

Igor

Technical Notes

WaveMetrics Technical Support

#020-INFO: Choosing the Right TN #020

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TN #020: Peak Measurement and Fitting

In the beginning, there was Technical Note #020, the Peak Measurement experiment. Well, okay, it was actually October 1990. It fit the sum of Gaussian or Lorentzian peaks and a baseline function to your data. It handled 1-6 peaks. The experiment was way cool, but impervious to customization.

TN#020-A: Custom Peak Measurement

Then customers wanted to fit other kinds of peaks, and TN020-A saw the light of day. It contains **two** experiments much like TN020 which are easier to modify to add a different peak type. The Custom Peak Measurement experiment already fits the sum of Voigt peaks and a baseline. Detailed instructions show you how to modify the experiment to fit to a different kind of peak. The Template Peak Measurement experiment fits the sum of interpolated and scaled versions of arbitrary peaks and a baseline to your data. The peak template is stored in an x-y pair of waves. The template originally contains a raised cosine peak. Both of these experiments handle 1-6 peaks.

TN#020-B: Peak Areas

And lo! Other customers saw that six peaks was too few, and couldn't we help them with their two hundred peaks? Yes, we could. Thus was born the Peak Areas experiment.

This experiment is useful when you have data containing a large number of peaks and need "rough and ready" estimates of peak parameters. This experiment does not fit a peak function to your data; it just measures the amplitude, width, and areas of peaks. There is no programmed limit to the number of peaks, but each peak measurement takes about 1 second on a Mac IIfx.

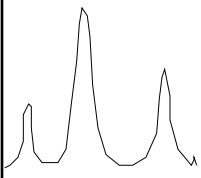
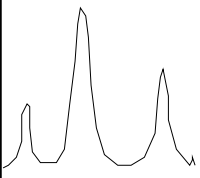
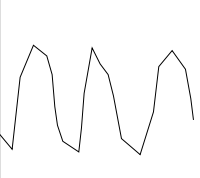
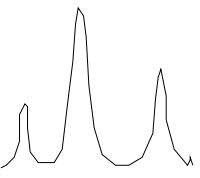
NOTE: The Peak Areas experiment's automatic peak finder assumes the data has regularly spaced periodic BIPOLAR PEAKS (peaks that have easily minima and maxima). If your data is unipolar (gaussian-like peaks on a baseline), use TN#020-C Unipolar Peak Areas.

The automatic peak identifier is crude, but can be modified by the knowledgeable user. If the automatic peak finder doesn't work with your data, you can still make peak measurements. Just use the cursors to identify the peak start, center, and end. The experiment does the rest: it can create and subtract a piecewise linear baseline, and make the measurements automatically.

TN#020-C: Unipolar Peak Areas

This is essentially a re-write of TN#020-B to handle unipolar peaks. Thresholds are used to locate the start and peak ends (instead of local minima). This experiment doesn't have its own documentation; refer to TN#020-B documentation.

Summary

Feature	Technical Note			
	020 & 020-H	020-A	020-B	020-C
Number of Peaks	1-6	1-6	1-∞	1-∞
Peak Fitting	Yes	Yes	No	No
Peak Measurements Based On	Fit Parameters	Fit Parameters	Direct Measurement	Direct Measurement
Peak Identification Algorithm	FindAPeak XOP	FindAPeak XOP	Local Min/Max	Min Threshold, Local Maxima
Compatible Peak Shape				
Peak Shape Functions	gauss, lor	voigt, template, custom	n/a	n/a
Ease of Modification	Difficult	Moderate	Easier	Easier
Documentation	TN020, TN020-H	TN020, TN020-A	TN020, TN020-B	TN020, TN020-B (really)

TN#020-D through G:

There aren't any (at least not yet).

TN#020-H: Holding Peak Fitting Estimates Constant

This is a small modification of the original Technical Note #020, the Peak Measurement experiment. The 'Peak Measurement' experiment estimates the position, width and amplitude of peaks automatically or semi-automatically. If you *know* any of these parameters and don't want Igor to vary them during peak fitting, TN020 does not provide an easy way to that.

This experiment (Peak Meas Enter Est & Hold) provides those capabilities, in addition to all of the capabilities of the original TN020 Peak Measurement experiment. It remains difficult to modify.

TN020-INFO: Continuing the Peak Fit (more iterations)

This note describes how you can change TN020 Peak Measurement and Fitting to cause the fitting of peaks to proceed after Igor gives up trying to fit. Sometimes this results in a successful fit in very difficult situations.

These changes do not provide you with more iterations of 'FitBaselineAtRegions'.

TN020-INFO: Entering Peak Estimates Directly

Often you want to enter the peak parameters directly rather than have Igor automatically estimate them, or use the cursors to manually identify the peaks.

This note describes how you can change TN020-A: Custom Peak Measurement and TN020-A: Template experiments by adding a new 'Enter New Peak Estimate' macro, similar to TN020-H, but without the "hold" capability.