrix:Smooth**. After clicking OK at the prompt, Origin performs the following:

1) If either the number of columns or the number of rows in the matrix is less than 32, Origin expands the matrix by a factor of two, and then shrinks the matrix by a factor of two. Origin then repeats this process once more.

2) If either the number of columns or the number of rows in the matrix is greater than 32, Origin shrinks the matrix by a factor of two, and then expands the matrix by a factor of two.

For information on shrinking and expanding the matrix, see "Shrinking" on page 109 and "Expanding" on page 109.

Integrating

To compute the volume beneath the surface defined by the matrix, select **Matrix:Integrate**. Origin performs a double integral over X and Y to compute the volume and reports the value in the Script window.

Converting a Worksheet into a Matrix

Origin provides several methods for converting worksheets to matrices, including direct, expand columns, 2D binning, regular XYZ, random XYZ, and sparse XYZ conversions. The method that you use will depend on the type of data in the worksheet.

Direct Conversion

To directly convert the active worksheet to a matrix, select **Edit:Convert to Matrix:Direct**. This menu command creates a new matrix that contains the same number of rows and columns as the associated

worksheet. Origin fills the matrix with the worksheet values, maintaining the same row and column positions in the matrix.

Note: To convert the active Excel workbook to a matrix using direct conversion, select the desired Excel workbook data and then select **Window:Create Matrix**.

To learn more about direct conversion, review the WORKSHEET TO MATRIX.OPJ project located in your Origin \SAMPLES\ANALYSIS\WORKSHEET TO MATRIX folder.

Expanding Columns During Conversion

There may be cases where a screen editor which is used to create an ASCII file has an upper limit for the number of characters allowed on a single line. This upper limit may even be less than the number of columns required in the matrix. To compensate for this, one row of matrix data can be stored in multiple rows of an ASCII file. Displaying this type of ASCII file in a matrix requires two steps. The first step is creating a new worksheet and importing the ASCII file into it. The second step is expanding the worksheet data into a matrix. To do this, select **Edit:Convert To Matrix:Expand Columns**. This menu command opens a dialog box in which you specify the number of ASCII file rows corresponding to one matrix row. After clicking OK, Origin copies your worksheet data from the first set of specified rows into the first row of a matrix. Origin repeats this procedure to convert all rows in the worksheet.

For example, if a matrix of 24 columns is stored in an ASCII file that only allows 8 columns of data to be stored in it, then each row of matrix data (24 different values) would take up 3 rows in the ASCII file. In this case, you would type 3 in the Expand for Every Row dialog box. After clicking OK, a new matrix is created with 3 rows of ASCII file data in each row of the matrix.

To learn more about expanding columns during conversion, review the WORKSHEET TO MATRIX.OPJ project located in your Origin \SAMPLES\ANALYSIS\WORKSHEET TO MATRIX folder.

2D Binning

Often in physical measurements, you may have raw values of two parameters, X and Y, from a sequence of measurements. An example of such a raw list of values could be paired values of energy and position of particles measured from many events, in a particle physics experiment. To explore the relationship between the two variables in a 3D graph, you must first construct a matrix by binning the X-Y paired data in two dimensions. For this purpose, Origin provides a 2D binning tool.

To perform 2D binning, select the desired Y column in your worksheet and select **Edit:Convert to Matrix:2D Binning**. Origin will use your selected Y column as Y values, and this column's associated X column as X values. The **2D Binning** menu command opens the Create Bin Matrix dialog box.

Specify the bin limits and bin size for the X and Y variables. The default values for bin limits are the minimum and maximum values of the X and Y columns. After clicking OK, a matrix is created by binning the X-Y paired data in two dimensions.

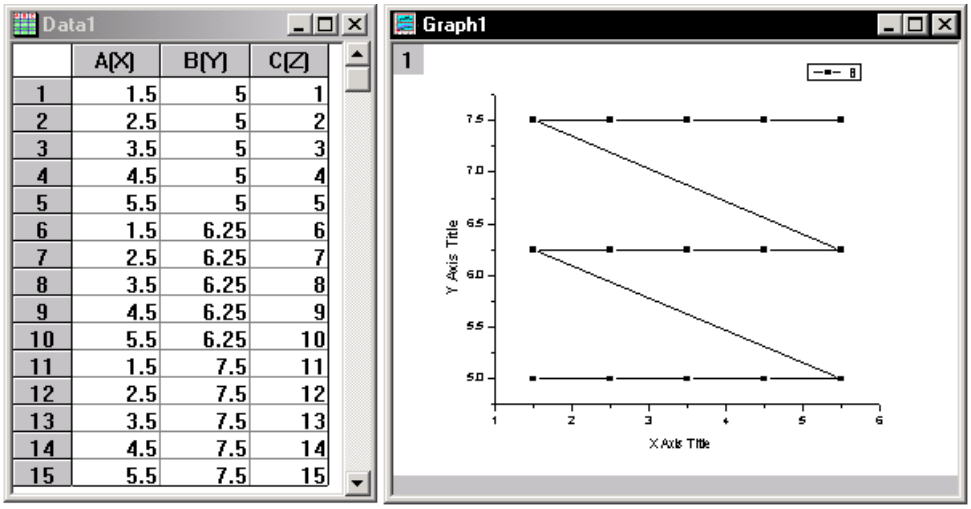
This tool can be versatile in data exploration, where you have values of more than two parameters from a sequence of measurements. You can explore the dependencies among any two of the parameters at a time, by selecting those two as your X and Y columns and creating a 2D matrix.

To learn more about 2D binning, review the 2D BINNING.OPJ project located in your Origin \SAMPLES\ANALYSIS\2D BINNING folder. Additionally, review the WORKSHEET TO MATRIX.OPJ project located in your Origin \SAMPLES\ANALYSIS\WORKSHEET TO MATRIX folder.

Converting Regular XYZ Data

In order for XYZ worksheet data to be classified as Regular, the XY data must meet the following requirements. Each X value must have the same number of Y values and each Y value must have the same number of X values. In addition, both the X and the Y data values must be equally spaced. To check for regularity, you can plot the XY data sets as a line and symbol graph.

Plotting Worksheet Data to Check Regularity



	A(X)	B(Y)	C(Z)
1	1.5	5	1
2	2.5	5	2
3	3.5	5	3
4	4.5	5	4
5	5.5	5	5
6	1.5	6.25	6
7	2.5	6.25	7
8	3.5	6.25	8
9	4.5	6.25	9
10	5.5	6.25	10
11	1.5	7.5	11
12	2.5	7.5	12
13	3.5	7.5	13
14	4.5	7.5	14
15	5.5	7.5	15

To convert regular XYZ worksheet data to a matrix, select the Z column and then select **Edit:Convert to Matrix:Regular XYZ**. The data is analyzed and put into a new matrix. To do this, Origin performs the following:

1) Origin first looks for duplicates in the data set and replaces them with mean values. Specifically, if there are multiple (x,y,z) points that have the same x,y values, these are replaced with just one (x,y,z) point where the new z value is the mean of all the z values of the duplicate points.

2) Origin then analyzes the x,y data sets to identify the locations of the steps in the data, thereby also determining how many groups are present in both data sets.

3) Origin then goes through each group of the x,y data set to look for fluctuations in the data values around the median value. If the fluctuations are larger than 25% of the step size (determined in step 2), then the conversion quits.

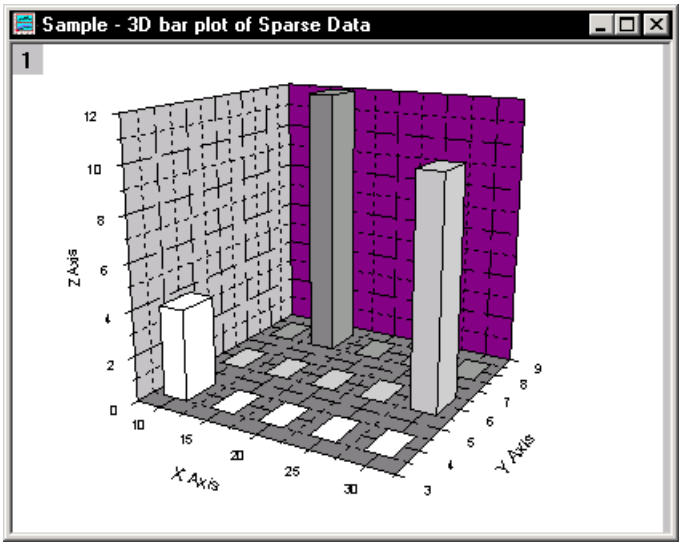
4) If the x,y data sets pass the test in step 3, then the data is sent to Origin's regular conversion routine, after setting the **mat.res** property to 0. Thus, the **mat.res** property is now only an internal parameter - you no longer need to set this property value.

Note: Because of the condition imposed in step 3, if there is too much fluctuation in the x,y data within each group, the algorithm will reject the data. The assumption is that there are only a few points within each group that deviate from the median. Therefore, if all the data points within a group are slightly different from each other and different only by a small amount compared to the step size from one group to the other, the algorithm may still reject the data set.

To learn more about converting regular XYZ data, review the WORKSHEET TO MATRIX.OPJ project located in your Origin \SAMPLES\ANALYSIS\WORKSHEET TO MATRIX folder.

Converting Sparse XYZ Data

The Sparse XYZ conversion is provided for the those who need to create a 3D plot with Z values plotted at specific X and Y values, as in the accompanying 3D bar plot.



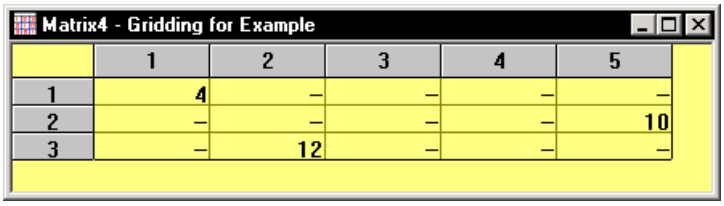
An Origin worksheet of the values might look something like this:

Example - Sparse XYZ

	A(X)	B(Y)	C(Z)
1	10	4	4
2	15	8	12
3	30	6	10
4			

The sparse conversion is similar to the regular XYZ conversion, except in the case of the sparse conversion, missing XY pairs are acceptable. During the conversion, these missing XY pairs are carried

over (no interpolation is performed). Thus, when converting the previous worksheet, if the X increment is set to 5 and the Y increment to 2 in the Gridding Parameters dialog box (all else left at the default), then the following matrix is created:



	1	2	3	4	5
1	4	–	–	–	–
2	–	–	–	–	10
3	–	12	–	–	–

To convert your worksheet to a matrix using the Sparse conversion, select the Z column and then select **Edit:Convert to Matrix:Sparse XYZ**.

To learn more about converting sparse XYZ data, review the WORKSHEET TO MATRIX.OPJ project located in your Origin \SAMPLES\ANALYSIS\WORKSHEET TO MATRIX folder.

To learn more about regular conversion, see "Converting Regular XYZ Data" on page 111.

Converting Random XYZ Data

If your worksheet data does not fall into any of the previously mentioned types (regular, direct, expand, 2D binning, sparse), then it can be classified as random data. The procedure for converting random XYZ data to a matrix is called gridding. To convert random XYZ data to a matrix, select the Z column and then select **Edit:Convert to Matrix:Random XYZ**. This menu command opens the Random XYZ Gridding tool.

Origin offers a number of gridding methods, including the method of Renka and Cline and a modification of Shepard's method. Both methods are implemented by calling the `nag_2d_scat_interpolant` function provided in the NAG C Library eo1 Interpolation. This function is documented in the NAG file e01sac_cl05.pdf. The documentation includes a discussion of the NQ, NW, and RNQ parameters for the modified Shepard's method. (When you install Origin, you are provided the option to install the NAG PDF files which document the NAG functions. If you clicked Yes to install these files, a \NAG PDFs folder is created with a subfolder for each library. If you did not install the PDFs, they remain accessible on your installation CD. Furthermore, you can install them at a later date by running the Origin "Add or Remove Files" program.)

The correlation method computes a new value for each cell in the regular matrix from the values of the points in the adjoining cells in the matrix that are included within the search radius. The computation is based on the Kriging method as can be found in Davis, John C., 1986. Statistics and Data Analysis in Geology. John Wiley & Sons, Inc. Second edition, pp. 383.

The weighted average method is a simple weighted average of the points with the weight equal to 1/r, where r is the distance of each point from the cell. If there is no value within the search radius, the radius is increased until at least one point is encountered. Increasing the search radius means that each point is more inter-related to neighboring points, producing a smoother surface that may lose fine details.

In addition to these new gridding methods, the Random XYZ Gridding tool provides a Show Plot check box and an Apply button. When the Show Plot check box is selected and Apply or OK are clicked, a graph is created that shows the raw data as an XYZ scatter plot and the grid as a mesh plot. If you clicked Apply,

you can then change the gridding method and click Apply again to view the raw data and updated gridding results in the graph. By changing the gridding method and re-clicking Apply, you can compare the graph output for the various methods and then choose the method which produces a surface that best includes the points.

Note: If duplicate XY pairs are found, this tool replaces all duplicate points with the average value.

Random Gridding Options for Correlation, Quick Correlation, and Weighted Average:

Number of Columns/Rows: Specifies the grid dimensions.

Search Radius: Minimum number of grid points from the current position used for computing the value of the current cell. If the given position has less than three points in any of the four adjacent quadrants, the search radius is increased until there are enough points or a boundary is reached.

Smoothness: Used by correlation (Kriging) method only. Relates values of points in the search radius to the computed value. Smaller values generate smoother surfaces.

To learn more about converting random XYZ data, review the WORKSHEET TO MATRIX.OPJ project located in your Origin \SAMPLES\ANALYSIS\WORKSHEET TO MATRIX folder.

Converting a Matrix into a Worksheet

Direct Conversion

To directly convert the active matrix to a worksheet, select **Edit:Convert to Worksheet:Direct**. This menu command creates a new worksheet and names the window Data*n*, where *n* is the lowest number available (not currently used in a worksheet name) in the project. The worksheet is created with the same number of rows and columns as the associated matrix. The first worksheet column is a designated X column by default. Remaining columns are designated Y. Origin fills the worksheet with the matrix values, maintaining the same row and column positions in the worksheet.

Creating a Worksheet with XYZ Columns

To convert the matrix to a worksheet with XYZ values, select **Edit:Convert to Worksheet:XYZ Columns**. This menu command opens the Convert Matrix to Worksheet dialog box. To display worksheet values sorted by the X mapping values, select X Constant 1st from the Conversion Type drop-down list. To display worksheet values sorted by the Y mapping values, select Y Constant 1st from the Conversion Type drop-down list. After clicking OK, this menu command creates a worksheet with X, Y, and Z columns. The cell values of the matrix are converted to Z data in the worksheet. The corresponding X and Y column values in the worksheet are set by the X and Y coordinate mapping information in the matrix.

Saving a Matrix Window

Select **File:Save Window As** to save a matrix window with all of its data. This menu command opens the Save As dialog box. 'Matrix (*.OGM)' is selected (by default) from the Save as Type drop-down list. Type the desired file name in the File Name text box and select the desired destination folder. You do not need to include the file extension in the File Name text box.

Saving a Matrix as a Template

To save a matrix with all formatting and relationships, but without any data, select **File:Save Template As**. This menu command opens the Save As dialog box. 'Matrix Template (*.OTM)' is selected (by default) from the Save as Type drop-down list. Type the desired file name in the File Name text box and select the desired destination folder. You do not need to include the file extension in the File Name text box.

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