# Table of Contents

Calculating Integrals and Statistics (Pro edition only) on Intervals using Fit Plot

Setting of intervals in `Fit interval` tab of Fit Plot was initially intended for specifying the range of data which are used for fitting by sum of fit curves. However, this tab can also be used to calculate integrals and statistics on these intervals (Statistics is only available in Pro edition). Data-Baseline is used to calculate the results.

Peak Moments

MagicPlot can integrate data on selected intervals and calculate peak moments (x mean, variance, skewness, kurtosis). Spectrum line is treated as probability distribution curve: *x* values are treated as 'independent variable' and *y* values are treated as 'probability'. Standard statistical formulas are used to calculate moments (see below).

Statistical data and integrals are automatically updated if *x* or *y* data are changed or intervals are changed.
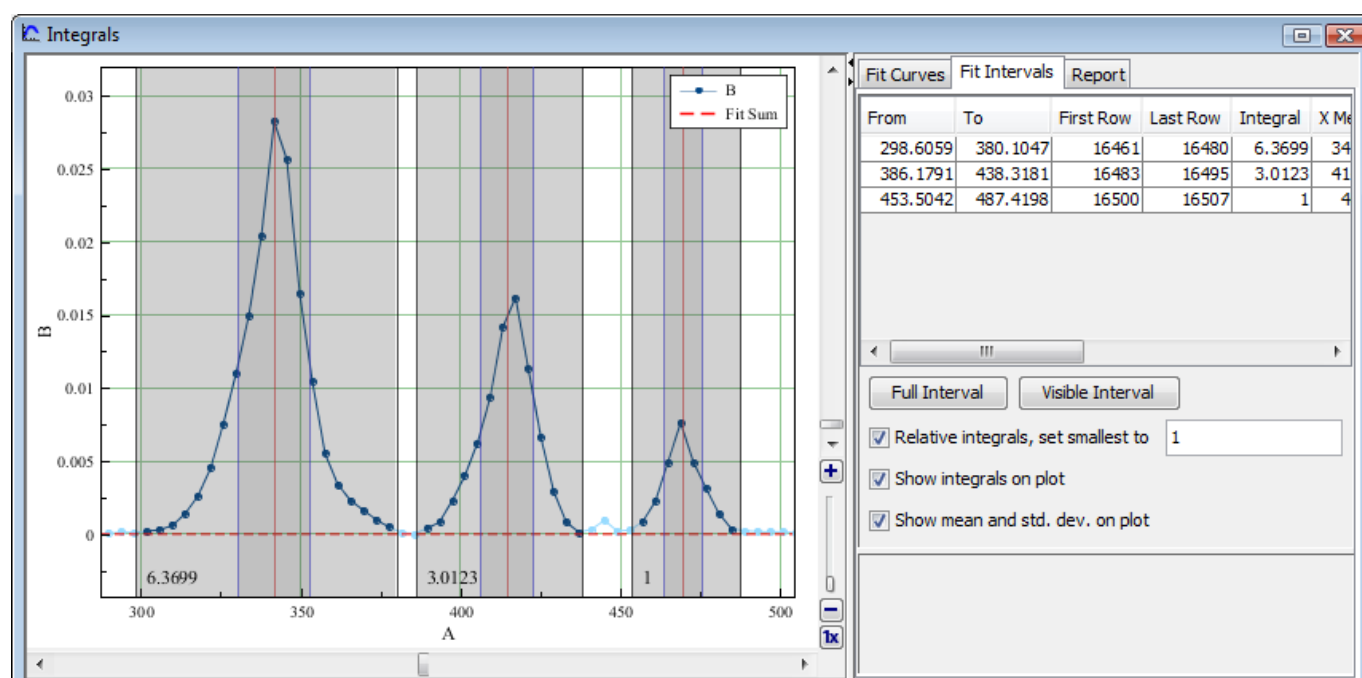
All statistical data are summarized in the intervals table:

From	To	First Row	Last Row	Integral	X Mean	Variance	Std.dev.	Skewness	Kurtosis	Y Sum	Points
298.6059	380.1047	16461	16480	6.3699	341.6323	128.0854	11.3175	8.7703e-4	0.6547	0.1588	20
386.1791	438.3181	16483	16495	3.0123	414.6365	68.0536	8.2495	-0.3499	0.0449	0.0752	13
453.5042	487.4198	16500	16507	1	469.668	35.0647	5.9215	0.1509	-0.2173	0.0255	8

Managing Intervals

Move interval borders with mouse. Double click on interval to split it at desired position. Right click opens context menu from which new intervals can be created on free space and existing intervals can be deleted or split.

Relative Integrals Calculation

MagicPlot can calculate relative integrals to compare the relative intensity of spectrum lines. To compute relative integrals set `Relative integrals` checkbox. MagicPlot designate the smallest integral as 1, but you can enter a custom value. If you want to set not the smallest integral as a reference point, enter 1 first and then enter the value of desired integral relative to 1 into this field, so that other integrals will be calculated relative to this new value.

Computational Formulas

Central moments are calculated as follows (see table). All sums are calculated using W compensated summation. Central moments are calculated on second pass after Mean calculation.

Property	Formula
n	The number of non-NaN (x,y) points
Y Sum (normalization)	$s = \sum_{i=1} y_i$
X Mean (first moment)	
2, 3, 4th W Central moments	$\nu_1 = \frac{1}{s}\sum_j y_j x_j$

$$\mu_k = \frac{1}{s}\sum_j y_j \left(x_j - \nu_1\right)^k, \quad k=2...4$$

MagicPlot uses the following formulas to calculate intervals statistics:

Property	Formula
Integral	Calculated using Trapezoidal rule
X Mean (expected value)	$\mu = \nu_1$
Variance	$\sigma^2 = \frac{n}{n-1}\mu_2$
Standard deviation	$\sigma = \sqrt{\sigma^2}$
Skewness	
Kurtosis	

$$\gamma_1 = \frac{\sqrt{n(n-1)}}{n-2}\frac{\mu_3}{\sigma^3}$$

$$\gamma_2 = \frac{1}{(n-2)(n-3)}\left((n+1)\frac{\mu_4}{\sigma^4} - 3(n-1)\right)$$

See Also

- Nonlinear Curve Fitting: Fit Plot
- Using Spline for Baseline Subtraction
- Descriptive Statistics

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<https://magicplot.com/wiki/> - **MagicPlot Manual**

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