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Overview

Igor Pro is a powerful data analysis environment. The power comes from a synergistic combination of
• An extensive set of basic built-in analysis operations
• A fast and flexible waveform arithmetic capability
• Immediate feedback from graphs and tables
• Extensibility through an interactive programming environment
• Extensibility through external code modules (XOPs and XFUNCs)

Analysis tasks in Igor range from simple experiments using no programming to extensive systems tailored for specific fields. Chapter I-2, Guided Tour of Igor Pro, shows examples of the former. WaveMetrics’ “Peak Measurement” procedure package is an example of the latter.

This chapter presents some of the basic analysis operations and discusses the more common analyses that can be derived from the basic operations. The end of the chapter shows a number of examples of using Igor’s programmability for “number crunching”.

Discussion of Igor Pro’s more specialized analytic capabilities is in chapters that follow.

See the WaveMetrics procedures, technical notes, and sample experiments that come with Igor Pro for more examples.

Analysis of Multidimensional Waves

Many of the analysis operations in Igor Pro operate on 1D (one-dimensional) data. However, Igor Pro includes the following capabilities for analysis of multidimensional data:
• Multidimensional waveform arithmetic
• Matrix math operations
• The MatrixOp operation
• Multidimensional Fast Fourier Transform
• 2D and 3D image processing operations
• 2D and 3D interpolation operations and functions

Some of these topics are discussed in Chapter II-6, Multidimensional Waves and in Chapter III-11, Image Processing. The present chapter focuses on analysis of 1D waves.

There are many analysis operations that are designed only for 1D data. Multidimensional waves do not appear in dialogs for these operations. If you invoke them on multidimensional waves from the command line or from an Igor procedure, Igor treats the multidimensional waves as if they were 1D. For example, the Histogram operation treats a 2D wave consisting of $n$ rows and $m$ columns as if it were a 1D wave with $n \times m$ rows. In some cases (e.g., WaveStats), the operation will be useful. In other cases, it will make no sense at all.

Waveform Versus XY Data

Igor is highly adapted for dealing with waveform data. In a waveform, data values are uniformly spaced in the X dimension. This is discussed under Waveform Model of Data on page II-57.

If your data is uniformly spaced, you can set the spacing using the SetScale operation. This is crucial because most of the built-in analysis operations and functions need to know this to work properly.

If your data is not uniformly spaced, you can represent it using an XY pair of waves. This is discussed under XY Model of Data on page II-58. Some of the analysis operations and functions in Igor can not handle XY pairs directly. To use these, you must either make a waveform representation of the XY pair or use Igor procedures that build on the built-in routines.
Converting XY Data to a Waveform

Sometimes the best way to analyze XY data is to make a uniformly-spaced waveform representation of it and analyze that instead. Most analysis operations are easier with waveform data. Other operations, such as the FFT, can be done only on waveform data. Often your XY data set is nearly uniformly-spaced so a waveform version of it is a very close approximation.

In fact, often XY data imported from other programs has an X wave that is completely unnecessary in Igor because the values in the X wave are actually a simple "series" (values that define a regular intervals, such as 2.2, 2.4, 2.6, 2.8, etc), in which case conversion to a waveform is a simple matter of assigning the correct X scaling to the Y data wave, using SetScale (or the Change Wave Scaling dialog):

```
SetScale/P x, xWave[0], xWave[1]-xWave[0], yWave
```

Now the X wave is superfluous and can be discarded:

```
KillWaves/Z xWave
```

The XY Pair to Waveform panel can be used to set the Y wave’s X scaling when it detects that the X wave contains series data. See Using the XY Pair to Waveform Panel on page III-104.

If your X wave is not a series, then to create a waveform representation of XY data you need to use interpolation. To create a waveform representation of XY data you need to do interpolation. Interpolation creates a waveform from an XY pair by sampling the XY pair at uniform intervals.

The diagram below shows how the XY pair defining the upper curve is interpolated to compute the uniformly-spaced waveform defining the lower curve. Each arrow indicates an interpolated waveform value:

Igor provides three tools for doing this interpolation: The XY Pair to Waveform panel, the built-in interp function and the Interpolate2 operation. To illustrate these tools we need some sample XY data. The following commands make sample data and display it in a graph:

```
Make/N=100 xData = .01*x + gnoise(.01)
Make/N=100 yData = 1.5 + 5*exp(-(xData-.5)/.1)^2)
Display yData vs xData
```

This creates a Gaussian shape. The x wave in our XY pair has some noise in it so the data is not uniformly spaced in the X dimension.

The x data goes roughly from 0 to 1.0 but, because our x data has some noise, it may not be monotonic. This means that, as we go from one point to the next, the x data usually increases but at some points may decrease. We can fix this by sorting the data.

```
Sort xData, xData, yData
```

This command uses the xData wave as the sort key and sorts both xData and yData so that xData always increases as we go from one point to the next.

Using the XY Pair to Waveform Panel

The XY Pair to Waveform panel creates a waveform from XY data using the SetScale or Interpolate2 operations, based on an automatic analysis of the X wave's data.
The required steps are:

1. Select XY Pair to Waveform from Igor's Data→Packages submenu.
   The panel is displayed:

   ![XY Pair to Waveform Panel](image)

   2. Select the X and Y waves (xData and yData) in the popup menus. When this example's xData wave
      is analyzed it is found to be "not regularly spaced (slope error avg= 0.52...)”, which means that Set-
      Scale is not appropriate for converting yData into a waveform.

   3. Use Interpolate is selected here, so you need a waveform name for the output. Enter any valid wave
      name.

   4. Set the number of output points. Using a number roughly the same as the length of the input waves
      is a good first attempt. You can choose a larger number later if the fidelity to the original is insuffi-
      cient. A good number depends on how uneven the X values are - use more points for more uneven-
      ness.

   5. Click Make Waveform.

   6. To compare the XY representation of the data with the waveform representation, append the wave-
      form to a graph displaying the XY pair. Make that graph the top graph, then click the "Append to
      <Name of Graph>" button.

   7. You can revise the Number of Points and click Make Waveform to overwrite the previously created
      waveform in-place.

**Using the Interp Function**

We can use the `interp` function (see page V-397) to create a waveform version of our Gaussian. The required
steps are:

1. Make a new wave to contain the waveform representation.
2. Use the `SetScale` operation to define the range of X values in the waveform.
3. Use the interp function to set the data values of the waveform based on the XY data.

Here are the commands:

```plaintext
Duplicate yData, wData
SetScale/I x 0, 1, wData
wData = interp(x, xData, yData)
```

To compare the waveform representation to the XY representation, we append the waveform to the graph.

```plaintext
AppendToGraph wData
```

Let's take a closer look at what these commands are doing.
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First, we cloned yData and created a new wave, wData. Since we used Duplicate, wData will have the same number of points as yData. We could have made a waveform with a different number of points. To do this, we would use the Make operation instead of Duplicate.

The SetScale operation sets the X scaling of the wData waveform. In this example, we are setting the X values of wData to go from 0 up to and including 1.0. This means that our waveform representation will contain 100 values at uniform intervals in the X dimension from 0 to 1.0.

The last step uses a waveform assignment to set the data values of wData. This assignment evaluates the right-hand expression once for each point in wData. For each evaluation, x takes on a different value from 0 to 1.0. The interp function returns the value of the curve yData versus xData at x. For instance, x=0.40404 (point number 40 of wData) falls between two points in the XY curve. The interp function linearly interpolates between those values to estimate a data value of 3.50537:

We can wrap these calculations up into an Igor procedure that can create a waveform version of any XY pair.

Function XYToWave1(xWave, yWave, wWaveName, numPoints)
    Wave/D xWave // X wave in the XY pair
    Wave/D yWave // Y wave in the XY pair
    String wWaveName // Name to use for new waveform wave
    Variable numPoints // Number of points for waveform
    Make/O/N=(numPoints) $wWaveName // Make waveform.
    Wave wWave= $wWaveName
    WaveStats/Q xWave // Find range of x coords
    SetScale/I x V_min, V_max, wWave // Set X scaling for wave
    wWave = interp(x, xWave, yWave) // Do the interpolation
End

This function uses the WaveStats operation to find the X range of the XY pair. WaveStats creates the variables V_min and V_max (among others). See Accessing Variables Used by Igor Operations on page IV-115 for details.

The function makes the assumption that the input waves are already sorted. We left the sort step out because the sorting would be a side-effect and we prefer that procedures not have nonobvious side effects.

To use the WaveMetrics-supplied XYToWave1 function, include the “XY Pair To Waveform” procedure file. See The Include Statement on page IV-155 for instructions on including a procedure file.

If you have blanks (NaNs) in your input data, the interp function will give you blanks in your output waveform as well. The Interpolate2 operation, discussed in the next section, interpolates across gaps in data and does not produce blanks in the output.

Using the Interpolate2 Operation

The Interpolate2 operation provides not only linear but also cubic and smoothing spline interpolation. Furthermore, it does not require the input to be sorted and can automatically make the destination waveform and set its X scaling. It also has a dialog that makes it easy to use interactively.

To use it on our sample XY data, choose Analysis→Interpolate and set up the dialog as shown:
Choosing “_auto_” for Y Destination auto-names the destination wave by appending “_L” to the name of the input “Y data” wave. Choosing “_none_” as the “X destination” creates a waveform from the input XY pair rather than a new XY pair.

Here is a rewrite of the XYToWave1 function that uses the Interpolate2 operation rather than the interp function.

```plaintext
Function XYToWave2(xWave, yWave, wWaveName, numPoints)
  Wave xWave // X wave in the XY pair
  Wave yWave // Y wave in the XY pair
  String wWaveName // Name to use for new waveform wave
  Variable numPoints // Number of points for waveform

  Interpolate2/T=1/N=(numPoints)/E=2/Y=$wWaveName xWave, yWave
End
```

Blanks in the input data are ignored.

For details on Interpolate2, see The Interpolate2 Operation on page III-110.

**Dealing with Missing Values**

A missing value is represented in Igor by the value NaN which means “Not a Number”. A missing value is also called a “blank”, because it appears as a blank cell in a table.

When a NaN is combined arithmetically with any value, the result is NaN. To see this, execute the command:

```plaintext
Print 3+NaN, NaN/5, sin(NaN)
```

By definition, a NaN is not equal to anything. Consequently, the condition in this statement:

```plaintext
if (myValue == NaN)
```

is always false.

The workaround is to use the `numtype` function:

```plaintext
if (NumType(myValue) == 2) // Is it a NaN?
```
See also NaNs, INFs and Missing Values on page II-76 for more about how NaN values.

Some routines deal with missing values by ignoring them. The CurveFit operation (see page V-105) is one example. Others may produce unexpected results in the presence of missing values. Examples are the FFT operation and the area and mean functions.

Here are some strategies for dealing with missing values.

### Replace the Missing Values With Another Value

You can replace NaNs in a wave with this statement:

```plaintext
wave0 = NumType(wave0)==2 ? 0:wave0 // Replace NaNs with zero
```

If you’re not familiar with the :? operator, see Operators on page IV-5.

For multi-dimensional waves you can replace NaNs using MatrixOp. For example:

```plaintext
Make/O/N=(3,3) matNaNTest = p + 10*q
Edit matNaNTest
matNaNTest[0][0] = NaN; matNaNTest[1][1] = NaN; matNaNTest[2][2] = NaN
MatrixOp/O matNaNTest=ReplaceNaNs(matNaNTest,0) // Replace NaNs with 0
```

### Remove the Missing Values

For 1D waves you can remove NaNs using WaveTransform zapNaNs. For example:

```plaintext
Make/N=5 NaNTest = p
Edit NaNTest
NaNTest[1] = NaN; NaNTest[4] = NaN
WaveTransform zapNaNs, NaNTest
```

There is no built-in operation to remove NaNs from an XY pair if the NaN appears in either the X or Y wave. You can do this, however, using the RemoveNaNsXY procedure in the "Remove Points" WaveMetrics procedure file which you can access through Help→Windows→WM Procedures Index.

There is no operation to remove NaNs from multi-dimensional waves as this would require removing the entire row and entire column where each NaN appeared.

### Work Around Gaps in Data

Many analysis routines can work on a subrange of data. In many cases you can just avoid the regions of data that contain missing values. In other cases you can extract a subset of your data, work with it and then perhaps put the modified data back into the original wave.

Here is an example of extract-modify-replace (even though Smooth properly accounts for NaNs):

```plaintext
Make/N=100 data1= sin(P/8)+gnoise(.05); data1[50]= NaN
Display data1
Duplicate/R=[0,49] data1,tmpdata1 // start work on first set
Smooth 5,tmpdata1
data1[0,49]= tmpdata1[P] // put modified data back
Duplicate/O/R=[51,,] data1,tmpdata1 // start work on 2nd set
Smooth 5,tmpdata1
data1[51,,]= tmpdata1[P-51]
KillWaves tmpdata1
```

### Replace Missing Data with Interpolated Values

You can replace NaN data values prior to performing operations that do not take kindly to NaNs by replacing them with smoothed or interpolated values using the Smooth operation (page V-748), the Loess operation (page V-454), or The Interpolate2 Operation.
Replace Missing Data Using the Interpolate2 Operation

By using the same number of points for the destination as you have source points, you can replace NaNs without modifying the other data.

If you have waveform data, simply duplicate your data and perform linear interpolation using the same number of points as your data. For example, assuming 100 data points:

\[ \text{Duplicate } \text{data1}, \text{data1a} \]
\[ \text{Interpolate } \text{T=1/N=100/Y=data1a/datal} \]

If you have XY data, the Interpolate2 operation has the ability to include the input x values in the output X wave. For example:

\[ \text{Duplicate } \text{data1, yData1, xData1} \]
\[ \text{xData1} = x \]
\[ \text{Display } \text{yData1 vs xData1} \]
\[ \text{Interpolate2 } \text{T=1/N=100/I/Y=yData1a/X=xData1a/xData1,yData1} \]

If, after performing an operation on your data, you wish to put the modified data back in the source wave while maintaining the original missing values you can use a wave assignment similar to this:

\[ \text{yData1 = (numtype(yData1) == 0) ? yData1 : yData1a} \]

This technique can also be applied using interpolated results generated by the Smooth operation (page V-748) or the Loess operation (page V-454).

Replace Missing Data Using Median Smoothing

You can use the Smooth dialog to replace each NaN with the median of surrounding values.

Select the Median smoothing algorithm, select "NaNs" from the Replace popup, and choose "Median" for the "with:" radio button. Enter the number of surrounding points used to compute the median (an odd number is best).

You can choose to overwrite the NaNs or create a new waveform with the result. The Smooth dialog produces commands like this:

\[ \text{Duplicate/O data1, data1_smth; DelayUpdate} \]
\[ \text{Smooth/M=(NaN) 5, data1_smth} \]

Interpolation

Igor Pro has a number of interpolation tools that are designed for different applications. We summarize these in the table below.

<table>
<thead>
<tr>
<th>Data</th>
<th>Operation/Function</th>
<th>Interpolation Method</th>
</tr>
</thead>
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<tr>
<td>1D waves</td>
<td>wave assignment, e.g., val=wave(x)</td>
<td>Linear</td>
</tr>
<tr>
<td>1D waves</td>
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<td>Running median, average, binomial, Savitsky-Golay</td>
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<tr>
<td>1D XY waves</td>
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<tr>
<td>1D single or XY waves</td>
<td>The Interpolate2 Operation</td>
<td>Linear, cubic spline, smoothing spline</td>
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<tr>
<td>1D or 2D single or XY</td>
<td>Loess</td>
<td>Locally-weighted regression</td>
</tr>
<tr>
<td>Triplet XYZ waves</td>
<td>ImageInterpolate</td>
<td>Voronoi</td>
</tr>
<tr>
<td>1D X, Y, Z waves</td>
<td>Data→Packages→XYZ to Matrix</td>
<td>Voronoi</td>
</tr>
<tr>
<td>1D X, Y, Z waves</td>
<td>Loess</td>
<td>Locally-weighted regression</td>
</tr>
<tr>
<td>2D waves</td>
<td>ImageInterpolate</td>
<td>Bilinear, splines, Kriging, Voronoi</td>
</tr>
</tbody>
</table>
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<table>
<thead>
<tr>
<th>Data</th>
<th>Operation/Function</th>
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<tbody>
<tr>
<td>2D waves</td>
<td>Interp2D()</td>
<td>Bilinear</td>
</tr>
<tr>
<td>2D waves (points on the surface of a sphere)</td>
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<tr>
<td>3D waves</td>
<td>Interp3D(), Interp3DPath, ImageTransform extractSurface</td>
<td>Trilinear</td>
</tr>
<tr>
<td>3D scatter data</td>
<td>Interpolate3D</td>
<td>Barycentric</td>
</tr>
</tbody>
</table>

All the interpolation methods in this table consist of two common steps. The first step involves the identification of data points that are nearest to the interpolation location and the second step is the computation of the interpolated value using the neighboring values and their relative proximity. You can find the specific details in the documentation of the individual operation or function.

The Interpolate2 Operation

The Interpolate2 operation performs linear, cubic spline and smoothing cubic spline interpolation on 1D waveform and XY data. The cubic spline interpolation is based on a routine in "Numerical Recipes in C". The smoothing spline is based on "Smoothing by Spline Functions", Christian H. Reinsch, Numerische Mathematische 10, 177-183 (1967).

Prior to Igor7, Interpolate2 was implemented as part of the Interpolate XOP. It is now built-in.

The Interpolate XOP also implemented an older operation named Interpolate which used slightly different syntax. If you are using the Interpolate operation, we recommend that you convert to using Interpolate2.

The main use for linear interpolation is to convert an XY pair of waves into a single wave containing Y values at evenly spaced X values so that you can use Igor operations, like FFT, which require evenly spaced data.

Cubic spline interpolation is most useful for putting a pleasingly smooth curve through arbitrary XY data. The resulting curve may contain features that have nothing to do with the original data so you should be wary of using the cubic spline for analytic rather than esthetic purposes.

Both linear and cubic spline interpolation are constrained to put the output curve through all of the input points and thus work best with a small number of input points. The smoothing spline does not have this constraint and thus works well with large, noisy data sets.

The Interpolate2 operation has a feature called "pre-averaging" which can be used when you have a large number of input points. Pre-averaging was added to Interpolate2 as a way to put a cubic spline through a large, noisy data set before it supported the smoothing spline. We now recommend that you use the smoothing spline instead of pre-averaging.


Spline Interpolation Example

Before going into a complete discussion of Interpolate2, let's look at a simple example first.

First, make some sample XY data using the following commands:

```
Make/N=10 xData, yData  // Make source data
xData = p; yData = 3 + 4*xData + gnoise(2)  // Create sample data
Display yData vs xData  // Make a graph
Modify mode=2, lsize=3  // Display source data as dots
```

Now, choose Analysis→Interpolate to invoke the Interpolate dialog.
Set Interpolation Type to Cubic Spline.
Choose yData from the Y Data pop-up menu.
Choose xData from the X Data pop-up menu.
Choose _auto_ from the Y Destination pop-up menu.
Choose _none_ from the X Destination pop-up menu.
Enter 200 in the Destination Points box.
Choose Off from the Pre-averaging pop-up menu.
Choose Evenly Spaced from the Dest X Coords pop-up menu.
Click Natural in the End Points section.
Notice that the dialog has generated the following command:
Interpolate2/T=2/N=200/E=2/Y=yData_CS xData, yData
This says that Interpolate2 will use yData as the Y source wave, xData as the X source wave and that it will
create yData_CS as the destination wave. _CS means "cubic spline".
Click the Do It button to do the interpolation.
Now add the yData_CS destination wave to the graph using the command:
AppendToGraph yData_CS; Modify rgb(yData_CS)=(0,0,65535)
Now let's try this with a larger number of input data points. Execute:
Redimension/N=500 xData, yData
xData = p/50; yData = 10*sin(xData) + gnoise(1.0)  // Create sample data
Modify lsize(yData)=1  // Smaller dots
Now choose Analysis→Interpolate to invoke the Interpolate dialog. All the settings should be as you left
them from the preceding exercise. Click the Do It button.
Notice that the resulting cubic spline attempts to go through all of the input data points. This is usually not
what we want.
Now, choose Analysis→Interpolate again and make the following changes:
Choose Smoothing Spline from the Interpolation Type pop-up menu. Notice the command generated now
references a wave named yData_SS. This will be the output wave.
Enter 1.0 for the smoothing factor. This is usually a good value to start from.
In the Standard Deviation section, click the Constant radio button and enter 1.0 as the standard deviation
value. 1.0 is correct because we know that our data has noise with a standard deviation of 1.0, as a result of
the "gnoise(1.0)" term above.
Click the Do It button to do the interpolation. Append the yData_SS destination wave to the graph using
the command:
AppendToGraph yData_SS; Modify rgb(yData_SS)=(0,0,0)
Notice that the smoothing spline adds a pleasing curve through the large, noisy data set. If necessary,
enlarge the graph window so you can see this.
You can tweak the smoothing spline using either the smoothing factor parameter or the standard deviation
parameter. If you are unsure of the standard deviation of the noise, leave the smoothing factor set to 1.0 and
try different standard deviation values. It is usually not too hard to find a reasonable value.
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The Interpolate Dialog

Choosing Analysis→Interpolate summons the Interpolate dialog from which you can choose the desired type of interpolation, the source wave or waves, the destination wave or waves, and the number of points in the destination waves. This dialog generates an **Interpolate2** command which you can execute, copy to the clipboard or copy to the command line.

From the Interpolation Type pop-up menu, choose Linear or Cubic Spline or Smoothing Spline. Cubic spline is good for a small input data set. Smoothing spline is good for a large, noisy input data set.

If you choose Cubic Spline, a Pre-averaging pop-up menu appear. The pre-averaging feature is largely no longer needed and is not recommended. Use the smoothing spline instead of the cubic spline with pre-averaging.

If you choose smoothing spline, a Smoothing Factor item and Standard Deviation controls appear. Usually it is best to set the smoothing factor to 1.0 and use the constant mode for setting the standard deviation. You then need to enter an estimate for the standard deviation of the noise in your Y data. Then try different values for the standard deviation until you get a satisfactory smooth spline through your data. See **Smoothing Spline Parameters** on page III-113 for further details.

From the Y Data and X Data pop-up menus, choose the source waves that define the data through which you want to interpolate. If you choose a wave from the X Data pop-up, Interpolate2 uses the XY curve defined by the contents of the Y data wave versus the contents of the X data wave as the source data. If you choose _calculated_ from the X Data pop-up, it uses the X and Y values of the Y data wave as the source data.

If you click the From Target checkbox, the source and destination pop-up menus show only waves in the target graph or table.

The X and Y data waves must have the same number of points. They do not need to have the same data type.

The X and Y source data does not need to be sorted before using Interpolate2. If necessary, Interpolate2 sorts a copy of the input data before doing the interpolation.

NaNs (missing values) and INFs (infinite values) in the source data are ignored. Any point whose X or Y value is NaN or INF is treated as if it did not exist.

Enter the number of points you want in the destination waves in the Destination Points box. 200 points is usually good.

From the Y Destination and X Destination pop-up menus, choose the waves to contain the result of the interpolation. For most cases, choose _auto_ for the Y destination wave and _none_ for the X destination wave. This gives you an output waveform. Other options, useful for less common applications, are described in the following paragraphs.

If you choose _auto_ from the Y Destination pop-up, Interpolate2 puts the Y output data into a wave whose name is derived by adding a suffix to the name of the Y data wave. The suffix is "_L" for linear interpolation, "_CS" for cubic spline interpolation and "_SS" for smoothing spline interpolation. For example, if the Y data wave is called "yData", then the default Y destination wave will be called "yData_L", "yData_CS" or "yData_SS".

If you choose _none_ for the X destination wave, Interpolate2 puts the Y output data in the Y destination wave and sets the X scaling of the Y destination wave to represent the X output data.

If you choose _auto_ from the X Destination pop-up, Interpolate2 puts the X output data into a wave whose name is derived by adding the appropriate suffix to the name of the X data wave. If the X data wave is "xData" then the X destination wave will be "xData_L", "xData_CS" or "xData_SS". If there is no X data wave then the X destination wave name is derived by adding the letter "x" to the name of the Y destination wave. For example, if the Y destination is "yData_CS" then the X destination wave will be "yData_CSx".
For both the X and the Y destination waves, if the wave already exists, Interpolate2 overwrites it. If it does not already exist, Interpolate2 creates it.

The destination waves will be double-precision unless they already exist when Interpolate2 is invoked. In this case, Interpolate2 leaves single-precision destination waves as single-precision. For any other precision, Interpolate2 changes the destination wave to double-precision.

The Dest X Coords pop-up menu gives you control over the X locations at which the interpolation is done. Usually you should choose Evenly Spaced. This generates interpolated values at even intervals over the range of X input values.

The Evenly Spaced Plus Input X Coords setting is the same as Evenly Spaced except that Interpolate2 makes sure that the output X values include all of the input X values. This is usually not necessary. This mode is not available if you choose _none_ for your X destination wave.

The Log Spaced setting makes the output evenly spaced on a log axis. Use this if your input data is graphed with a log X axis. This mode ignores any non-positive values in your input X data. It is not available if you choose _none_ for your X destination wave.

The From Dest Wave setting takes the output X values from the X coordinates of the destination wave. The Destination Points setting is ignored. You could use this, for example, to get a spline through a subset of your input data. You must create your destination waves before doing the interpolation for this mode. If your destination is a waveform, use the SetScale operation to define the X values of the waveform. Interpolate2 will calculate its output at these X values. If your destination is an XY pair, set the values of the X destination wave. Interpolate2 will create a sorted version of these values and will then calculate its output at these values. If the X destination wave was originally reverse-sorted, Interpolate2 will reverse the output.

The End Points radio buttons apply only to the cubic spline. They control the destination waves in the first and last intervals of the source wave. Natural forces the second derivative of the spline to zero at the first and last points of the destination waves. Match 1st Derivative forces the slope of the spline to match the straight lines drawn between the first and second input points, and between the last and next-to-last input points. In most cases it doesn't much matter which of these alternatives you use.

**Smoothing Spline Algorithm**

The smoothing spline algorithm is based on "Smoothing by Spline Functions", Christian H. Reinsch, *Numerische Mathematik* 10. It minimizes

\[ \int_{x_0}^{x_n} g''(x)^2 \, dx, \]

among all functions \( g(x) \) such that

\[ \sum_{i=0}^{n} \left( \frac{g(x_i) - y_i}{\sigma_i} \right)^2 \leq S, \]

where \( g(x_i) \) is the value of the smooth spline at a given point, \( y_i \) is the Y data at that point, \( \sigma_i \) is the standard deviation of that point, and \( S \) is the smoothing factor.

**Smoothing Spline Parameters**

The smoothing spline operation requires a standard deviation parameter and a smoothing factor parameter. The standard deviation parameter should be a good estimate of the standard deviation of the noise in your Y data. The smoothing factor should nominally be close to 1.0, assuming that you have an accurate standard deviation estimate.
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Using the Standard Deviation section of the Interpolate2 dialog, you can choose one of three options for the standard deviation parameter: None, Constant, From Wave.

If you choose None, Interpolate2 uses an arbitrary standard deviation estimate of 0.05 times the amplitude of your Y data. You can then play with the smoothing factor parameter until you get a pleasing smooth spline. Start with a smoothing factor of 1.0. This method is not recommended.

If you choose Constant, you can then enter your estimate for the standard deviation of the noise and Interpolate2 uses this value as the standard deviation of each point in your Y data. If your estimate is good, then a smoothing factor around 1.0 will give you a nice smooth curve through your data. If your initial attempt is not quite right, you should leave the smoothing factor at 1.0 and try another estimate for the standard deviation. For most types of data, this is the preferred method.

If you choose From Wave then Interpolate2 expects that each point in the specified wave contains the estimated standard deviation for the corresponding point in the Y data. You should use this method if you have an appropriate wave.

**Interpolate2’s Pre-averaging Feature**

A linear or cubic spline interpolation goes through all of the input data points. If you have a large, noisy data set, this is probably not what you want. Instead, use the smoothing spline.

Before Interpolate2 had a smoothing spline, we recommended that you use the cubic spline to interpolate through a decimated version of your input data. The pre-averaging feature was designed to make this easy.

Because Interpolate2 now supports the smoothing spline, the pre-averaging feature is no longer necessary. However, we still support it for backward compatibility.

When you turn pre-averaging on, Interpolate2 creates a temporary copy of your input data and reduces it by decimation to a smaller number of points, called nodes. Interpolate2 then usually adds nodes at the very start and very end of the data. Finally, it does an interpolation through these nodes.

**Identical Or Nearly Identical X Values**

This section discusses a degenerate case that is of no concern to most users.

Input data that contains two points with identical X values can cause interpolation algorithms to produce unexpected results. To avoid this, if Interpolate2 encounters two or more input data points with nearly identical X values, it averages them into one value before doing the interpolation. This behavior is separate from the pre-averaging feature. This is done for the cubic and smoothing splines except when the Dest X Coords mode is is Log Spaced or From Dest Wave. It is not done for linear interpolation.

Two points are considered nearly identical in X if the difference in X between them (dx) is less than 0.01 times the nominal dx. The nominal dx is computed as the X span of the input data divided by the number of input data points.

**Destination X Coordinates from Destination Wave**

This mode, which we call "X From Dest" mode for short, takes effect if you choose From Dest Wave from the Dest X Coords pop-up menu in the Interpolate2 dialog or use the Interpolate2 /I=3 flag. In this mode the number of output points is determined by the destination wave and the /N flag is ignored.

In X From Dest mode, the points at which the interpolation is done are determined by the destination wave. The destination may be a waveform, in which case the interpolation is done at its X values. Alternatively the destination may be an XY pair in which case the interpolation is done at the data values stored in the X destination wave.

Here is an example using a waveform as the destination:

```
Make /O /N=20 wave0 // Generate source data
SetScale x 0, 2*PI, wave0
wave0 = sin(x) + gnoise(.1)
```
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Display wave0
ModifyGraph mode=3
Make /O /N=1000 dest0 // Generate dest waveform
SetScale x 0, 2*PI, dest0
AppendToGraph dest0
ModifyGraph rgb(dest0)=(0,0,65535)
Interpolate2 /T=2 /I=3 /Y=dest0 wave0 // Do cubic spline interpolation

If your destination is an XY pair, Interpolate2 creates a sorted version of these values and then calculates its output at the X destination wave's values. If the X destination wave was originally reverse-sorted, as determined by examining its first and last values, Interpolate2 reverses the output after doing the interpolation to restore the original ordering.

In X From Dest mode with an XY pair as the destination, the X wave may contain NaNs. In this case, Interpolate2 creates an internal copy of the XY pair, removes the points where the X destination is NaN, does the interpolation, and copies the results to the destination XY pair. During this last step, Interpolate2 restores the NaNs to their original locations in the X destination wave. Here is an example of an XY destination with a NaN in the X destination wave:

Make/O xData={1,2,3,4,5}, yData={1,2,3,4,5} // Generate source data
Display yData vs xData
Make/O xDest={1,2,NaN,4,5}, yDest={0,0,0,0,0} // Generate dest XY pair
ModifyGraph mode=3,marker=19
AppendToGraph yDest vs xDest
ModifyGraph rgb(yDest)=(0,0,65535)
Interpolate2 /T=1 /I=3 /Y=yDest /X=xDest xData, yData // Do interpolation

Differentiation and Integration

The Differentiate operation (see page V-137) and Integrate operation (see page V-386) provide a number of algorithms for operation on one-dimensional waveform and XY data. These operations can either replace the original data or create a new wave with the results. The easiest way to use these operations is via dialogs available from the Analysis menu.

For most applications, trapezoidal integration and central differences differentiation are appropriate methods. However, when operating on XY data, the different algorithms have different requirements for the number of points in the X wave. If your X wave does not show up in the dialog, try choosing a different algorithm or click the help button to see what the requirements are.

When operating on waveform data, X scaling is taken into account; you can turn this off using the /P flag. You can use the SetScale operation (see page V-728) to define the X scaling of your Y data wave.

Although these operations work along just one dimension, they can be targeted to operate along rows or columns of a matrix (or even higher dimensions) using the /DIM flag.

The Integrate operation replaces or creates a wave with the numerical integral. For finding the area under a curve, see Areas and Means on page III-115.

Areas and Means

You can compute the area and mean value of a wave in several ways using Igor.

Perhaps the simplest way to compute a mean value is with the Wave Stats dialog in the Analysis menu. The dialog is pictured under Wave Statistics on page III-117. You select the wave, type in the X range (or use the current cursor positions), click Do It, and Igor prints several statistical results to the history area. Among them is V_avg, which is the average, or mean value. This is the same value that is returned by the mean function (see page V-503), which is faster because it doesn’t compute any other statistics. The mean function returns NaN if any data within the specified range is NaN. The WaveStats operation, on the other hand, ignores such missing values.
WaveStats and the `mean` function use the same method for computing the mean: find the waveform values within the given X range, sum them together, and divide by the number of values. The X range serves only to select the values to combine. The range is rounded to the nearest point numbers.

If you consider your data to describe discrete values, such as a count of events, then you should use either WaveStats or the mean function to compute the average value. You can most easily compute the total number of events, which is an area of sorts, using the `sum` function (see page V-872). It can also be done easily by multiplying the WaveStats outputs `V_avg` and `V_npnts`.

If your data is a sampled representation of a continuous process such as a sampled audio signal, you should use the `faverage` function to compute the mean, and the area function to compute the area. These two functions use the same linear interpolation scheme as does trapezoidal integration to estimate the waveform values between data points. The X range is not rounded to the nearest point. Partial X intervals are included in the calculation through this linear interpolation.

The diagram below shows the calculations each function performs for the data shown. The two values 43 and 92.2 are linear interpolation estimates.

![Diagram showing calculations for waveStats, mean, and faverage functions over interval (12.75, 13.32)]

<table>
<thead>
<tr>
<th>Function</th>
<th>Calculation</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>WaveStats/R=(12.75,13.32)</code> wave</td>
<td>$V_{\text{avg}} = (55+88+100+87)/4 = 82.5$</td>
</tr>
<tr>
<td><code>mean(wave,12.75,13.32)</code></td>
<td>$= (55+88+100+87)/4 = 82.5$</td>
</tr>
<tr>
<td><code>area(wave,12.75,13.32)</code></td>
<td>$= 0.05 \cdot (43+55) / 2 \quad \text{first trapezoid}$</td>
</tr>
<tr>
<td></td>
<td>$+ 0.20 \cdot (55+88) / 2 \quad \text{second trapezoid}$</td>
</tr>
<tr>
<td></td>
<td>$+ 0.20 \cdot (88+100) / 2 \quad \text{third trapezoid}$</td>
</tr>
<tr>
<td></td>
<td>$+ 0.12 \cdot (100+92.2) / 2 \quad \text{fourth trapezoid}$</td>
</tr>
<tr>
<td></td>
<td>$= 47.082$</td>
</tr>
<tr>
<td><code>faverage(wave,12.75,13.32)</code></td>
<td>$= \frac{\text{area(wave,12.75,13.32)}}{13.32-12.75}$ $= 47.082/0.57 = 82.6$</td>
</tr>
</tbody>
</table>

Note that only the area function is affected by the X scaling of the wave. `faverage` eliminates the effect of X scaling by dividing the area by the same X range that area multiplied by.

One problem with these functions is that they can not be used if the given range of data has missing values (NaNs). See `Dealing with Missing Values` on page III-107 for details.
X Ranges and the Mean, \textit{faverage}, and area Functions

The X range input for the mean, \textit{faverage} and area functions are optional. Thus, to include the entire wave you don’t have to specify the range:

\begin{verbatim}
Make/N=10 wave=2; Edit wave.xy // X ranges from 0 to 9
Print area(wave) // entire X range, and no more
\end{verbatim}

Sometimes, in programming, it is not convenient to determine whether a range is beyond the ends of a wave. Fortunately, these functions also accept X ranges that go beyond the ends of the wave.

\begin{verbatim}
Print area(wave, 0, 9) // entire X range, and no more
\end{verbatim}

You can use expressions that evaluate to a range beyond the ends of the wave:

\begin{verbatim}
Print leftx(wave),rightx(wave)
0 10
Print area(wave,leftx(wave),rightx(wave)) // entire X range, and more
\end{verbatim}

or even an X range of ±∞:

\begin{verbatim}
Print area(wave, -Inf, Inf)  // entire X range of the universe
\end{verbatim}

Finding the Mean of Segments of a Wave

Under \textbf{Analysis Programming} on page III-142 is a function that finds the mean of segments of a wave where you specify the length of the segments. It creates a new wave to contain the means for each segment.

Area for XY Data

To compute the area of a region of data contained in an XY pair of waves, use the \textit{areaXY} function (see page V-35). There is also an XY version of the \textit{faverage} function; see \textit{faverageXY} on page V-186.

In addition you can use the AreaXYBetweenCursors WaveMetrics procedure file which contains the AreaXYBetweenCursors and AreaXYBetweenCursorsLessBase procedures. For instructions on loading the procedure file, see \textbf{WaveMetrics Procedures Folder} on page II-32. Use the \textbf{Info Panel and Cursors} to delimit the X range over which to compute the area. AreaXYBetweenCursorsLessBase removes a simple trapezoidal baseline - the straight line between the cursors.

Wave Statistics

The \textbf{WaveStats} operation (see page V-934) computes various descriptive statistics relating to a wave and prints them in the history area of the command window. It also stores the statistics in a series of special variables or in a wave so you can access them from a procedure.

The statistics printed and the corresponding special variables are:

<table>
<thead>
<tr>
<th>Variable</th>
<th>Meaning</th>
</tr>
</thead>
<tbody>
<tr>
<td>V_npnts</td>
<td>Number of points in range excluding points whose value is NaN or INF.</td>
</tr>
<tr>
<td>V_numNaNs</td>
<td>Number of NaNs.</td>
</tr>
<tr>
<td>V_numINFs</td>
<td>Number of INFs.</td>
</tr>
<tr>
<td>V_avg</td>
<td>Average of data values.</td>
</tr>
<tr>
<td>V_sum</td>
<td>Sum of data values.</td>
</tr>
</tbody>
</table>
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<table>
<thead>
<tr>
<th>Variable</th>
<th>Meaning</th>
</tr>
</thead>
<tbody>
<tr>
<td>V_sdev</td>
<td>Standard deviation of data values, $\sigma = \sqrt{\frac{1}{V_{npnts} - 1} \sum (Y_i - V_{avg})^2}$</td>
</tr>
<tr>
<td>V_sem</td>
<td>Standard error of the mean $sem = \frac{\sigma}{\sqrt{V_{npnts}}}$</td>
</tr>
<tr>
<td>V_rms</td>
<td>RMS (Root Mean Square) of Y values $= \sqrt{\frac{1}{V_{npnts} \sum Y_i^2}}$</td>
</tr>
<tr>
<td>V_adev</td>
<td>Average deviation $= \frac{1}{V_{npnts}} \sum_{i=0}^{V_{npnts} - 1}</td>
</tr>
<tr>
<td>V_skew</td>
<td>Skewness $= \frac{1}{V_{npnts}} \sum_{i=0}^{V_{npnts} - 1} \left[ \frac{x_i - \bar{x}}{\sigma} \right]^3$</td>
</tr>
<tr>
<td>V_kurt</td>
<td>Kurtosis $= \frac{1}{V_{npnts}} \sum_{i=0}^{V_{npnts} - 1} \left[ \frac{x_i - \bar{x}}{\sigma} \right]^4 - 3$</td>
</tr>
<tr>
<td>V_minloc</td>
<td>X location of minimum data value.</td>
</tr>
<tr>
<td>V_min</td>
<td>Minimum data value.</td>
</tr>
<tr>
<td>V_maxloc</td>
<td>X location of maximum data value.</td>
</tr>
<tr>
<td>V_max</td>
<td>Maximum data value.</td>
</tr>
<tr>
<td>V_minRowLoc</td>
<td>Row containing minimum data value.</td>
</tr>
<tr>
<td>V_maxRowLoc</td>
<td>Row containing maximum data value.</td>
</tr>
<tr>
<td>V_minColLoc</td>
<td>Column containing minimum data value (2D or higher waves).</td>
</tr>
<tr>
<td>V_maxColLoc</td>
<td>Column containing maximum data value (2D or higher waves).</td>
</tr>
<tr>
<td>V_minLayerLoc</td>
<td>Layer containing minimum data value (3D or higher waves).</td>
</tr>
<tr>
<td>V_maxLayerLoc</td>
<td>Layer containing maximum data value (3D or higher waves).</td>
</tr>
<tr>
<td>V_minChunkLoc</td>
<td>Chunk containing minimum v value (4D waves only).</td>
</tr>
<tr>
<td>V_maxChunkLoc</td>
<td>Chunk containing maximum data value (4D waves only).</td>
</tr>
<tr>
<td>V_startRow</td>
<td>The unscaled index of the first row included in calculating statistics.</td>
</tr>
<tr>
<td>V_endRow</td>
<td>The unscaled index of the last row included in calculating statistics.</td>
</tr>
<tr>
<td>V_startCol</td>
<td>The unscaled index of the first column included in calculating statistics. Set only when /RMD is used.</td>
</tr>
<tr>
<td>V_endCol</td>
<td>The unscaled index of the last column included in calculating statistics. Set only when /RMD is used.</td>
</tr>
</tbody>
</table>
To use the WaveStats operation, choose Wave Stats from the Statistics menu.

Igor ignores NaNs and INFs in computing the average, standard deviation, RMS, minimum and maximum. NaNs result from computations that have no defined mathematical meaning. They can also be used to represent missing values. INFs result from mathematical operations that have no finite value.

This procedure illustrates the use of WaveStats. It shows the average and standard deviation of a source wave, assumed to be displayed in the top graph. It draws lines to indicate the average and standard deviation.

Function `ShowAvgStdDev(source)`

```plaintext
    Wave source // source waveform
    Variable left=leftx(source),right=rightx(source) // source X range
    WaveStats/Q source
    SetDrawLayer/K ProgFront
    SetDrawEnv xcoord=bottom,ycoord=left,dash= 7
    DrawLine left, V_avg, right, V_avg // show average
    SetDrawEnv xcoord=bottom,ycoord=left,dash= 7
    DrawLine left, V_avg+V_sdev, right, V_avg+V_sdev // show +std dev
    SetDrawEnv xcoord=bottom,ycoord=left,dash= 7
    DrawLine left, V_avg-V_sdev, right, V_avg-V_sdev // show -std dev
    SetDrawLayer UserFront
End
```

You could try this function using the following commands.

```plaintext
    Make/N=100 wave0 = gnoise(1)
    Display wave0; ModifyGraph mode(wave0)=2, lsize(wave0)=3
    ShowAvgStdDev(wave0)
```

When you use WaveStats with a complex wave, you can choose to compute the same statistics as above for the real, imaginary, magnitude and phase of the wave. By default WaveStats only computes the statistics for the real part of the wave. When computing the statistics for other components, the operation stores the results in a multidimensional wave `M_WaveStats`.

If you are working with large amounts of data and you are concerned about computation speed you might be able to take advantage of the `/M` flag that limits the calculation to the first order moments.
If you are working with 2D or 3D waves and you want to compute the statistics for a domain of an arbitrary shape you should use the **ImageStats** operation (see page V-356) with an ROI wave.

### Histograms

A histogram totals the number of input values that fall within each of a number of value ranges (or “bins”) usually of equal extent. For example, a histogram is useful for counting how many data values fall in each range of 0-10, 10-20, 20-30, etc. This calculation is often made to show how students performed on a test:

![Histogram Example](image.png)

The usual use for a histogram in this case is to figure out how many students fall into certain numerical ranges, usually the ranges associated with grades A, B, C, and D. Suppose the teacher decides to divide the 0-100 range into 4 equal parts, one per grade. The **Histogram** operation (see page V-297) can be used to show how many students get each grade by counting how many students fall in each of the 4 ranges.

We start by creating a wave to hold the histogram output:

```plaintext
Make/N=4/D/O studentsWithGrade
```

Next we execute the Histogram command which we generated using the Histogram dialog:

```plaintext
Histogram/B={0,25,4} scores,studentsWithGrade
```

The /B flag tells Histogram to create four bins, starting from 0 with a bin width of 25. The first bin counts values from 0 up to but not including 25.

The Histogram operation analyzes the source wave (**scores**), and puts the histogram result into a destination wave (**studentsWithGrade**).

Let’s create a text wave of **grades** to plot **studentsWithGrade** versus a grade letter in a category plot:

```plaintext
Make/O/T grades = {"D", "C", "B", "A"}
Display studentsWithGrade vs grades
SetAxis/A/E=1 left
```

Everything looks good in the category plot. Let’s double-check that all the students made it into the bins:

```plaintext
Print sum(studentsWithGrade)
```

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There are two missing students. They are ones who scored 100 on the test. The four bins we defined are actually:

- **Bin 1**: 0 - 24.99999
- **Bin 2**: 25 - 49.99999
- **Bin 3**: 50 - 74.99999
- **Bin 4**: 75 - 99.99999
The problem is that the test scores actually encompass 101 values, not 100. To include the perfect scores in the last bin, we could add a small number such as 0.001 to the bin width:

- Bin 1: 0 - 25.009999
- Bin 2: 25.001 - 49.001999
- Bin 3: 50.002 - 74.002999
- Bin 4: 75.003 - 100.0399

The students who scored 25, 50 or 75 would be moved down one grade, however. Perhaps the best solution is to add another bin for perfect scores:

```
Make/O/T grades= {"D", "C", "B", "A", "A+"}
Histogram/B={0,25,5} scores,studentsWithGrade
```

For information on plotting a histogram, see Chapter II-13, Category Plots and Graphing Histogram Results on page III-122.

This example was intended to point out the care needed when choosing the histogram binning. Our example used “manual binning”.

The Histogram operation provides five ways to set binning. They correspond to the radio buttons in the Histogram dialog:

<table>
<thead>
<tr>
<th>Bin Mode</th>
<th>What It Does</th>
</tr>
</thead>
<tbody>
<tr>
<td>Manual bins</td>
<td>Sets number of points and X scaling of the destination (output) wave based on parameters that you explicitly specify.</td>
</tr>
<tr>
<td>Auto-set bins</td>
<td>Sets X scaling of destination wave to cover the range of values in the source wave. Does not change the number of points (bins) in the destination wave.</td>
</tr>
<tr>
<td></td>
<td>Thus, you must set the number of destination wave points before computing the histogram.</td>
</tr>
<tr>
<td></td>
<td>When using the Histogram dialog, if you select Make New Wave or Auto from the Output Wave menu, the dialog must be told how many points the new wave should have. It displays the Number of Bins box to let you specify the number.</td>
</tr>
<tr>
<td>Set bins from destination wave</td>
<td>Does not change the X scaling or the number of points in the destination wave. Thus, you need to set the X scaling and number of points of the destination wave before computing the histogram.</td>
</tr>
<tr>
<td></td>
<td>When using the Histogram dialog, the Set from destination wave radio button is only available if you choose Select Existing Wave from the Output Wave menu.</td>
</tr>
<tr>
<td>Auto-set bins: 1+\log_2(N)</td>
<td>Examines the input data and sets the number of bins based on the number of input data points. Sets the bin range the same as if Auto-set bin range were selected.</td>
</tr>
<tr>
<td>Auto-set bins: 3.49<em>Sdev</em>N^-1/3</td>
<td>Examines the input data and sets the number of bins based on the number of input data points and the standard deviation of the data. Sets the bin range the same as if Auto-set bin range were selected.</td>
</tr>
<tr>
<td>Freedman-Diaconis method</td>
<td>Sets the optimal bin width to ( \text{binWidth} = 2 \times \text{IQR} \times N^{-1/3} ) where IQR is the interquartile distance (see StatsQuantiles) and the bins are evenly-distributed between the minimum and maximum values.</td>
</tr>
</tbody>
</table>

Added in Igor Pro 7.00.
Histogram Caveats

If you use the “Set bins from destination wave” mode, you must create the destination wave, using the **Make** operation, before computing the histogram. You also must set the X scaling of the destination wave, using the **SetScale**.

The Histogram operation does not distinguish between 1D waves and multidimensional waves. If you use a multidimensional wave as the source wave, it will be analyzed as if the wave were one dimensional. This may still be useful - you will get a histogram showing counts of the data values from the source wave as they fall into bins.

If you would like to perform a histogram of 2D or 3D image data, you may want to use the **ImageHistogram** operation (see page V-323), which supports specific features that apply to images only.

**Graphing Histogram Results**

Our example above displayed the histogram results as a category plot because the bins corresponded to text values. Often histogram bins are displayed on a numeric axis. In this case you need to know how Igor displays a histogram result.

For example, this histBins destination wave has 12 points (bins), the first bin starting at -3, and each bin is 0.5 wide. The X scaling is shown in the table:

<table>
<thead>
<tr>
<th>Point</th>
<th>histBins.x</th>
<th>histBins.d</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>-3</td>
<td>14</td>
</tr>
<tr>
<td>1</td>
<td>-2.5</td>
<td>8</td>
</tr>
<tr>
<td>2</td>
<td>-2</td>
<td>8</td>
</tr>
<tr>
<td>3</td>
<td>-1.5</td>
<td>7</td>
</tr>
<tr>
<td>4</td>
<td>-1</td>
<td>8</td>
</tr>
<tr>
<td>5</td>
<td>-0.5</td>
<td>14</td>
</tr>
<tr>
<td>6</td>
<td>0</td>
<td>14</td>
</tr>
<tr>
<td>7</td>
<td>0.5</td>
<td>6</td>
</tr>
<tr>
<td>8</td>
<td>1</td>
<td>8</td>
</tr>
<tr>
<td>9</td>
<td>1.5</td>
<td>13</td>
</tr>
<tr>
<td>10</td>
<td>2</td>
<td>14</td>
</tr>
<tr>
<td>11</td>
<td>2.5</td>
<td>15</td>
</tr>
</tbody>
</table>

When histBins is graphed in both bars and markers modes, it looks like this:

Note that the markers are positioned at the start of the bars. You can offset the marker trace by half the bin width if you want them to appear in the center of the bin.

Alternatively, you can make a second histogram using the Bin-Centered X Values option. In the Histogram dialog, check the Bin-Centered X Values checkbox.
Histogram Dialog

To use the Histogram operation, choose Histogram from the Analysis menu.

To use the “Manually set bins” or “Set from destination wave” bin modes, you need to decide the range of data values in the source wave that you want the histogram to cover. You can do this visually by graphing the source wave or you can use the WaveStats operation to find the exact minimum and maximum source values.

The dialog requires that you enter the starting bin value and the bin width. If you know the starting bin value and the ending bin value then you need to do some arithmetic to calculate the bin width.

A line of text at the bottom of the Destination Bins box tells you the first and last values, as well as the width and number of bins. This information can help with trial-and-error settings.

If you use the “Manually set bins” or any of the “Auto-set” modes, Igor will set the X units of the destination wave to be the same as the Y units of the source wave.

If you enable the Accumulate checkbox, Histogram does not clear the destination wave but instead adds counts to the existing values in it. Use this to accumulate results from several histograms in one destination. If you want to do this, don’t use the “Auto-set bins” option since it makes no sense to change bins in mid-stream. Instead, use the “Set from destination wave” mode. To use the Accumulate option, the destination wave must be double-precision or single-precision and real.

The “Bin-Centered X Values” and “Create Square Root(N) Wave” options are useful for curve fitting to a histogram. If you do not use Bin-Centered X Values, any X position parameter in your fit function will be shifted by half a bin width. The Square Root(N) Wave creates a wave that estimates the standard deviation of the histogram data; this is based on the fact that counting data have a Poisson distribution. The wave created by this option does not try to do anything special with bins having zero counts, so if you use the square root(N) wave to weight a curve fit, these zero-count bins will be excluded from the fit. You may need to replace the zeroes with some appropriate value.

The binning modes were added in Igor Pro. In earlier versions of Igor, the accumulate option had two effects:

- Did not clear the destination wave.
- Effectively used the “Set bins from destination wave” mode.

To maintain backward compatibility, the Histogram operation still behaves this way if the accumulate (“/A”) flag is used and no bin (“/B”) flag is used. This dialog always generates a bin flag. Thus, the accumulate flag just forces accumulation and has no effect on the binning.

You can use the Histogram operation on multidimensional waves but they are treated as though the data belonged to a single 1D wave. If you are working with 2D or 3D waves you may prefer to use the Image-Histogram operation (see page V-323), which computes the histogram of one layer at a time.

Histogram Example

The following commands illustrate a simple test of the histogram operation.

```
Make/N=10000 noise = gnoise(1) // make raw data
Make hist // make destination wave
Histogram/B={-3, (3 - -3)/100, 100} noise, hist // do histogram
Display hist; Modify mode(hist)=1
```

These commands produce the following graph:
Because the values in the source wave are Gaussian deviates generated by the gnoise function, the histogram should have the familiar Gaussian bell-shape. You can estimate the characteristics of the population the samples were taken from by fitting a Gaussian curve to the data. First try fitting a Gaussian curve to the example histogram:

```plaintext
CurveFit gauss hist /D // curve fit to histogram
```

The solution from the curve fit was (if you try this example on your computer, the results will be somewhat different because the random noise added by gnoise will be different):

- \( y_0 = 1.7489 \pm 2.62 \)
- \( A = 238.73 \pm 3.06 \)
- \( x_0 = -0.03346 \pm 0.0113 \)
- \( \text{width} = 1.3914 \pm 0.0261 \)

Note that the peak position (\( x_0 \)) is shifted approximately half a bin below zero. Since the gnoise() function produces random numbers with mean of zero, we would expect \( x_0 \) to be close to zero. The shifted value of \( x_0 \) is a result of Igor’s way of storing the X values for histogram bins. Setting the X value to the left edge is good for displaying a bar chart, but bad for curve fitting.

By default, a histogram wave has the X scaling set such that an X value gives the value at the left end of a bin. Usually if you are going to fit a curve to a histogram, you want centered X values. You can change the
X scaling to centered values using SetScale. But it is easier to simply use the option to have the Histogram operation produce output with bin-centered X values by adding the /C flag to the Histogram command:

\[
\text{Histogram/C=B={-3, (3 - -3)/100, 100} noise, hist // do histogram}
\]

\[
\text{CurveFit gauss hist /D // curve fit to histogram}
\]

The result of the curve fit is closer to what we expect:

\[
\begin{align*}
y_0 & = 1.7489 \pm 2.62 \\
A & = 238.73 \pm 3.06 \\
x_0 & = -0.0034602 \pm 0.0113 \\
\text{width} & = 1.3914 \pm 0.0261
\end{align*}
\]

But this shifts the trace showing the histogram by half a bin on the graph. If the trace is displayed using markers or dots, this may be what is desired, but if you have used bars, the display is incorrect.

Another possibility is to make an X wave to go with the histogram data. This X wave would contain X values shifted by half a bin. Use this X wave as input to the curve fit, but don’t use it on the graph:

\[
\text{Histogram/B={-3, (3 - -3)/100, 100} noise, hist // Histogram without /C}
\]

\[
\text{Duplicate hist, hist_x}
\]

\[
\text{hist_x = x + deltax(hist)/2}
\]

\[
\text{CurveFit gauss hist /X=hist_x/D}
\]

Use this method to graph the original histogram wave without modifying the X scaling, so a graph using bars is correct. It also gives a curve fit that uses the center X values, giving the correct x0. You could also use the Histogram operation twice, once with the /C flag to get bin-centered X values, and once without to get the shifted X scaling appropriate for bars. Both methods have the drawback of creating an extra wave that you must track.

There is one last refinement to curve fitting to a histogram. Since the histogram represents counts, the values in a histogram should have uncertainties described by a Poisson distribution. The standard deviation of a Poisson distribution is equal to the square root of the mean, which implies that the estimated error of a histogram bin depends on the magnitude of the value. This, in turn, implies that the errors are not constant and a curve fit will give a biased solution.

The correct solution is to use a weighting wave; use the /N flag with the Histogram operation to get the appropriate wave. This example makes a new data set using gnoise to make gaussian-distributed values, makes a histogram with bin-centered X values and the appropriate weighting wave, and then does two curve fits, one without weighting and one with:

\[
\text{Make/N=1024 gdata=gnoise(1)}
\]

\[
\text{Make/N=20/O gdata_Hist}
\]

\[
\text{Histogram/C/N/B=4 gdata,gdata_Hist}
\]

\[
\text{Display gdata_Hist}
\]

\[
\text{ModifyGraph mode=3,marker=8}
\]

\[
\text{CurveFit gauss gdata_Hist /D}
\]

\[
\text{CurveFit gauss gdata_Hist /W=W_SqrtN /I=1 /D}
\]

Note the “/W=W_SqrtN /I=1” addition to the second CurveFit command; this adds the weighting using the weighting wave created by the Histogram operation. Also, /B=4 was used to have the Histogram operation set the number of bins and bin range appropriately for the input data.

The results from the unweighted fit:

\[
\begin{align*}
y_0 & = -3.3383 \pm 2.98 \\
A & = 133.26 \pm 3.51 \\
x_0 & = 0.024088 \pm 0.0252 \\
\text{width} & = 1.5079 \pm 0.0578
\end{align*}
\]

And from the weighted fit:

\[
\begin{align*}
y_0 & = 0.33925 \pm 0.804 \\
A & = 135.21 \pm 5.25 \\
x_0 & = 0.0038416 \pm 0.031 \\
\text{width} & = 1.3604 \pm 0.0405
\end{align*}
\]
Computing an “Integrating” Histogram

In a histogram, each bin of the destination wave contains a count of the number of occurrences of values in the source that fell within the bounds of the bin. In an *integrating* histogram, instead of *counting* the occurrences of a value within the bin, we *add* the value itself to the bin. When we’re done, the destination wave contains the sum of all values in the source which fell within the bounds of the bin.

Igor comes with an example experiment called “Integrating Histogram” that illustrates how to do this with a user function. To see the example, choose File→Example Experiments→Analysis→Integrating Histogram.

Sorting

The **Sort** operation (see page V-753) sorts one or more 1D numeric or text waves in ascending or descending order.

The Sort operation is often used to prepare a wave or an XY pair for subsequent analysis. For example, the interp function assumes that the X input wave is monotonic.

There are other sorting-related operations: MakeIndex and IndexSort. These are used in rare cases and are described in the section **MakeIndex and IndexSort Operations** on page III-127. The **SortColumns** operation sorts columns of multidimensional waves. Also see the **SortList** function for sorting string lists.

To use the Sort operation, choose Sort from the Analysis menu.

The sort key wave controls the reordering of points. However, the key wave itself is not reordered unless it is also selected as a destination wave in the “Waves to Sort” list.

The number of points in the destination wave or waves must be the same as in the key wave. When you select a wave from the dialog’s Key Wave list, Igor shows only waves with the same number of points in the Waves to Sort list.

The key wave can be a numeric or text wave, but it must not be complex. The destination wave or waves can be text, real or complex except for the MakeIndex operation in which case the destination must be text or real.

The number of destination waves is limited by the 1000 character limit in Igor’s command buffer. To sort a very large number of waves, use several Sort commands in succession, being careful not to sort the key wave until the very last.

By default, text sorting is case-insensitive. Use the /C flag with the Sort operation to make it case-sensitive.

Simple Sorting

In the simplest case, you would select a single wave as both the source and the destination. Then Sort would merely sort that wave.

If you want to sort an XY pair such that the X wave is in order, you would select the X wave as the source and both the X and Y waves as the destination.

Sorting to Find the Median Value

The following user-defined function illustrates a simple use of the Sort operation to find the median value of a wave.

```
Function FindMedian(w, x1, x2) // Returns median value of wave w
    Wave w
    Variable x1, x2 // Range of interest
    Variable result
    Duplicate/R=(x1,x2)/FREE w, medianWave // Make a clone of wave
    Sort tempMedianWave, medianWave // Sort clone
```
SetScale/P x 0,1,medianWave
result = medianWave((numpnts(medianWave)-1)/2)

return result
End

It is easier and faster to use the built-in **median** function to find the median value in a wave.

**Multiple Sort Keys**

If the key wave has two or more identical values, you may want to use a secondary source to determine the order of the corresponding points in the destination. This requires using multiple sort keys. The Sorting dialog does not provide a way to specify multiple sort keys but the Sort operation does. Here is an example demonstrating the difference between sorting by single and by multiple keys. Notice that the sorted wave (tdest) is a text wave, and the sort keys are text (tsrc) and numeric (nw1):

Make/O/T tsrc={"hello","there","hello","there"}
Duplicate/O tsrc,tdest
Make nw1= \{3,5,2,1\}
tdest= tsrc + " " + num2str(nw1)
Edit tsrc,nw1,tdest

<table>
<thead>
<tr>
<th>Point</th>
<th>tsrc</th>
<th>nw1</th>
<th>tdest</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>hello</td>
<td>3</td>
<td>hello 3</td>
</tr>
<tr>
<td>1</td>
<td>there</td>
<td>5</td>
<td>there 5</td>
</tr>
<tr>
<td>2</td>
<td>hello</td>
<td>2</td>
<td>hello 2</td>
</tr>
<tr>
<td>3</td>
<td>there</td>
<td>1</td>
<td>there 1</td>
</tr>
</tbody>
</table>

Single-key text sort:
Sort tsrc,tdest      // nw1 not used

<table>
<thead>
<tr>
<th>Point</th>
<th>tsrc</th>
<th>nw1</th>
<th>tdest</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>hello</td>
<td>3</td>
<td>hello 3</td>
</tr>
<tr>
<td>1</td>
<td>there</td>
<td>5</td>
<td>hello 2</td>
</tr>
<tr>
<td>2</td>
<td>hello</td>
<td>2</td>
<td>there 1</td>
</tr>
<tr>
<td>3</td>
<td>there</td>
<td>1</td>
<td>there 5</td>
</tr>
</tbody>
</table>

Execute this to scramble tdest again:
tdest= tsrc + " " + num2str(nw1)

Execute this to see a two key sort (nw1 breaks ties):
Sort \{tsrc,nw1\},tdest

<table>
<thead>
<tr>
<th>Point</th>
<th>tsrc</th>
<th>nw1</th>
<th>tdest</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>hello</td>
<td>3</td>
<td>hello 2</td>
</tr>
<tr>
<td>1</td>
<td>there</td>
<td>5</td>
<td>hello 3</td>
</tr>
<tr>
<td>2</td>
<td>hello</td>
<td>2</td>
<td>there 1</td>
</tr>
<tr>
<td>3</td>
<td>there</td>
<td>1</td>
<td>there 5</td>
</tr>
</tbody>
</table>

The reason that “hello 3” sorts after “hello 2” is because nw1[0] = 3 is greater than nw1[2] = 2.

You can sort by more than two keys by specifying more than two waves inside the braces.

**MakeIndex and IndexSort Operations**

The MakeIndex and IndexSort operations are infrequently used. You will normally use the Sort operation.

Applications of MakeIndex and IndexSort include:
- Sorting large quantities of data
- Sorting individual waves from a group one at a time
- Accessing data in sorted order without actually rearranging the data
- Restoring data to the original ordering
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The MakeIndex operation creates a set of index numbers. IndexSort can then use the index numbers to rearrange data into sorted order. Together they act just like the Sort operation but with an extra wave and an extra step.

The advantage is that once you have the index wave you can quickly sort data from a given set of waves at any time. For example, if you have hundreds of waves you can not use the normal sort operation on a single command line. Also, when writing procedures it is more convenient to loop through a set of waves one at a time than to try to generate a single command line with multiple waves.

You can also use the index values to access data in sorted order without using the IndexSort operation. For example, if you have data and index waves named wave1 and wave1index, you can access the data in sorted order on the right hand side of a wave assignment like so:

```
wave1[wave1index[p]]
```

If you create an index wave, you can undo a sort and restore data to the original order. To do this, simply use the Sort operation with the index wave as the source.

To understand the MakeIndex operation, consider that the following commands

```
Duplicate data1,data1index
MakeIndex data1,data1index
```

are identical in effect to

```
Duplicate data1,data1index
data1index= P
Sort data1,data1index
```

Like the Sort operation, the MakeIndex operation can handle multiple sort keys.

Decimation

If you have a large data set it may be convenient to deal with a smaller but representative number of points. In particular, if you have a graph with millions of points, it probably takes a long time to draw or print the graph. You can do without many of the data points without altering the graph much. Decimation is one way to accomplish this.

There are at least two ways to decimate data:

1. Keep only every nth data value. For example, keep the first value, discard 9, keep the next, discard 9 more, etc. We call this Decimation by Omission (see page III-128).
2. Replace every nth data value with the result of some calculation such as averaging or filtering. We call this Decimation by Smoothing (see page III-129).

Decimation by Omission

To decimate by omission, create the smaller output wave and use a simple assignment statement (see Waveform Arithmetic and Assignments on page II-69) to set their values. For example, If you are decimating by a factor of 10 (omitting 9 out of every 10 values), create an output wave with 1/10th as many points as the input wave.

For example, make a 1000 point test input waveform:

```
Make/O/N=1000 wave0
SetScale x 0, 5, wave0
wave0 = sin(x) + gnoise(.1)
```

Now, make a 100 point waveform to contain the result of the decimation:

```
Make/O/N=100 decimated
SetScale x 0, 5, decimated // preserve the x range
decimated = wave0[p*10]  // for(p=0;p<100; p+=1) decimated[p] = wave0[p*10]
```

Decimation by omission can be obtained more easily using the Resample operation and dialog by using an interpolation factor of 1 and a decimation factor of (in this case) 10, and a filter length of 1.
Decimation by Smoothing

While decimation by omission completely discards some of the data, decimation by smoothing combines all of the data into the decimated result. The smoothing can take many forms: from simple averaging to various kinds of lowpass digital filtering.

The simplest form of smoothing is averaging (sometimes called “boxcar” smoothing). You can decimate by averaging some number of points in your original data set. If you have 1000 points, you can create a 100 point representation by averaging every set of 10 points down to one point. For example, make a 1000 point test waveform:

Make/O/N=1000 wave0
SetScale x 0, 5, wave0
wave0 = sin(x) + gnoise(.1)

Now, make a 100 point waveform to contain the result of the decimation:

Make/O/N=100 wave1
SetScale x 0, 5, wave1
wave1 = mean(wave0, x, x+9*deltax(wave0))

Notice that the output wave, wave1, has one tenth as many points as the input wave.

The averaging is done by the waveform assignment

wave1 = mean(wave0, x, x+9*deltax(wave0))

This evaluates the right-hand expression 100 times, once for each point in wave1. The symbol “x” returns the X value of wave1 at the point being evaluated. The right-hand expression returns the average value of wave0 over the segment that corresponds to the point in wave1 being evaluated.

It is essential that the X values of the output wave span the same range as the X values of the input range. In this simple example, the SetScale commands satisfy this requirement.

Results similar to the example above can be obtained more easily using the Resample operation (page V-682) and dialog.

Resample is based on a general sample rate conversion algorithm that optionally interpolates, low-pass filters, and then optionally decimates the data by omission. The lowpass filter can be set to “None” which averages an odd number of values centered around the retained data points. So decimation by a factor of 10 would involve averaging 11 values centered around every 10th point.

The decimation by averaging above can be changed to be 11 values centered around the retained data point instead 10 values from the beginning of the retained data point this way:

Make/O/N=100 wave1Centered
SetScale x 0, 5, wave1Centered
wave1Centered = mean(wave0, x-5*deltax(wave0), x+5*deltax(wave0))

Each decimated result (each average) is formed from different values than wave1 used, but it isn’t any less valid as a representation of the original data.
Using the Resample operation:

Duplicate/O wave0, wave2
Resample/DOWN=10/WINF=None/N=11 wave2        // no /UP means no interpolation

gives nearly identical results to the wave1Centered = mean(...) computation, the exceptions being only the initial and final values, which are simple end-effect variations.

The /WINF and /N flags of Resample define simple low-pass filtering options for a variety of decimation-by-smoothing choices. The default /WINF=Hanning window gives a smoother result than /WINF=None. See the WindowFunction operation (page V-946) for more about these window options.

Miscellaneous Operations

WaveTransform

When working with large amounts of data (many waves or multiple large waves), it is frequently useful to replace various wave assignments with wave operations which execute significantly faster. The WaveTransform operation (see page V-938) is designed to help in these situations. For example, to flip the data in a 1D wave you can execute the following code:

Function flipWave(inWave)
   wave inWave
   Variable num=numPnts(inWave)
   Variable n2=num/2
   Variable i,tmp
   num-=1
   Variable j
   for(i=0;i<n2;i+=1)
      tmp=inWave[i]
      j=num-i
      inWave[i]=inWave[j]
      inWave[j]=tmp
   endfor
End

You can obtain the same result much faster using the command:

WaveTransform/O flip, waveName

In addition to “flip”, WaveTransform can also fill a wave with point index or the inverse point index, shift data points, normalize, convert to complex-conjugate, compute the squared magnitude or the phase, etc.


Compose Expression Dialog

The Compose Expression item in the Analysis menu brings up the Compose Expression dialog.

This dialog generates a command that sets the value of a wave, variable or string based on a numeric or string expression created by pointing and clicking. Any command that you can generate using the dialog could also be typed directly into the command line.

The command that you generate with the Compose Expression dialog consists of three parts: the destination, the assignment operator and the expression. The command resembles an equation and is of the form:

<destination> <assignment-operator> <expression>

For example:
wave1 = K0 + wave2 // a wave assignment command
K0 += 1.5 * K1 // a variable assignment command
str1 = "Today is" + date() // a string assignment command

Table Selection Item

The Destination Wave pop-up menu contains a "table selection" item. When you choose "table selection", Igor assigns the expression to whatever is selected in the table. This could be an entire wave or several entire waves, or it could be a subset of one or more waves.

To use this feature, start by selecting in a table the numeric wave or waves to which you want to assign a value. Next, choose Compose Expression from the Analysis menu. Choose "table selection" in the Destination Wave pop-up menu. Next, enter the expression that you want to assign to the waves. Notice the command that Igor has created which is displayed in the command box toward the bottom of the dialog. If you have selected a subset of a wave, Igor will generate a command for that part of the wave only. Finally, click Do It to execute the command.

Create Formula Checkbox

The Create Formula checkbox in the Compose Expression dialog generates a command using the := operator rather than the = operator. The := operator establishes a dependency such that, if a wave or variable on the right hand side of the assignment statement changes, Igor will reassign values to the destination (left hand side). We call the right hand side a formula. Chapter IV-9, Dependencies, provides details on dependencies and formulas.

Matrix Math Operations

There are three basic methods for performing matrix calculations: normal wave expressions, the MatrixXXX operations, and the MatrixOp operation.

Normal Wave Expressions

You can add matrices to other matrices and scalars using normal wave expressions. You can also multiply matrices by scalars. For example:

Make matA={{1,2,3},{4,5,6}}, matB={{7,8,9},{10,11,12}}
matA = matA+0.01*matB
gives new values for
matA = {{1.07,2.08,3.09},{4.1,5.11,6.12}}

MatrixXXX Operations

A number of matrix operations are implemented in Igor. Most have names starting with the word “Matrix”. For example, you can multiply a series of matrices using the MatrixMultiply operation (page V-482). This operation. The /T flag allows you to specify that a given matrix’s data should be transposed before being used in the multiplication.

Many of Igor’s matrix operations use the LAPACK library. To learn more about LAPACK see:


or the LAPACK web site:
http://www.netlib.org/lapack/lug/lapack_lug.html

Unless noted otherwise, LAPACK routines support real and complex, IEEE single-precision and double-precision matrix waves. Most matrix operations create the variable V_flag and set it to zero if the operation is successful. If the flag is set to a negative number it indicates that one of the parameters passed to the LAPACK routines is invalid. If the flag value is positive it usually indicates that one of the rows/columns of the input matrix caused the problem.
MatrixOp Operation

The MatrixOp operation (page V-483) improves the execution efficiency and simplifies the syntax of matrix expressions. For example, the command

\[ \text{MatrixOp matA = (matD - matB \times matC) \times matD} \]

is equivalent to matrix multiplications and subtraction following standard precedence rules.


Matrix Commands

Here are the matrix math operations and functions.

General:

- \text{MatrixCondition}(\text{matrixA})
- \text{MatrixConvolve coefMatrix, dataMatrix}
- \text{MatrixCorr}[\text{flags}] \text{waveA [, waveB]}
- \text{MatrixDet}(\text{matrixA})
- \text{MatrixDot(\text{waveA, waveB})}
- \text{MatrixFilter}[\text{flags}] \text{Method \ dataMatrix}
- \text{MatrixGLM}[/Z] \text{matrixA, matrixB, waveD}
- \text{MatrixMultiply matrixA[/T], matrixB[/T] [, additional matrices]}
- \text{MatrixOp} [/O] \text{destwave = expression}
- \text{MatrixRank}(\text{matrixA [, maxConditionNumber]})
- \text{MatrixTrace}(\text{matrixA})
- \text{MatrixTranspose} [/H] \text{matrix}

EigenValues, eigenvectors and decompositions:

- \text{MatrixEigenV}[\text{flags}] \text{matrixWave}
- \text{MatrixGLM} \text{matrixA, matrixB, waveD}
- \text{MatrixInverse}[\text{flags}] \text{srcWave}
- \text{MatrixLUD} \text{matrixA}
- \text{MatrixLUDTD srcMain, srcUpper, srcLower}
- \text{MatrixSchur} [/Z] \text{srcMatrix}
- \text{MatrixSVD} \text{matrixA}

Linear equations and least squares:

- \text{MatrixGaussJ} \text{matrixA, vectorsB}
- \text{MatrixLinearSolve}[\text{flags}] \text{matrixA, matrixB}
- \text{MatrixLinearSolveTD} [/Z] \text{upperW, mainW, lowerW, matrixB}
- \text{MatrixLSS}[\text{flags}] \text{matrixA, matrixB}
- \text{MatrixLUBkSub matrixL, matrixU, index, vectorB}
- \text{MatrixSolve method, matrixA, vectorB}
- \text{MatrixSVBkSub matrixU, vectorW, matrixV, vectorB}

Using MatrixOp

When performing mathematical calculations your first choice may be to write standard wave assignments such as:

\[ \text{wave1} = \text{wave2 + wave3} \]

When the expression on the right-hand-side (RHS) is complicated or when the waves are large you can gain a significant performance improvement using MatrixOp (short for "matrix operation"). MatrixOp was originally conceived to perform calculations on 2D waves and was later extended to waves of any dimension.

To use the basic form of MatrixOp simply prepend its name to the assignment statement:
MatrixOp wave1 = wave2 + wave3

Although the two commands appear similar, having the general form:

destWave = expression

they are different in behavior.

A significant difference is that MatrixOp operates on pure array elements without regard to wave scaling and does not support indexing using x, y, z, t, p, q, r, or s on the RHS.

The wave assignment requires that the destination wave exist at the time of execution but MatrixOp creates its destination wave automatically. In these commands:

Make/O wave2 = 1/(p+1), wave3 = 1
MatrixOp/O wave1 = wave2 + wave3

MatrixOp creates a single precision (SP) wave named wave1 and stores the result in it.

When MatrixOp creates a destination wave its data type and dimensions depend on the expression on the RHS. In the preceding example, MatrixOp created wave1 as SP because wave2 and wave3 are SP. The rules that MatrixOp uses to determine the data type and dimensions of the destination are discussed below under MatrixOp Data Promotion Policy on page III-138.

These rules leads to the following difference between MatrixOp and wave assignments:

Make/O wave1 = 42 // wave1 is 128 points wave, all points are set to 42
MatrixOp/O wave1 = 42 // wave1 is now 1 point wave set to 42

Assignment statements evaluate the RHS and store the result in a point-by-point manner. Because of this, you sometimes get unexpected results if the destination wave appears on the RHS. In this example, WaveMin(wave2) changes during the evaluation of the assignment statement:

wave2 = wave2 - WaveMin(wave2)

By contrast, MatrixOp evaluates the RHS for all points in the destination before storing anything in the destination wave. Consequently this command behaves as expected:

MatrixOp/O wave2 = wave2 - minVal(wave2)

Another important difference appears when the RHS involves complex numbers. If you try, for example,

Make/O/C cwave2
Make/O wave1, wave3
wave1 = cwave2 + wave3

you get an error, "Complex wave used in real expression".

By contrast, MatrixOp creates the destination as complex so this command works without error:

MatrixOp/O wave1 = cwave2 + wave3

In this example the RHS mixes real and complex waves, something MatrixOp handles without problems.

In addition to the standard math operators, MatrixOp supports a list of functions that can be applied to operands on the RHS. Examples are abs, sin, cos, mean, minVal and maxVal. There are many more described in the MatrixOp reference documentation and listed below under MatrixOp Functions by Category on page III-140.

MatrixOp Data Tokens

A MatrixOp command has the general form:

MatrixOp [flags] destWave = expression
The expression on the RHS is a combination of data tokens with MatrixOp operators and MatrixOp functions. A data token is one of the following:

- A literal number
- A numeric constant declared with the Constant keyword
- A numeric local variable
- A numeric global variable
- A numeric wave
- A numeric wave layer
- The result from a MatrixOp function

You can not call a user-defined function or external function from expression.

This function illustrates each type of data token:

```
Constant kConstant = 234
Function Demo()
    // Literal number
    MatrixOp/O dest = 123

    // Constant
    MatrixOp/O dest = kConstant

    // Local Variable
    Variable localVariable = 345
    MatrixOp/O dest = localVariable

    // Global Variable
    Variable/G root:gVar = 456
    NVAR globalVariable = root:gVar
    MatrixOp/O dest = globalVariable

    // Wave
    Make/O/N=(3,3) mat = p + 10*q
    MatrixOp/O tMat = mat^t

    // Wave layer
    Make/O/N=(3,3,3) w3D = p + 10*q + 100*r
    MatrixOp/O layer1 = w3D[1][1][1]

    // Output from a MatrixOp function
    MatrixOp/O invMat = inv(mat)
End
```

**MatrixOp Wave Data Tokens**

MatrixOp uses only the numeric data and the dimensions of waves. All other properties, in particular wave scaling, are ignored. If wave scaling is important in your application, follow MatrixOp with CopyScales or SetScale or use a wave assignment statement instead of MatrixOp.

From the command line you can reference a wave in expression using the simple wave name, the partial data folder path to the wave or the full data folder path to a wave. In a user-defined function you can reference a wave using a simple wave name or a wave reference variable pointing to an existing wave. We call all of these methods of referencing waves “wave references”.

A wave data token consists of a wave reference optionally qualified by indices that identify a subset of the wave. For example:

```
Function Demo()
    // Creates automatic wave reference for w3D
    Make/O/N=(3,4,5) w3D = p + 10*q + 100*r
```
MatrixOp/O dest = w3D  // dest is a 3D wave
MatrixOp/O dest = w3D[0][1][2]  // dest is a 1D wave with 1 point
MatrixOp/O dest = w3D[0][1][]  // dest is a 2D wave with 1 layer
End

MatrixOp supports only two kinds of subsets of waves:

- A subset that evaluates to a scalar (a single value)
- A subset that evaluates to one or more layers (2D arrays)

Subsets that evaluate to a row \((w3D[1][][2])\) or a column \((w3D[][1][2])\) are not supported.

**Scalars:** The following expressions evaluate to scalars:

- \(\text{wave1d}[a]\) where \(a\) is a literal number or a local variable. MatrixOp clips the index \(a\) to the valid range for \(\text{wave1d}\). The expression evaluates to a scalar equal to the referenced wave element.

- \(\text{wave2d}[a][b]\) where \(a\) and \(b\) are literal numbers or local variables. MatrixOp clips the indices to the valid range of the corresponding dimensions. The expression evaluates to a scalar equal to the referenced wave element.

- \(\text{wave3d}[a][b][c]\) where \(a\), \(b\), and \(c\) are literal numbers or local variables. MatrixOp clips the indices to the valid range of the corresponding dimensions. The expression evaluates to a scalar equal to the referenced wave element.

**Layers:** The following evaluate to one or more 2D layers:

- \(\text{wave3d}[][][a]\) Layer \(a\) from the 3D wave is treated as a 2D matrix. The first and second bracket pairs must be empty. MatrixOp clips \(a\) to the valid range of layers. The result is a 2D wave.

- \(\text{wave3d}[][a,b]\) expression is evaluated for all layers between layer \(a\) and layer \(b\). MatrixOp clips \(a\) and \(b\) to the valid range of layers. The result is a 3D wave.

- \(\text{wave3d}[][a,b,c]\) expression is evaluated for layers starting with layer \(a\) and increasing to layer \(b\) incrementing by \(c\). Layers are clipped to the valid range and \(c\) must be a positive integer. The result is a 3D wave.

You can use waves of any dimensions as parameters to MatrixOp functions. For example:

Make/O/N=128 wave1d = x
MatrixOp/O outWave = exp(wave1d)

MatrixOp does not support expressions that include the same 3D wave on both sides of the equation:

MatrixOp/O wave3D = wave3D + 3  // Not allowed

Instead use:

MatrixOp/O newWave3D = wave3D + 3

You can use any combination of data types for operands. In particular, you can mix real and complex types in expression. MatrixOp determines data types of inputs and the appropriate output data type at runtime without regard to any type declaration such as Wave/C.

MatrixOp functions can create certain types of 2D data tokens. Such tokens are used on the RHS of the assignment. The const and zeroMat functions create matrices of specified dimensions containing fixed values. The identity function creates identity matrices and triDiag creates a tridiagonal matrix from 1D input waves. The rowRepeat and colRepeat functions also construct matrices from 1D waves. The setRow, setCol and setOffDiag functions transfer data from 1D waves to elements of 2D waves.
MatrixOp and Wave Dimensions

MatrixOp was designed to optimize operations on 2D arrays (matrices) but it also supports other wave dimensions in various expressions. However it does not support zero point waves.

A 1D wave is treated as a matrix with one column. 3D and 4D waves are treated as arrays of layers so their assignments are processed on a layer-by-layer basis. For example:

```
Make/O/N=(4,5) wave2 = q
Make/O/N=(4,5,6) wave3 = r
MatrixOp/O wave1 = wave2 * wave3 // 2D multiplies 3D one layer at a time
```

wave1 winds up as a 3D wave of dimensions (4,5,6). Each layer of wave1 contains the contents of the corresponding layer of wave3 multiplied on an element-by-element basis by the contents of wave2.

Exceptions for layer-by-layer processing are special MatrixOp functions such as `beam` and `transposeVol`.

Some binary operators have dimensional restrictions for their wave operands. For example, matrix multiplication (wave2 x wave3) requires that the number of columns in wave2 be equal to the number of rows in wave3. Regular multiplication (wave2*wave3) requires that the number of rows and the columns of the two be equal. For example,

```
Make/O/N=(4,6) wave2
Make/O/N=(3,8) wave3
MatrixOp/O wave1 = wave2 * wave3 // Error: "Matrix Dimensions Mismatch"
```

The exception to this rule is when the righthand operand is a single wave element:

```
MatrixOp/O wave1 = wave2 * wave3[2][3] // Equivalent to scalar multiplication
```

Some MatrixOp functions operate on each column of the matrix and result in a 1 row by N column wave which may be confusing when used elsewhere in Igor. If what you need is an N row 1D wave you can re-dimension the wave or simply include a transpose operator in the MatrixOp command:

```
Make/O/N=(4,6) wave2=gnoise(4)
MatrixOp/O wave1=sumCols(wave2)^t // wave1 is a 1D wave with 6 rows
```

MatrixOp Operators

MatrixOp defines 8 binary operators and two postfix operators which are available for use in the RHS expression. The operators are listed in the Operators section of the reference documentation for MatrixOp on page V-483.

MatrixOp does not support operator combinations such as `+=`.

The basic operators, `+`, `-`, `*`, and `/`, operate in much the same way as they would in a regular wave assignment with one exception: when the `-` or `/` operation involves a matrix and a scalar, it is only supported if the matrix is the first operand and the scalar is the second. For example:

```
Make/O wave2 = 1
Variable var1 = 7
MatrixOp/O wave1 = wave2 - var1 // OK: Subtract var1 to each point in wave2
MatrixOp/O wave1 = var1 - wave2 // Error: Can't subtract a matrix from a scalar
MatrixOp/O wave1 = var1 / wave2 // Error: Can't divide a scalar by a matrix
```

Division of a scalar by a matrix can be accomplished using the reciprocal function as in:

```
MatrixOp/O wave1 = scalar * rec(wave2)
```

The dot operator `.` is used to compute the generalized dot product:

```
MatrixOp/O wave1 = wave2 . wave3 // Spaces around '.' are optional
```

The x operator designates matrix-matrix multiplication.
MatrixOp/O wave1 = wave2 x wave3 // Spaces around 'x' are required!

The logical operators && and || are restricted to real-valued data tokens and produce unsigned byte
numeric tokens with the value 0 or 1.

The two postfix operators ^t (matrix transpose) and ^h (Hermitian transpose) operate on the first token to
their left:

MatrixOp/O wave1 = wave2^t + wave3

The transpose operation has higher precedence and therefore executes before the addition.

The left token may be a compound token as in:

MatrixOp/O wave1 = sumCols(wave2)^t

MatrixOp supports the ^ character only in the two postfix operators ^t and ^h. For exponentiation use the
powR and powC functions.

**MatrixOp Multiplication and Scaling**

MatrixOp provides a number of multiplication and scaling capabilities. They include matrix-scalar multi-

lication:

MatrixOp/O wave1 = wave2 * scalar // Equivalent to a wave assignment

and wave-wave multiplication:

MatrixOp wave1 = wave2 * wave3 // Also includes layer-by-layer support

and matrix-matrix multiplication:

MatrixOp wave1 = wave2 x wave3

The latter is equivalent to the **MatrixMultiply** operation with the convenience of allowing you to write and
execute complicated compound expressions in one line.

MatrixOp adds two specialized scaling functions that are frequently used. The *scaleCols* function multi-
plies each column by a different scalar and the *scale* function scales its input to a specified range.

**MatrixOp Data Rearrangement and Extraction**

MatrixOp is often used to rearrange data in a matrix or to extract a subset of the data for further calculation.

You can extract an element or a layer from a wave using square-bracket indexing:

// Extract scalar from point a of the wave
MatrixOp destWave = wave1d[a]

// Extract scalar from element a,b of the wave
MatrixOp destWave = wave2d[a][b]

// Extract scalar from element a,b,c of the wave
MatrixOp destWave = wave3d[a][b][c]

// Extract layer a from the 3D wave
MatrixOp destWave = wave3d[][][a]

You can also extract layers from a 3D wave starting with layer a and increasing the layer number up to layer
b using increments c:

MatrixOp destWave = wave3d[][][a,b,c]

a, b and c must be scalars. Layers are clipped to the valid range and c must be a positive integer.
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If you need to loop over rows, columns, layers or chunks it is often useful to extract the relevant data using the MatrixOp functions row, col, layer and chunk. You can extract matrix diagonals using getDiag. You can use subRange to extract more than one row or more than one column.

The Rotate operation works on 1D waves. MatrixOp extends this to higher dimensions with the functions: rotateRows, rotateCols, rotateLayers, and rotateChunks.

MatrixOp transposeVol is similar to ImageTransform transposeVol but it supports complex data types.

The MatrixOp redimension function is designed to convert 1D waves into 2D arrays but it can also extract data from higher-dimensional waves.

MatrixOp Data Promotion Policy

MatrixOp chooses the data type of the destination wave based on the data types and operations used in the expression on the RHS. Here are some examples:

```
Make/O/B/U wave2, wave3  // Create two unsigned byte waves
MatrixOp/O wave1 = wave2  // wave1 is unsigned byte
MatrixOp/O wave1 = wave2 + wave3  // wave1 is unsigned word (16 bit)
MatrixOp/O wave1 = wave2 * wave3  // wave1 is unsigned word (16 bit)
MatrixOp/O wave1 = wave2 / wave3  // wave1 is SP
MatrixOp/O wave1 = magsqr(wave2)  // wave1 is SP
```

The examples show the destination wave's data type changing to represent the range of possible results of the operation. MatrixOp does not inspect the data in the waves to determine if the promotion is required for the specific waves.

Igor variables are usually treated as double precision data tokens. MatrixOp applies special rules for variables that contain integers. Here is an example:

```
Make/O/B/U wave2  // Create unsigned byte wave
Variable vv = 2.1  // Variable containing DP value
MatrixOp/O wave1 = wave2*vv  // wave1 is DP
```

Now change the variable to store various integers:

```
vv = 2
MatrixOp/O wave1 = wave2*vv  // wave1 is unsigned word (16 bit)
vv = 257
MatrixOp/O wave1 = wave2*vv  // wave1 is unsigned integer (32 bit)
vv = 65538
MatrixOp/O wave1 = wave2*vv  // wave1 is DP
```

These examples show that MatrixOp represents the variable vv as a token with a data type that fits its contents. If the variable does not contain an integer value the token is treated as DP.

MatrixOp is convenient for complex math calculations because it automatically creates real or complex destination waves as appropriate. For example:

```
Make/O/C wave2, wave3  // SP complex
Make/O wave4  // SP real
MatrixOp/O wave1 = wave2 * wave3 * wave4  // wave1 is SP complex
MatrixOp/O wave1 = abs(wave2*wave3) * wave4  // wave1 is SP real
```

An exception to the complex policy is the sqrt function which returns NaN when its input is real and negative.
If you want to restrict data type promotion you can use the /NPRM flag:

Make/O/B/U wave2, wave3
MatrixOp/O wavel = wave2 * wave3   // wavel is unsigned word (16 bit).

A number of MatrixOp functions convert integer tokens to SP prior to processing and are not affected by the /NPRM flag. These include all the trigonometric functions, chirp and chirpZ, fft, ifft, normalization functions, sqrt, log, exp and forward/backward substitutions.

**MatrixOp Compound Expressions**

You can use compound expressions with most MatrixOp functions that operate on regular data tokens. In a compound expression you pass the result from one MatrixOp operator or function as the input to another. For example:

MatrixOp/O wavel = sum(abs(wave2-wave3))

This is particularly convenient for transformations and filtering:

MatrixOp/O wavel = IFFT(FFT(wave1,2)*filterWave,3)

Some MatrixOp functions, such as beam and transposeVol, do not support compound expressions because they require input that has more than two-dimensions while compound expressions are evaluated on a layer by layer basis:

Make/O/N=(10,20,30) wave3
MatrixOp/O wavel = beam(wave3+wave3,5,5)   // Error: Bad MatrixOp token
MatrixOp/O wavel = beam(wave3,5+1,5)   // Compound expression allowed here

**MatrixOp Multithreading**

Common CPUs are capable of running multiple threads. Some calculations are well suited to run in parallel. There are several ways to take advantage of multithreading using MatrixOp:

- **User-created preemptive threads**
  MatrixOp is thread-safe so you can call it from preemptive threads. See [ThreadSafe Functions and Multitasking](#) on page IV-308 for details.

- **Layer threads**
  If you are evaluating expressions that involve multiple layers you can use the /NTHR flag to run each layer calculation in a separate thread. When you account for thread overhead it makes sense to use /NTHR when the per-layer calculations are on the order of 1 million CPU cycles or more.

- **Internal multithreading of operations or functions**
  Some MatrixOp functions are automatically multithreaded for SP and DP data. These include matrix-matrix multiplication, trigonometric functions, hypot, sqrt, erf, erfc, inverseErf, and inverseErfc. The **MultiThreadingControl** operation provides fine-tuning of automatic multithreading but you normally do not need to tinker with it.

**MatrixOp Performance**

In most situations MatrixOp is faster than a wave assignment statement or FastOp. However, for small waves the extra overhead may make it slower.

MatrixOp works fastest on floating point data types. For maximum speed, convert integer waves to single-precision floating point before calling MatrixOp.

Some MatrixOp expressions are evaluated with automatic multithreading. See [MatrixOp Multithreading](#) on page III-139 for details.

**MatrixOp Optimization Examples**

The section shows examples of using MatrixOp to improve performance.
• Replace matrix manipulation code with MatrixOp calls. For example, replace this:
  Make/O/N=(vecSize,vecSize) identityMatrix = p==q ? 1 : 0
  MatrixMultiply matB, matC
  identityMatrix -= M_Product
  MatrixMultiply identityMatrix, matD
  MatrixInverse M_Product
  Rename M_Inverse, matA
  
  with:
  MatrixOp matA = Inv((Identity(vecSize) - matB x matC) x matD)

• Replace waveform assignment statements with MatrixOp calls. For example, replace this:
  Duplicate/O wave2,wave1
  wave1 = wave2*2
  
  with:
  MatrixOp/O wave1 = wave2*2

• Factor and compute only once any repeated sub-expressions. For example, replace this:
  MatrixOp/O wave1 = var1*wave2*wave3
  MatrixOp/O wave4 = var2*wave2*wave3
  
  with:
  MatrixOp/O/FREE tmp = wave2*wave3 // Compute the product only once
  MatrixOp/O wave1 = var1*tmp
  MatrixOp/O wave4 = var2*tmp

• Replace instances of the ?: conditional operator in wave assignments with MatrixOp calls. For ex-
  ample, replace this:
  wave1 = wave1[p]==0 ? NaN : wave1[p]
  
  with:
  MatrixOp/O wave1 = setNaNs(wave1,equal(wave1,0))

MatrixOp Functions by Category
This section lists the MatrixOp functions by category to help you select the appropriate function.

Numbers and Arithmetic
  e     inf    Pi    nan    maxAB    mod

Trigonometric
  acos  asin  atan  atan2  cos  hypot
  phase sin  sqrt  tan

Exponential
  acosh  asinh  atanh  cosh  exp  ln
  log    powC  powR  sinh  tanh

Complex
  cmplx  conj  imag  magSqr  p2Rect  phase
  powC   r2Polar real
Rounding and Truncation

abs
ceil
clip
floor
mag
round

Conversion

cmplx
fp32
fp64
int8
int16
int32
uint8
uint16
uint32

Data Properties

numCols	numPoints	numRows	numType
waveChunks
waveLayers
wavePoints

Data Characterization

averageCols
crossCovar
chol
det
frobenius
integrate
intMatrix
maxCols
maxVal
mean
minVal
productCol
productCols
productDiagonal
productRows
sgn
sum
sumBeams
sumCols
sumRows
sumSqr
trace
varCols

Data Creation and Extraction

beam
catCols
catRows
col
colRepeat
rowRepeat
chunk
const
getDiag
identity
insertMat
inv
layer
rec
subRange
subWaveC
subWaveR
tridiag
waveIndexSet
waveMap
zeroMat

Data Transformation

diagonal
diagRC
normalize
normalizeCols
normalizeRows
redimension
replace
replaceNaNs
reverseCol
reverseCols
reverseRow
reverseRows
rotateChunks
rotateCols
rotateLayers
rotateRows
scale
scaleCols
setCol
setNaNs
setOffDiag
setRow
shiftVector
subtractMean
transposeVol

Time Domain

asyncCorrelation
convolve
correlate
limitProduct
syncCorrelation
### Analysis Programming

This section contains data analysis programming examples. There are many more examples in the WaveMetrics Procedures, Igor Technical Notes, and Examples folders.

#### Passing Waves to User Functions and Macros

As you look through various examples you will notice two different ways to pass a wave to a function: using a Wave parameter or using a String parameter.

<table>
<thead>
<tr>
<th>Using a Wave Parameter</th>
<th>Using a String Parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>Function Test1(w)</td>
<td>Function Test2(wn)</td>
</tr>
<tr>
<td>Wave w</td>
<td>String wn</td>
</tr>
<tr>
<td>Usable in functions, not in macros.</td>
<td>Usable in functions and macros.</td>
</tr>
<tr>
<td>w is a “formal” name. Use it just as if it were the name of an actual wave.</td>
<td>Use the $ operator to convert from a string to wave name.</td>
</tr>
</tbody>
</table>

The string method is used in macros and in user functions for passing the name of a wave that may not yet exist but will be created by the called procedure. The wave parameter method is used in user functions when the wave will always exist before the function is called. For details, see Accessing Waves in Functions on page IV-76.

#### Returning Created Waves from User Functions

A function can return a wave as the function result. For example:

```plaintext
Function Test()  
  Wave w = CreateNoiseWave(5, "theNoiseWave")  
  WaveStats w  
  Display w as "Noise Wave"  
End
```
Function/WAVE CreateNoiseWave(noiseValue, destWaveName)
    Variable noiseValue
    String destWaveName
    Make/O $destWaveName = gnoise(noiseValue)
    Wave w = $destWaveName
    return w
End

If the returned wave is intended for temporary use, you can create it as a free wave:

Function Test()
    Wave w = CreateFreeNoiseWave(5) // w is a free wave
    WaveStats w
    // w is killed when the function exist
End

Function/WAVE CreateFreeNoiseWave(noiseValue)
    Variable noiseValue
    Make/O/FREE aWave = gnoise(noiseValue)
    return aWave
End

To return multiple waves, you can return a “wave reference wave”. See Wave Reference Waves on page IV-71 for details.

Writing Functions that Process Waves

The user function is a powerful, general-purpose analysis tool. You can do practically any kind of analysis. However, complex analyses require programming skill and patience.

It is useful to think about an analysis function in terms of its input parameters, its return value and any side effects it may have. By return value, we mean the value that the function directly returns. For example, a function might return a mean or an area or some other characteristic of the input. By side effects, we mean changes that the function makes to any objects. For example, a function might change the values in a wave or create a new wave.

This table shows some of the common types of analysis functions. Examples follow.

<table>
<thead>
<tr>
<th>Input Parameters</th>
<th>Return Value</th>
<th>Side Effects</th>
<th>Example Function</th>
</tr>
</thead>
<tbody>
<tr>
<td>A source wave</td>
<td>A number</td>
<td>None</td>
<td>WaveSum</td>
</tr>
<tr>
<td>A source wave</td>
<td>Not used</td>
<td>The source wave is modified</td>
<td>RemoveOutliers</td>
</tr>
<tr>
<td>A source wave</td>
<td>Wave reference</td>
<td>A new destination wave is created</td>
<td>LogRatio</td>
</tr>
<tr>
<td>A source wave and a destination wave</td>
<td>Not used</td>
<td>The destination wave is modified</td>
<td></td>
</tr>
<tr>
<td>An array of wave references</td>
<td>A number</td>
<td>None</td>
<td>WavesMax</td>
</tr>
<tr>
<td>An array of wave references</td>
<td>Wave reference</td>
<td>A new wave is created</td>
<td>WavesAverage</td>
</tr>
</tbody>
</table>

The following example functions are intended to show you the general form for some common analysis function types. We have tried to make the examples useful while keeping them simple.
WaveSum Example

Input: Source wave
Return value: Number
Side effects: None

// WaveSum(w)
// Returns the sum of the entire wave, just like Igor’s sum function.
Function WaveSum(w)
    Wave w
    Variable i, n=numpnts(w), total=0
    for(i=0;i<n;i+=1)
        total += w[i]
    endfor
    return total
End

To use this, you would execute something like
Print "The sum of wave0 is:", WaveSum(wave0)

RemoveOutliers Example

Input: Source wave
Return value: Number
Side effects: Source wave is modified

Often a user function used for number-crunching needs to loop through each point in an input wave. The following example illustrates this.

// RemoveOutliers(theWave, minVal, maxVal)
// Removes all points in the wave below minVal or above maxVal.
// Returns the number of points removed.
Function RemoveOutliers(theWave, minVal, maxVal)
    Wave theWave
    Variable minVal, maxVal
    Variable i, numPoints, numOutliers
    Variable val
    numOutliers = 0
    numPoints = numpnts(theWave) // number of times to loop
    for (i = 0; i < numPoints; i += 1)
        val = theWave[i]
        if ((val < minVal) || (val > maxVal)) // is this an outlier?
            numOutliers += 1
        else // if not an outlier
            theWave[i - numOutliers] = val // copy to input wave
        endif
    endfor
    // Truncate the wave
    DeletePoints numPoints-numOutliers, numOutliers, theWave
    return numOutliers
End

To test this function, try the following commands.
Make/O/N=10 wave0= gnoise(1); Edit wave0
Print RemoveOutliers(wave0, -1, 1), "points removed"

RemoveOutliers uses the for loop to iterate through each point in the input wave. It uses the built-in numpnts function to find the number of iterations required and a local variable as the loop index. This is a very common practice.
The line “if ((val < minVal) || (val > maxVal))” decides whether a particular point is an outlier. 
|| is the logical OR operator. It operates on the logical expressions “(val < minVal)” and “(val > maxVal)”. This is discussed in detail under Bitwise and Logical Operators on page IV-39.

To use the WaveMetrics-supplied RemoveOutliers function, include the Remove Points.ipf procedure file:
#include <Remove Points>

See The Include Statement on page IV-155 for instructions on including a procedure file.

**LogRatio Example**

**Input:** Source waves  
**Return value:** Wave reference  
**Side effects:** Output wave created

// LogRatio(source1, source2, outputWaveName)  
// Creates a new wave that is the log of the ratio of input waves.  
// Returns a reference to the output wave.

Function/WAVE LogRatio(source1, source2, outputWaveName)
   Wave source1, source2  
   String outputWaveName  
   Duplicate/O source1, $outputWaveName  
   WAVE wOut = $outputWaveName  
   wOut = log(source1/source2)  
   return wOut
End

To call this from a function, you would execute something like:

Wave wRatio = LogRatio(wave0, wave1, "ratio")  
Display wRatio

The LogRatio function illustrates how to treat input and output waves. Input waves must exist before the function is called and therefore are passed as wave reference parameters. The output wave may or may not already exist when the function is called. If it does not yet exist, it is not possible to create a wave reference for it. Therefore we pass to the function the desired name for the output wave using a string parameter. The function creates or overwrites a wave with that name in the current data folder and returns a reference to the output wave.

**WavesMax Example**

**Input:** Array of wave references  
**Return value:** Number  
**Side effects:** None

// WavesMax(waves)  
// Returns the maximum value in waves in the waves array.

Function WavesMax(waves)
   Wave/WAVE waves  
   Variable theMax = -INF  
   Variable numWaves = numpnts(waves)  
   Variable i  
   for(i=0; i<numWaves; i+=1)  
      Wave w = waves[i]  
      Variable tmp = WaveMax(w)  
      theMax = max(tmp, theMax)  
   endfor  
   return theMax
End

This function illustrates how you might call WavesMax from another function:
Function DemoWavesMax()
    Make/FREE/N=10 w0 = p
    Make/FREE/N=10 w1 = p + 1

    Make/FREE/WAVE waves = {w0, w1}

    Variable theMax = WavesMax(waves)

    Printf "The maximum value is %g\r", theMax
End

WavesAverage Example
Input: An array of wave references
Return value: Wave reference
Side effects: Creates output wave

// WavesAverage(waves, outputWaveName)
// Returns a reference to a new wave, each point of which contains the
// average of the corresponding points of a number of source waves.
// waves is assumed to contain at least one wave reference and
// all waves referenced by waves are expected to have the same
// number of points.
Function/WAVE WavesAverage(waves, outputWaveName)
    Wave/WAVE waves // A wave containing wave references
    String outputWaveName

    // Make output wave based on the first source wave
    Wave first = waves[0]
    Duplicate/O first, $outputWaveName
    Wave wOut = $outputWaveName
    wOut = 0

    Variable numWaves = numpnts(waves)
    Variable i
    for(i=0; i<numWaves; i+=1)
        Wave source = waves[i]
        wOut += source // Add source to output
    endfor

    wOut /= numWaves // Divide by number of waves

    return wOut
End

This function shows how you might call WavesAverage from another function:

Function DemoWavesAverage()
    Make/FREE/N=10 w0 = p
    Make/FREE/N=10 w1 = p + 1

    Make/FREE/WAVE waves = {w0, w1}

    Wave wAverage = WavesAverage(waves, "averageOfWaves")
    Display wAverage
End

Finding the Mean of Segments of a Wave

An Igor user who considers each of his waves to consist of a number of segments with some number of
points in each segment asked us how he could find the mean of each of these segments. We wrote the Find-
SegmentMeans function to do this.
Function/WAVE FindSegmentMeans(source, n)

    Wave source
    Variable n

    String dest // name of destination wave
    Variable segment, numSegments
    Variable startX, endX, lastX

    dest = NameOfWave(source)+"_m" // derive name of dest from source
    numSegments = trunc(numpnts(source) / n)
    if (numSegments < 1)
        DoAlert 0, "Destination must have at least one point"
        return $"" // Null wave reference
    endif

    Make/O/N=(numSegments) $dest
    WAVE destw = $dest
    for (segment = 0; segment < numSegments; segment += 1)
        startX = pnt2x(source, segment*n) // start X for segment
        endX = pnt2x(source, (segment+1)*n - 1)// end X for segment
        destw[segment] = mean(source, startX, endX)
    endfor

    return destw
End

This diagram illustrates a source wave with three ten-point segments and a destination wave that will contain the mean of each of the source segments. The FindSegmentMeans function makes the destination wave.

To test FindSegmentMeans, try the following commands.

Make/N=100 wave0=p+1; Edit wave0
FindSegmentMeans(wave0,10)
Append wave0_m

The loop index is the variable “segment”. It is the segment number that we are currently working on, and also the number of the point in the destination wave to set.

Using the segment variable, we can compute the range of points in the source wave to work on for the current iteration: segment*n up to (segment+1)*n - 1. Since the mean function takes arguments in terms of a wave’s X values, we use the pnt2x function to convert from a point number to an X value.

If it is guaranteed that the number of points in the source wave is an integral multiple of the number of points in a segment, then the function can be speeded up and simplified by using a waveform assignment statement in place of the loop. Here is the statement.

    destw = mean(source, pnt2x(source,p*n), pnt2x(source,(p+1)*n-1))

The variable p, which Igor automatically increments as it evaluates successive points in the destination wave, takes on the role of the segment variable used in the loop. Also, the startX, endX and lastX variables are no longer needed.
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Using the example shown in the diagram, \( p \) would take on the values 0, 1 and 2 as Igor worked on the destination wave. \( n \) would have the value 10.

Working with Mismatched Data

Occasionally, you may find yourself with several sets of data each sampled at a slightly different rate or covering a different range of the independent variable (usually time). If all you want to do is create a graph showing the relationship between the data sets then there is no problem.

However, if you want to subtract one from another or do other arithmetic operations then you will need to either:

- Create representations of the data that have matching X values. Although each case is unique, usually you will want to use the Interpolate2 operation (see Using the Interpolate2 Operation on page III-106) or the interp function (see Using the Interp Function on page III-105) to create data sets with common X values. You can also use the Resample to create a wave to match another.

- Properly set each wave’s X scaling, and perform the waveform arithmetic using X scaling values and Igor’s automatic linear interpolation. See Mismatched Waves on page II-75.

The WaveMetrics procedure file Wave Arithmetic Panel uses these techniques to perform a variety of operations on data in waves. You can access the panel by choosing Packages→Wave Arithmetic from the Analysis menu. This will open the procedure file and display the control panel. Click the help button in the panel to learn how to use it.

References
