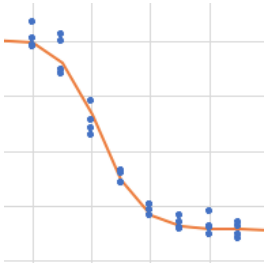
Oct 15, 2019

Sigmoid fitting in Excel (Excel Solver Add-In)



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Protocol status: Working
We use this protocol and it's working

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Abstract

This protocol covers how to fit sigmoidal curve to data within Excel, and allows rapid estimation of EC50/IC50 values from experimental dose-response data. Although R or other specialized software is more suitable for detailed analyses, it is sometimes useful to perform sigmoidal fitting within Excel. Note that this is just a simplified version (only sigmoid fitting) of the protocol reported in Gerdi Kemmer & Sandro Keller (2010) Nat. Protocol 5: 267–281, and intended for routine laboratory use.

Before start

Excel Solver Add-In is currently bundled with Excel by default, but you need to load the add-in for the first time. To load the add-in, select "Excel Add-Ins" from "Tools" menu, check the Solver Add-In, and click OK.

1 Download the following excel file. Copy the excel sheet into your excel file if needed.
The file contains a sheet set up for sigmoidal fitting with an example data set, for which you can test the fitting procedure.

ExcelSolver_Sigmoid.xlsx

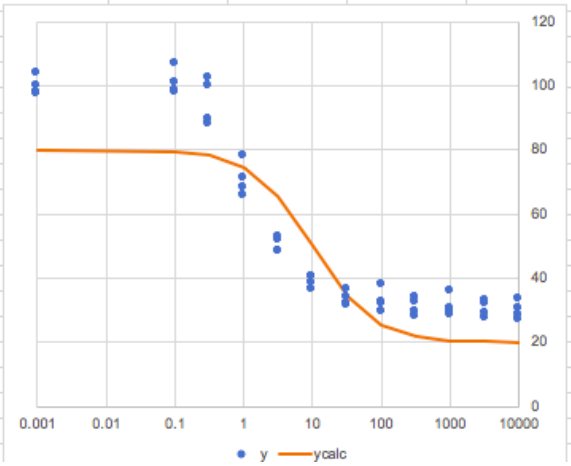
2 Open the excel file, and enter your data in the "x" and "y" column. Delete unnecessary data.

Note

The data in the "x" column should be in decreasing or increasing order. Otherwise, the plot will not be correctly displayed.

Expected result

	A	B	C	D	E	F	G	H	I
1	**Sigmoid Fitting**					x	y	ycalc	
2	min	20	<- named cell "min"			0.001	99.7975709	79.9940006	
3	max	80	<- named cell "max"			0.001	103.846154	79.9940006	
4	n	1	<- named cell "n"			0.001	97.3684211	79.9940006	
5	ec50	10	<- named cell "ec_50"			0.001	97.9757085	79.9940006	
6						0.1	106.882591	79.4059406	
7	SSR	8364.50359				0.1	101.012146	79.4059406	
8						0.1	98.1781377	79.4059406	
9						0.1	98.582996	79.4059406	
10	FUN	min+(max-min)/(1+10^(n*(log10(x)-log10(ec_50))))				0.316	89.2712551	78.1620783	
11						0.316	88.0566802	78.1620783	
12						0.316	102.226721	78.1620783	
13						0.316	99.7975709	78.1620783	
14						1	78.340081	74.5454545	
15						1	65.7894737	74.5454545	
16						1	71.0526316	74.5454545	
17						1	68.2186235	74.5454545	
18						3.16	51.8218623	65.5927052	
19						3.16	48.3805668	65.5927052	
20						3.16	52.6315789	65.5927052	
21						3.16	48.582996	65.5927052	
22						10	40.2834008	50	
23						10	36.2348178	50	
24						10	38.4615385	50	
25						10	40.48583	50	
26						31.6	31.9838057	34.4230769	
27						31.6	31.3765182	34.4230769	
28						31.6	36.2348178	34.4230769	
29						31.6	33.805668	34.4230769	
30						100	37.854251	25.4545455	



3 Guess initial parameters for the sigmoid (minimum, max, n, and ec50), which can be easily guessed from the plot, and enter the estimated initial values into the cells (B2, B3, B4, B5).

> **Note**
>
> If the initial guess is too far from the real values, the fitting algorithm may not result in reasonable fit.

4 Start Excel Solver by selecting "Solver" from "Tools" menu.

4.1 Set "Target cells" to "$B$7", which contains SSR (Sum of Squared Residuals).

4.2 Set "equall to" section to "Value of 0".

> **Note**
>
> This results in a warning saying "unable to find solution", but you can ignore it.

4.3 Set "Changing cells" to the cells that contains initial values ("$B$2:$B$5").

4.4 Add constraints if needed. We recommend to add "ec_50 >= 0.000001" etc., to avoid EC50 becoming negative values or zero.

4.5 Uncheck "Assume non-negative", if checked.

4.6 Basically, no need to change the other options.

5 Click "Solve" to run the Solver, wait several seconds. Close the Solver window when the calculation finished. Then you can get fitted parameters and a curve overlaid over the raw data points. Check if the sigmoid curve is reasonably fitted over the data.

Expected result

	A	B	C	D	E	F	G	H
1	**Sigmoid Fitting**					x	y	ycalc
2	min	31.4307228	<- named cell "min"			0.001	99.7975709	102.260797
3	max	102.270164	<- named cell "max"			0.001	103.846154	102.260797
4	n	1.23828456	<- named cell "n"			0.001	97.3684211	102.260797
5	ec50	1.35595482	<- named cell "ec_50"			0.001	97.9757085	102.260797
6						0.1	106.882591	99.5702057
7	SSR	619.934068				0.1	101.012146	99.5702057
8						0.1	98.1781377	99.5702057
9						0.1	98.582996	99.5702057
10	FUN	min+(max-min)/(1+10^(n*(log10(x)-log10(ec_50))))				0.316	89.2712551	92.2523877
11						0.316	88.0566802	92.2523877
12						0.316	102.226721	92.2523877
13						0.316	99.7975709	92.2523877
14						1	78.340081	73.4502001
15						1	65.7894737	73.4502001
16						1	71.0526316	73.4502001
17						1	68.2186235	73.4502001
18						3.16	51.8218623	49.8257882
19						3.16	48.3805668	49.8257882
20						3.16	52.6315789	49.8257882
21						3.16	48.582996	49.8257882
22						10	40.2834008	36.9340573
23						10	36.2348178	36.9340573
24						10	38.4615385	36.9340573
25						10	40.48583	36.9340573
26						31.6	31.9838057	32.837679
27						31.6	31.3765182	32.837679
28						31.6	36.2348178	32.837679
29						31.6	33.805668	32.837679
30						100	37.854251	31.7737709
31						100	32.5910931	31.7737709