Non-linear least squares fitting two Gaussians in Excel

The Gaussians are given by C column, which is plotted vs. the B column. The initial guess for the parameters is given in the cells H7, I7, J7 and H8, I8 and J8

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We can use the STDEV function (in another worksheet as needed) to calculate the noise in the data. This is shown below. Note that there are 50 data points in the file.

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Using the estimate for the noise the value of chi-squared can be estimated and is given in cell L9 in this sheet. This step is essential for Solver to work.

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4		2	-0.00631	0.000472	9.9692E-23	0.006312		First make	a graph of	both		00						+
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6		4	0.01636	0.000614	1.9288E-22	-0.01636												T
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11		9	0.002571	-0.00029	9.85E-22	-0.00257												
12		10	-0.00437	-0.00027	1.3602E-21	0.004368												
13		11	0.002607	0.000603	1.8763E-21	-0.00261			Two O	verlappi	ng Gaus	ssians wi	th Initia	l Guess				
14		12	0.015395	-0.00041	2.5854E-21	-0.01539		0.5										
15		13	0.007243	0.000352	3.5585E-21	-0.00724					٨							
16		14	0.001776	0.000526	4.8923E-21	-0.00178		0.4										
17		15	0.008453	0.000182	6.7186E-21	-0.00845		0.3										
18		16	0.005783	-0.00031	9.2165E-21	-0.00578		0.0				*						
19		17	-0.00068	0.000773	1.2629E-20	0.000684		0.2			- Y	<u> </u>						
20		18	0.004804	0.000701	1.7286E-20	-0.0048					11	1						
21		19	-0.0052	0.00044	2.3633E-20	0.005205		0.1			1							
22		20	0.013383	0.000968	3.2276E-20	-0.01338		o 👾	1. In Party	May Jack and	4	~	Marine Marine					
23		21	0.002537	-0.00053	4.4031E-20	-0.00254		0	100	20	0	300	400	500	600			
24		22	0.002272	0.000315	5.9999E-20	-0.00227		-0.1										
25		23	0.012812	-0.00051	8.1668E-20	-0.01281					noi	se 1 —						
26		24	0.010398	0.000281	1.1104E-19	-0.0104							1					
27		25	-0.0024	0.000344	1.5081E-19	0.002396												
4	> Peak overlap data	TGA da	ata She	et3 (÷						•							
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(6 💿 📋 🛓	<u> </u>		<u>ک</u>	1 0)										· ·	Pr ENG	

Then we run Solver, which will alter the parameters given in the 6 cells indicated previously to minimize the value of chi-squared. If you cannot find Solver then you need to install the Add-in as shown in a previous segment.

🚺 🔒 🗲 e e e e e e e e e e e e e e e e e e					tutorial_6_g	aussians_B	[Comp	patibility N	lode] - Excel						? 🛧 –	8 ×			
FILE HOME INSERT PAG	E LAYOUT	FORMUL	AS DA	TA REVIE	W VIEW AC	ROBAT										Sign in			
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6	4	0.01636	0.000614	1.9288E-22	-0.01636	THE DOLL	autu	Sets with	ru combin	ation of t	.wo daassii	and doing the be		calculate th	e target cell.				
7	5	-0.00495	0.000613	2.6785E-22	0.004947		15	250	15					SOLVE	R				
8	- 6	0.010262	-0.00042	3.7153E-22	-0.01026		20	300	30					Tell me	more				
9	7	-0.00261	0.000746	5.1479E-22	0.002614						2.791264			-					
10	8	-0.02278	-0.0006	7.1248E-22	0.02278						· · · · ·								
11	9	0.002571	-0.00029	9.85E-22	-0.00257														
12	10	-0.00437	-0.00027	1.3602E-21	0.004368														
13	11	0.002607	0.000603	1.8763E-21	-0.00261			Two O	verlappi	ng Gaus	ssians wi	th Initial Gue	SS						
14	12	0.015395	-0.00041	2.5854E-21	-0.01539	0.5													
15	13	0.007243	0.000352	3.5585E-21	-0.00724					٨									
16	14	0.001776	0.000526	4.8923E-21	-0.00178	0.4	-												
17	15	0.008453	0.000182	6.7186E-21	-0.00845	0.3	;												
18	16	0.005783	-0.00031	9.2165E-21	-0.00578						*								
19	17	-0.00068	0.000773	1.2629E-20	0.000684	0.2	2			_) ¥									
20	18	0.004804	0.000701	1.7286E-20	-0.0048	0.1													
21	19	-0.0052	0.00044	2.3633E-20	0.005205														
22	20	0.013383	0.000968	3.2276E-20	-0.01338	0	-	A State	the had and		7	the the state							
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20	24	0.010398	0.000281	1.1104E-19	-0.0104														
27	25	-0.0024	0.000344	1.5081E-19	0.002390														
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Note that the Gaussians have been fit reasonably well and the value of chi-squared is 0.9. If the estimate for the noise were perfect then chi-squared should be 1.0



We focus on the fit. Now if we subtract the fitted function from the data we will obtain the residuals.



Amplitude	Position	Width
9.75	250.0	9.84
20.4	299.0	30.3

In this case the residuals have the appearance of noise. They have no structure. This is an indication of a good fit as well.

Residuals from fit to two Gaussian functions

