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Simultaneous fitting of sigmoid curves in Excel (Excel Solver Add-in)

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Abstract

Sometimes it is desirable to fit sigmoid curves with shared parameters against several data sets. Such simultaneous fitting procedure is available in most of the specialized statistical softwares (R, Prism etc.), but also possible with Excel. Here, this protocol explains how to perform simultaneous fitting using Excel Solver plug-in against a pair of data set. For more basic protocol to fit sigmoid curve, see Kenji Ohgane (2019) Sigmoid fitting in Excel (Excel Solver Add-In). **protocols.io** <u>dx.doi.org/10.17504/protocols.io.78ihrue</u>. See Gerdi Kemmer & Sandro Keller (2010) **Nat. Protocols** 5: 267–281 for more detail on the use of Excel Solver in nonlinear least square fitting.

Guidelines

Although this protocol explains how to set up simultaneous fitting of two curves, you can easily accommodate this protocol to more complex data sets. However, for more sophisticated analysis, the use of Prism (commercial software) or R (open source software) is recommended for more clear analytical workflow and reproducibility. To perform simultaneous fitting of dose-response curves in R, the use of *drc* package would be a convenient option.

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.

The file contains a sheet set up for simultaneous sigmoidal fitting with two set of example data, for which you can test the fitting procedure.

ExcelSolver_SimultaneousFitting.xlsx

2 Open the excel file, and enter your data set in the two set of "x" and "y" columns. 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.



Guess initial parameters for the sigmoids (minimum, max, n, and ec_50), which can be easily guessed from the plot, and enter the estimated initial values into the cells (B2, B3, B4, and B5 for the first data set, and K2, K3, K4, and K5 for the second data set).

Note

Note that these cells for parameters are "named cells". So you can reference these cells from within equations by using "=min" (first data set) or "=min_" (second data set), where an underbar denotes parameters for the second data set. If you want to modify the equation for the curves, please modify equations within the cells in the "ycalc" columns.

4 Start the Excel Solver add-in from Tool > Solver on the menu bar.

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4.1 Set "Objective / Target cells" to "\$B\$8", which contains the sum of SSR (Sum of Squared Residuals) calculated for the two data sets.

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4.2 Set "equal 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 variable cells" to the cells that contains initial values for the two sigmoid curves ("\$B\$2:\$B\$5, \$K\$2:\$K\$5").
- 4.4 Add constraints.

(1) We recommend to add "ec_50 >= 0.000001" etc., to avoid EC50 becoming negative values or zero.

(2) In this example, we fit two sigmoid curves that share minimum and maximum values against the pair of data set. So add two constraints as shown in the figure ("min = min_" and "max=max_").

Expected result
Adding constraints By Changing Variable Cells: SB52:3B55,5K52:3K55 Subject to the Constraints: Common parameters (min & max) By Changing Variable Cells: Subject to the Constraints: Common parameters (min & max) Add Constraint Change Add Constraint: Cell Reference: Constraint: Min Add Cancel OK

4.5 Confirm that "Assume non-negative" is unchecked, and click "Solve" to run the Solver. 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.

Solver Results Solver could not find a feasible solution. Ignore this message Reports Reports Feasibility Feasibility Feasibility-Bounds Return to Solver Parameters Dialog Outline Reports Save Scenario Cancel OK	ected result				
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5 Then you can get fitted parameters and curves overlaid over the raw data points. Check if the sigmoid curve is reasonably fitted over the data.



