Week 7

Goodness/Badness of Fits:

Using χ^2 to choose parent function

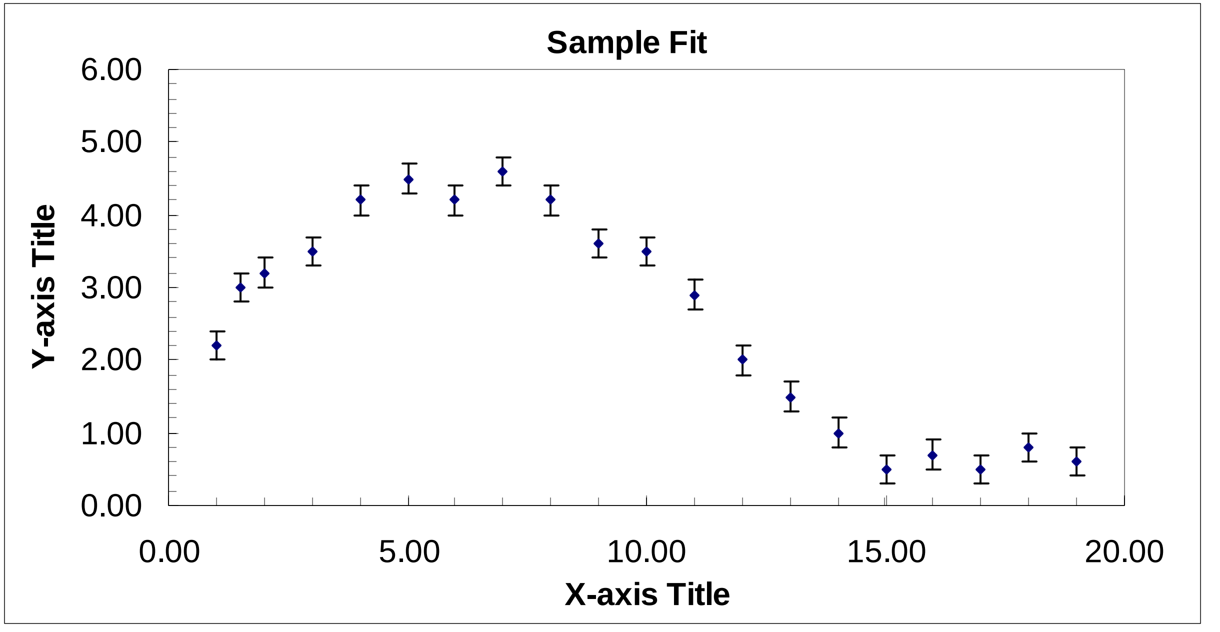
False or Local Minima

New and Improved MPL Fitting:

- Henceforth you can use the "full power" version of our MPL fitting program
- look for: mpl_DATAFIT10
  - password on some machines is "<see board>"
- fits all parameters sequentially, using the grid search method (to be explained next week)
- estimates parameter uncertainties for you using two methods (to be explained)

Using χ^2 to choose parent function

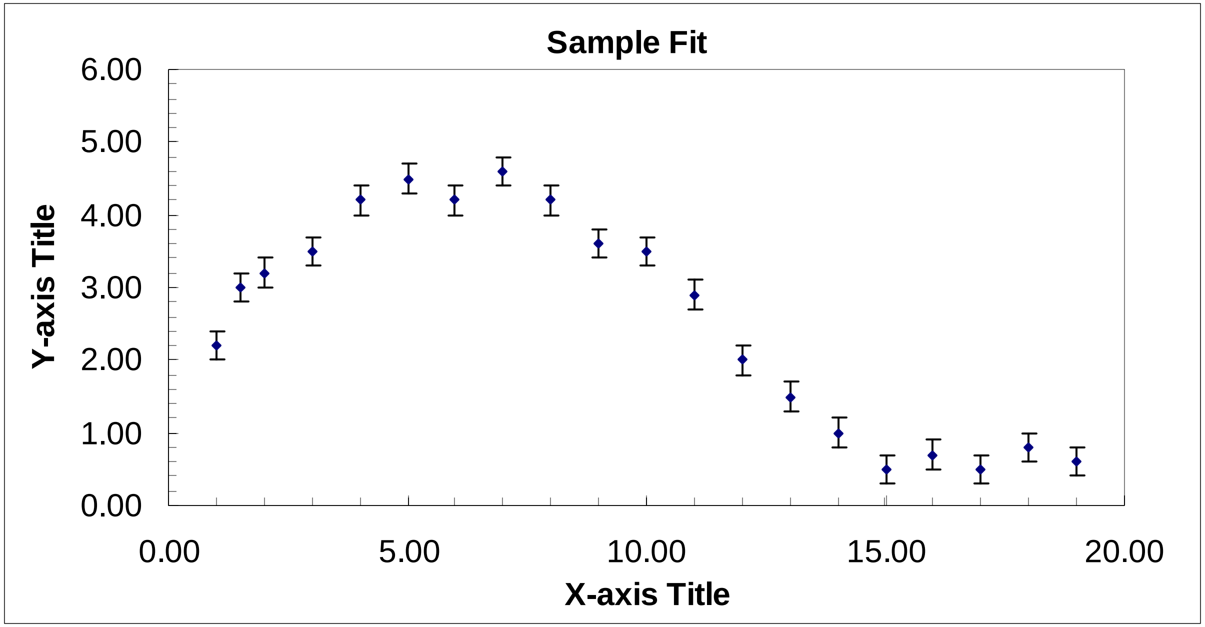
- What is a reasonable "parent" function to fit this data?
- Suppose we have competing views of reality:
  - sine function
  - polynomial function



$$y(x) = a_1 \sin(a_2 x + a_3) + a_4$$

$$y(x) = a_1 + a_2(x - a_5) + a_3(x - a_5)^2 + a_4(x - a_5)^3$$

Using χ^2 to choose parent function



$$y(x) = a_1 \sin(a_2 x + a_3) + a_4$$

Run demo of mpl_DATAFIT10 for sine-function case...

Using χ^2 to choose parent function

Modern Physics Lab Data Fitting

R.A.Sch. v.10b

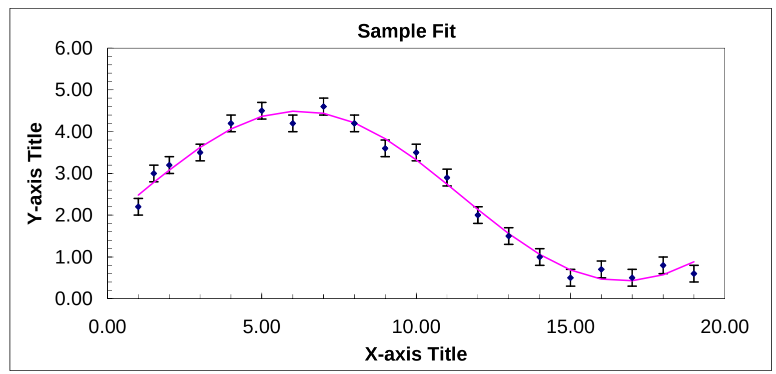
Date Now: 22-Feb-2009 **Time Now:** 9:25:41 PM **Log Book Page:** ________

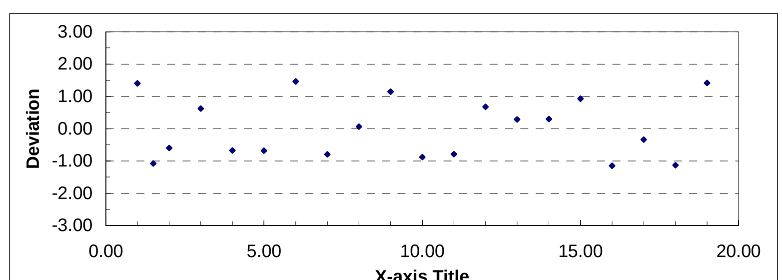
	Value	Initial Step Size	Final Step Size	Estimated Uncertainty	Refined Uncertainty
Fit Parameter 1=	-2.04	0.1	0.0063		
Fit Parameter 2=	0.30	0.1	0.0002		
Fit Parameter 3=	2.85	0.1	0.0063		
Fit Parameter 4=	2.46	0.1	0.0063		
Fit Parameter 5=					
χ^2 =	16.50				
χ^2/d.o.f. =	1.03				

Entries	Constraints	d.o.f.	$\sigma(\chi^2/\text{dof})$
20	4	16	0.35

Substitute your data (up to 1090 lines) below. Program "FIT Theory" column with your fitting function.

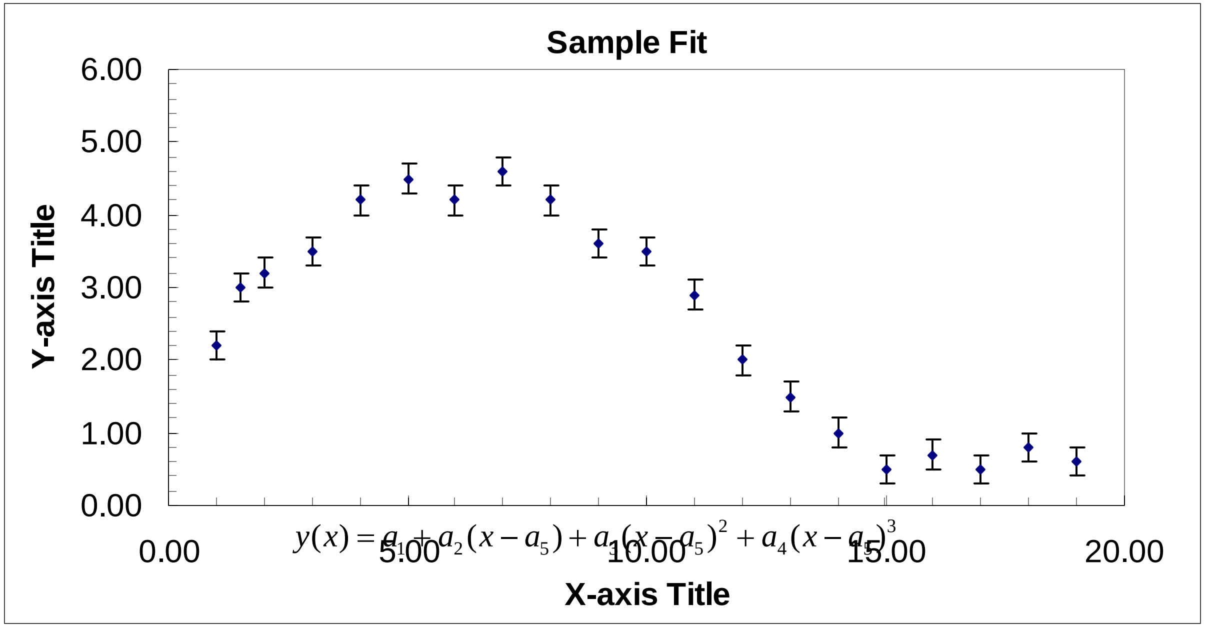
	X Data	Y Data	DY Data	FIT Theory	Deviation	Dev. ^{2}
1	1.00	2.20	0.20	2.48	1.40	1.97
2	1.50	3.00	0.20	2.78	-1.08	1.16
3	2.00	3.20	0.20	3.08	-0.60	0.36
4	3.00	3.50	0.20	3.62	0.62	0.39
5	4.00	4.20	0.20	4.07	-0.67	0.45
6	5.00	4.50	0.20	4.36	-0.68	0.47
7	6.00	4.20	0.20	4.49	1.46	2.13
8	7.00	4.60	0.20	4.44	-0.80	0.64
9	8.00	4.20	0.20	4.21	0.06	0.00
10	9.00	3.60	0.20	3.83	1.15	1.31
11	10.00	3.50	0.20	3.32	-0.88	0.77
12	11.00	2.90	0.20	2.74	-0.79	0.62
13	12.00	2.00	0.20	2.13	0.67	0.46
14	13.00	1.50	0.20	1.56	0.28	0.08
15	14.00	1.00	0.20	1.06	0.30	0.09
16	15.00	0.50	0.20	0.69	0.93	0.86
17	16.00	0.70	0.20	0.47	-1.15	1.32
18	17.00	0.50	0.20	0.43	-0.34	0.12
19	18.00	0.80	0.20	0.57	-1.13	1.28
20	19.00	0.60	0.20	0.88	1.41	2.00





χ^2 **Tolerance = +-** 0.010

Using χ^2 to choose parent function



$$y(x) = a_1 + a_2(x - a_5) + a_3(x - a_5)^2 + a_4(x - a_5)^3$$

Run demo of 5_param_fit for polynomial case...

Using χ^2 to choose parent function

Modern Physics Lab Data Fitting

R.A.Sch. v.10b

Date Now: 22-Feb-2009 **Time Now:** 9:14:02 PM **Log Book Page:** ________

	Value	Initial Step Size	Final Step Size	Estimated Uncertainty	Refined Uncertainty
Fit Parameter 1=	3.20	0.1	0.0063		
Fit Parameter 2=	-0.50	0.1	0.0004		
Fit Parameter 3=	-0.0214	0.0020	0.0001		
Fit Parameter 4=	0.00516	0.00050	0.0000		
Fit Parameter 5=	[illegible]	1	0.0039		
χ^2 =	21.81				
χ^2/d.o.f. =	1.45				

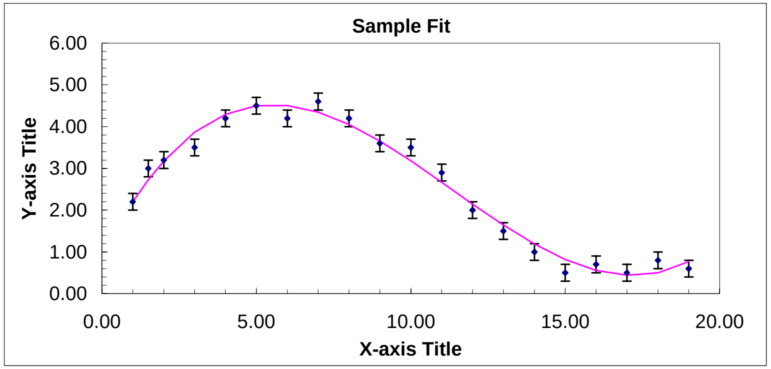
Polynomial: loser

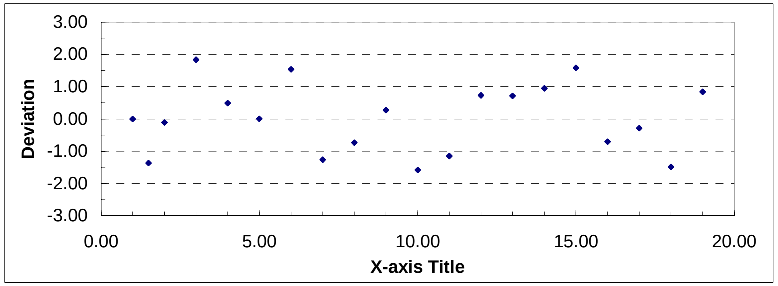
Entries	Constraints	d.o.f.	$\sigma(\chi^2/dof)$
20	5	15	0.37

Substitute your data (up to 1090 lines) below. Program "FIT Theory" column with your fitting function

Both fits "look" reasonable...

	X Data	Y Data	DY Data	FIT Theory	Deviation	Dev. ^{2}
						0.00
						1.87
						0.01
						3.37
						0.24
						0.00
						2.35
						1.60
						0.54
						0.07
11	10.00	3.50	0.20	3.18	-1.58	2.51
12	11.00	2.90	0.20	2.67	-1.15	1.32
13	12.00	2.00	0.20	2.15	0.73	0.53
14	13.00	1.50	0.20	1.64	0.71	0.50
15	14.00	1.00	0.20	1.19	0.94	0.89
16	15.00	0.50	0.20	0.82	1.59	2.51
17	16.00	0.70	0.20	0.56	-0.71	0.50
18	17.00	0.50	0.20	0.44	-0.28	0.08
19	18.00	0.80	0.20	0.50	-1.49	2.21
20	19.00	0.60	0.20	0.77	0.84	0.71





χ^2 **Tolerance = +-** 0.010

Using χ^2 to choose parent function

Modern Physics Lab Data Fitting

R.A.Sch. v.10b

Date Now: 22-Feb-2009 **Time Now:** 9:25:41 PM **Log Book Page:** ________

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Fit Parameter 5=					
χ^2 =	16.50				
χ^2/d.o.f. =	1.03				

Entries	Constraints	d.o.f.	$\sigma(\chi^2/\text{dof})$
20	4	16	0.35

Sine: winner

Substitute your data (up to 1090 lines) below. Program "FIT Theory" column with your fitting function

Both fits "look" reasonable...

	X Data	Y Data	DY Data	FIT Theory	Deviation	Dev. ^{2}
						1.97
						1.16
						0.36
						0.39
						0.45
						0.47
						2.13
						0.64
						0.00
						1.31
11	10.00	3.50	0.20	3.32	-0.88	0.77
12	11.00	2.90	0.20	2.74	-0.79	0.62
13	12.00	2.00	0.20	2.13	0.67	0.46
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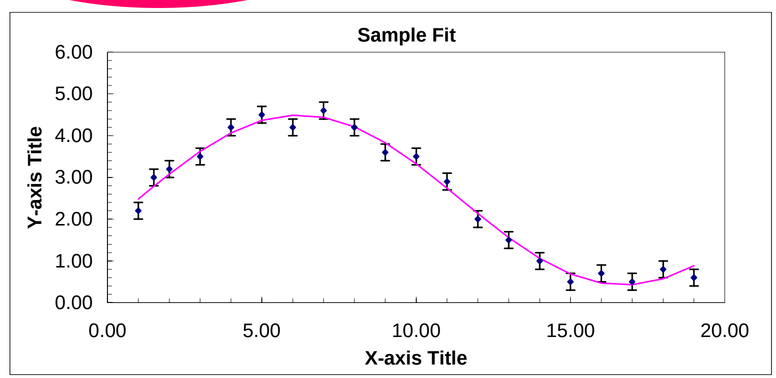
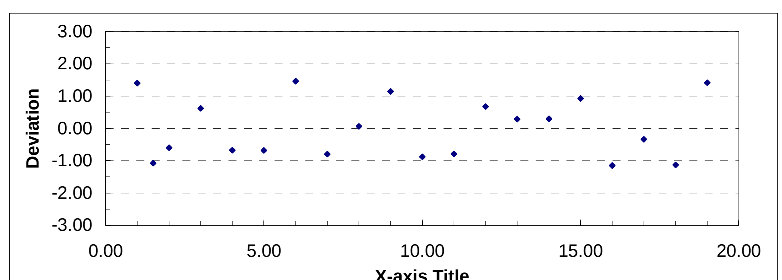
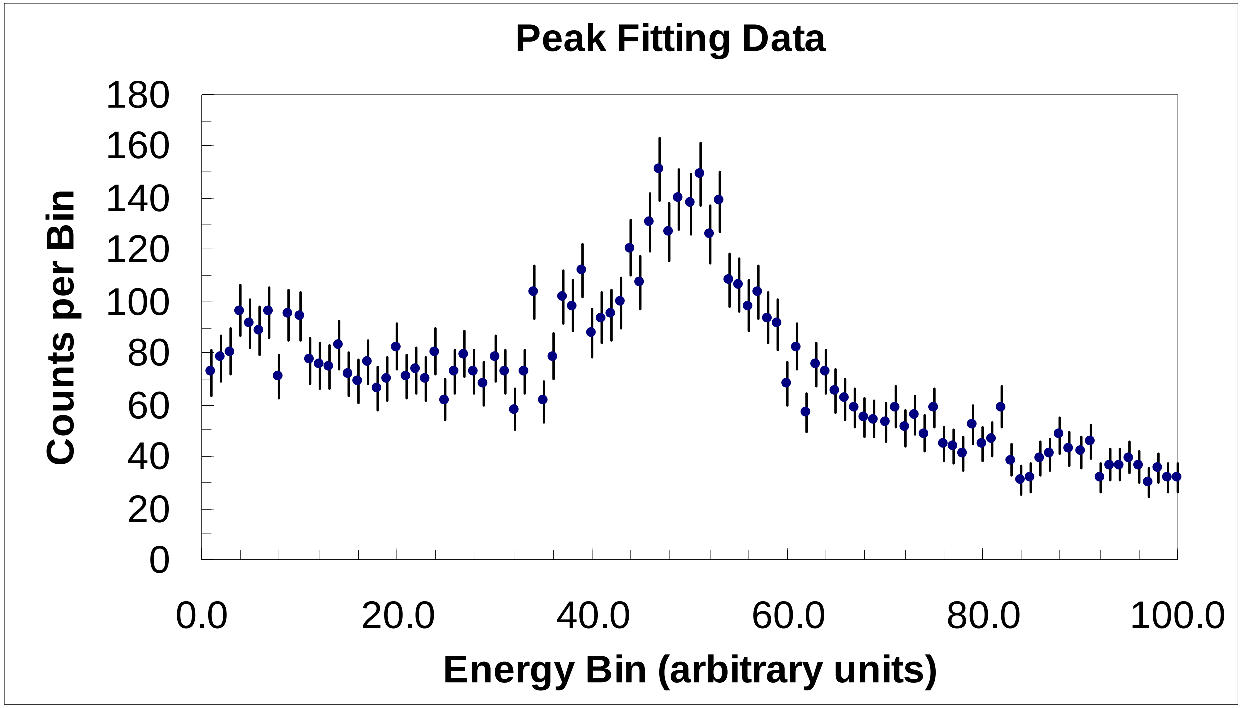
15	14.00	1.00	0.20	1.06	0.30	0.09
16	15.00	0.50	0.20	0.69	0.93	0.86
17	16.00	0.70	0.20	0.47	-1.15	1.32
18	17.00	0.50	0.20	0.43	-0.34	0.12
19	18.00	0.80	0.20	0.57	-1.13	1.28
20	19.00	0.60	0.20	0.88	1.41	2.00





χ^2 Tolerance = +- 0.010

Gaussian vs. Lorentzian Lineshapes

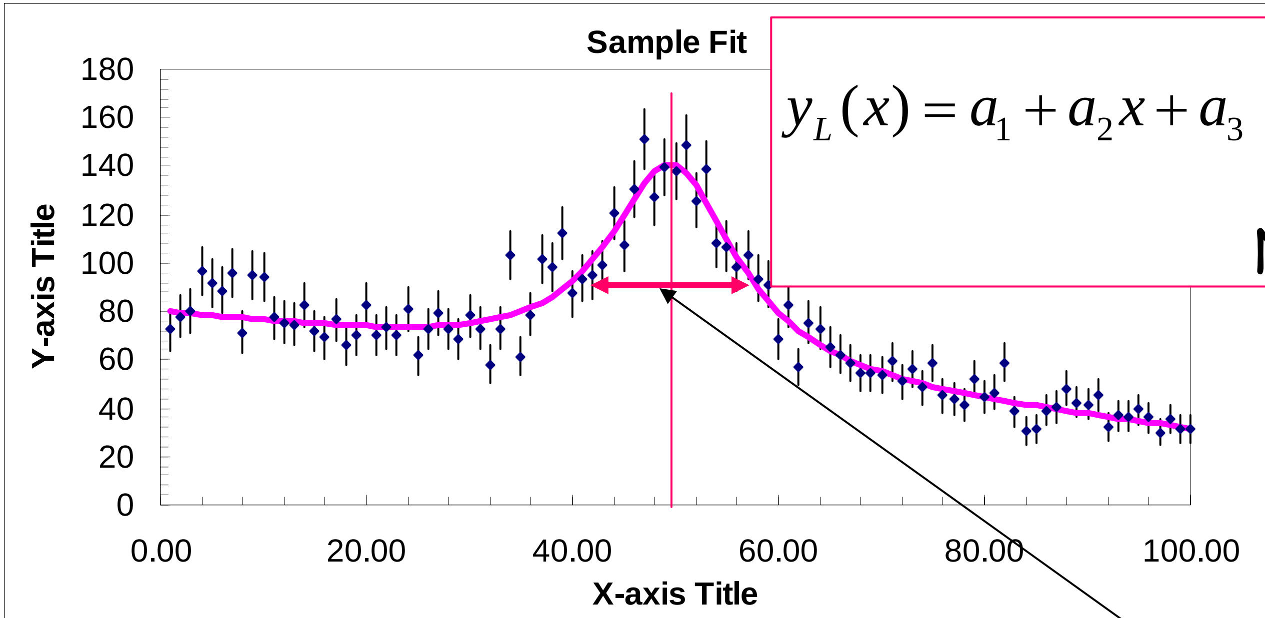


- Often we have to fit a "peak" above "background"
- Examples in: Mossbauer, Compton, Neutron, ESR, X-Ray

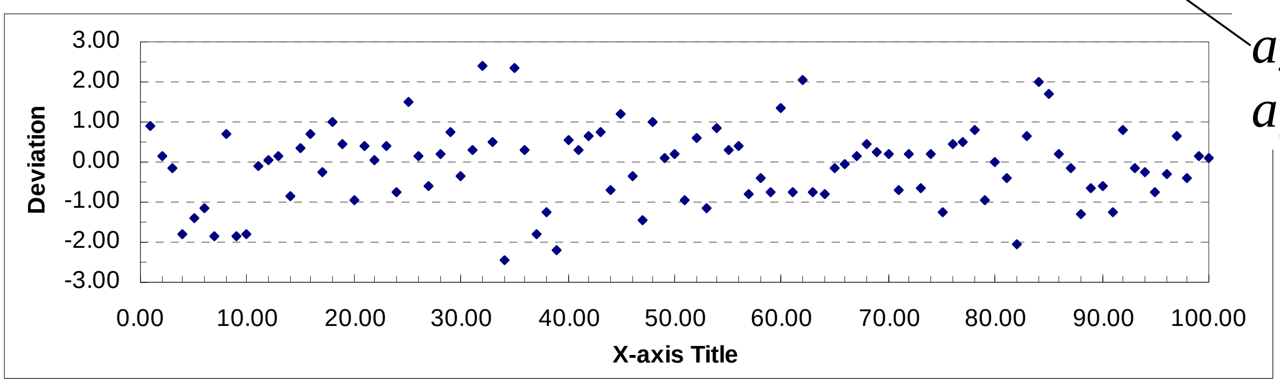
What parent function should you pick?

mpl_Gaussian
mpl_Lorentzian

Try a "Lorentzian" + polynomial



$$y_L(x) = a_1 + a_2 x + a_3 \underbrace{\left\{ \frac{a_4 / 2\pi}{(x - a_5)^2 + (a_4/2)^2} \right\}}_{\text{Normalized Lorentzian}}$$

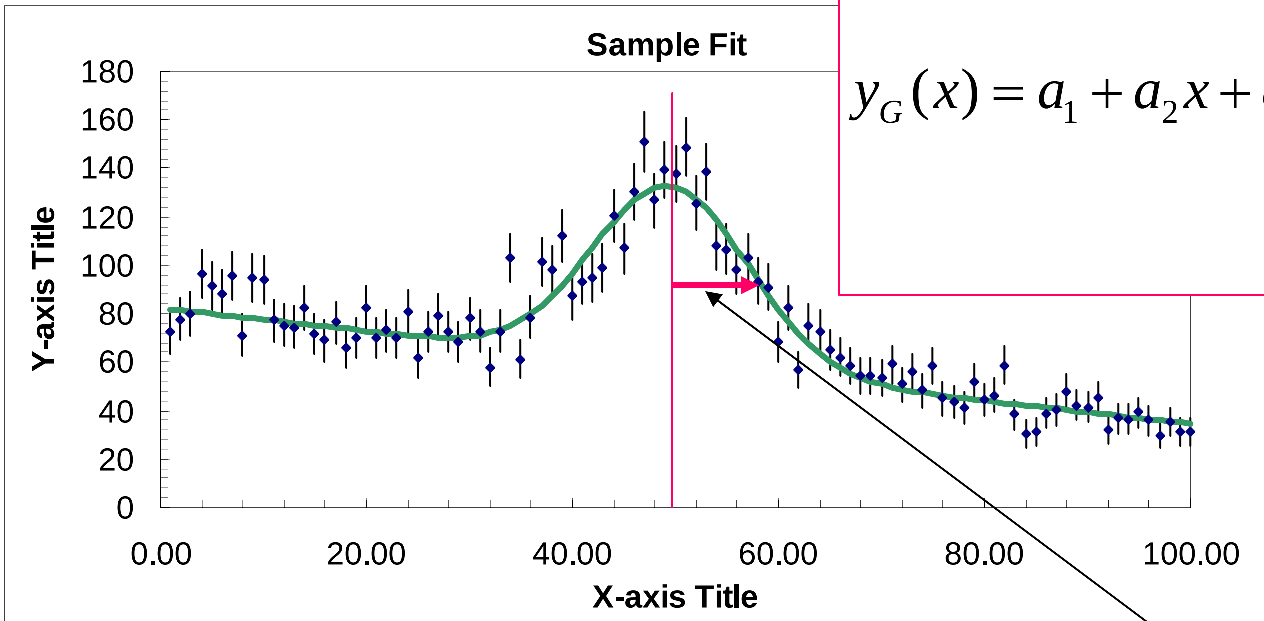


a_4 = 2.354σ = "FWHM"

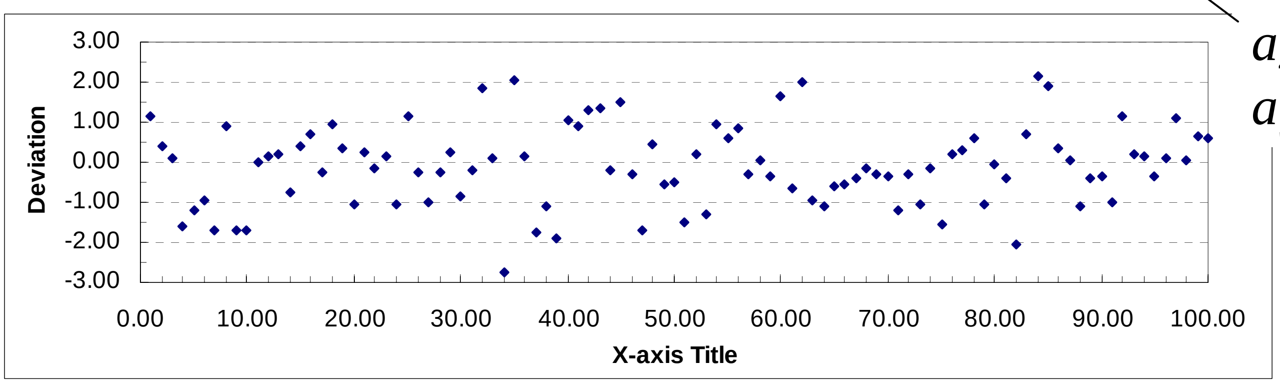
a_3 = "area under curve"

χ^2/ν = 1.00 ± 0.15

Try a "Gaussian" + polynomial



$$y_G(x) = a_1 + a_2 x + a_3 \underbrace{\left\{ \frac{1}{\sqrt{2\pi}} \frac{1}{a_4} e^{-\frac{1}{2}\left(\frac{x-a_5}{a_4}\right)^2} \right\}}_{\text{Normalized Gaussian}}$$



a_4 = σ = "width"

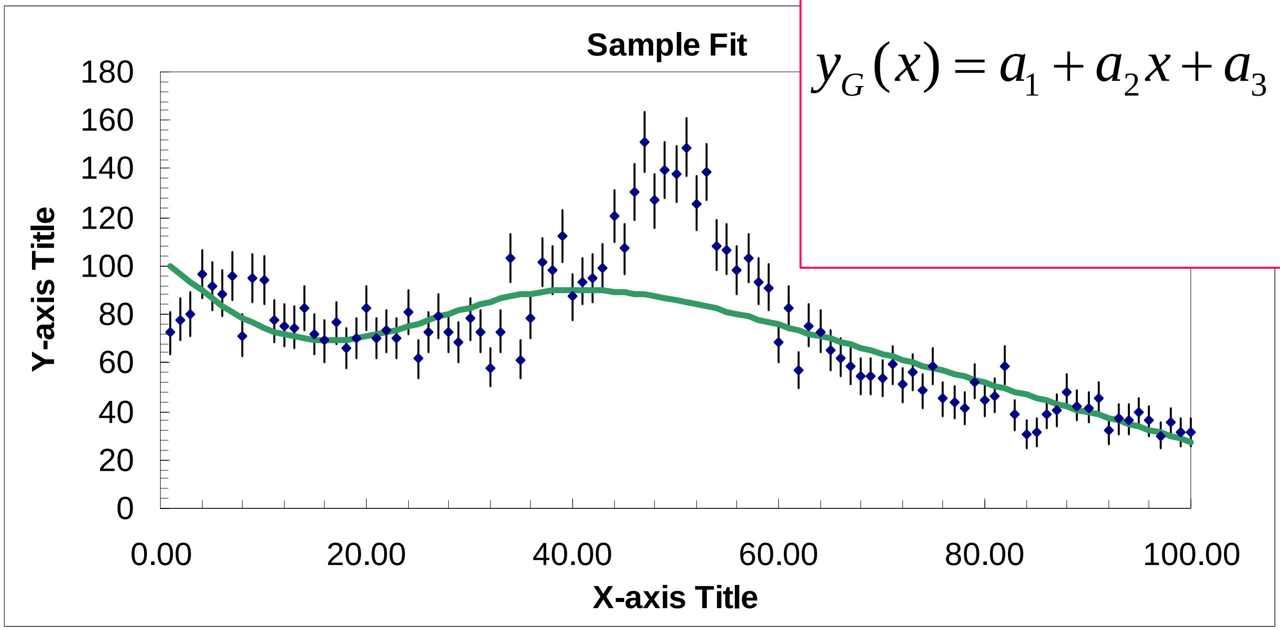
a_3 = "area under curve"

χ^2/ν = 1.06 ± 0.15

Gaussian vs. Lorentzian Lineshapes

- Both parent functions were linear in a1, a2, a3, but non-linear in a4 and a5
  - necessitated iterated fit solutions
  - cf. Bevington Chap. 7 & 8 on non-linear fitting
- In this case, the χ^2 values were too close to "tell" whether one parent function or the other was better
  - How to answer the question? Get more and better data !

False/Local Minima



$$y_G(x) = a_1 + a_2 x + a_3 \underbrace{\left\{ \frac{1}{\sqrt{2\pi}} \frac{1}{a_4} e^{-\frac{1}{2}\left(\frac{x-a_5}{a_4}\right)^2} \right\}}_{\text{Normalized Gaussian}}$$

χ^2/ν =
3.50 ± 0.15

- A major problem when fitting many parameters
- Even sophisticated computer programs are often fooled
- Try random starting values to see whether convergence is stable

FalseMinimum

Summary

- If you are confident the errors on the data are correct, fitting to various parent functions can distinguish among "physics" options
- Take care to consider the "goodness" of the fit when deciding where one parent or another is better
- Beware the lure of false minima: restart the search at various places to test for lower minima
- Program mpl_DATAFIT10 (password given) is available to use

Backup Slides…