

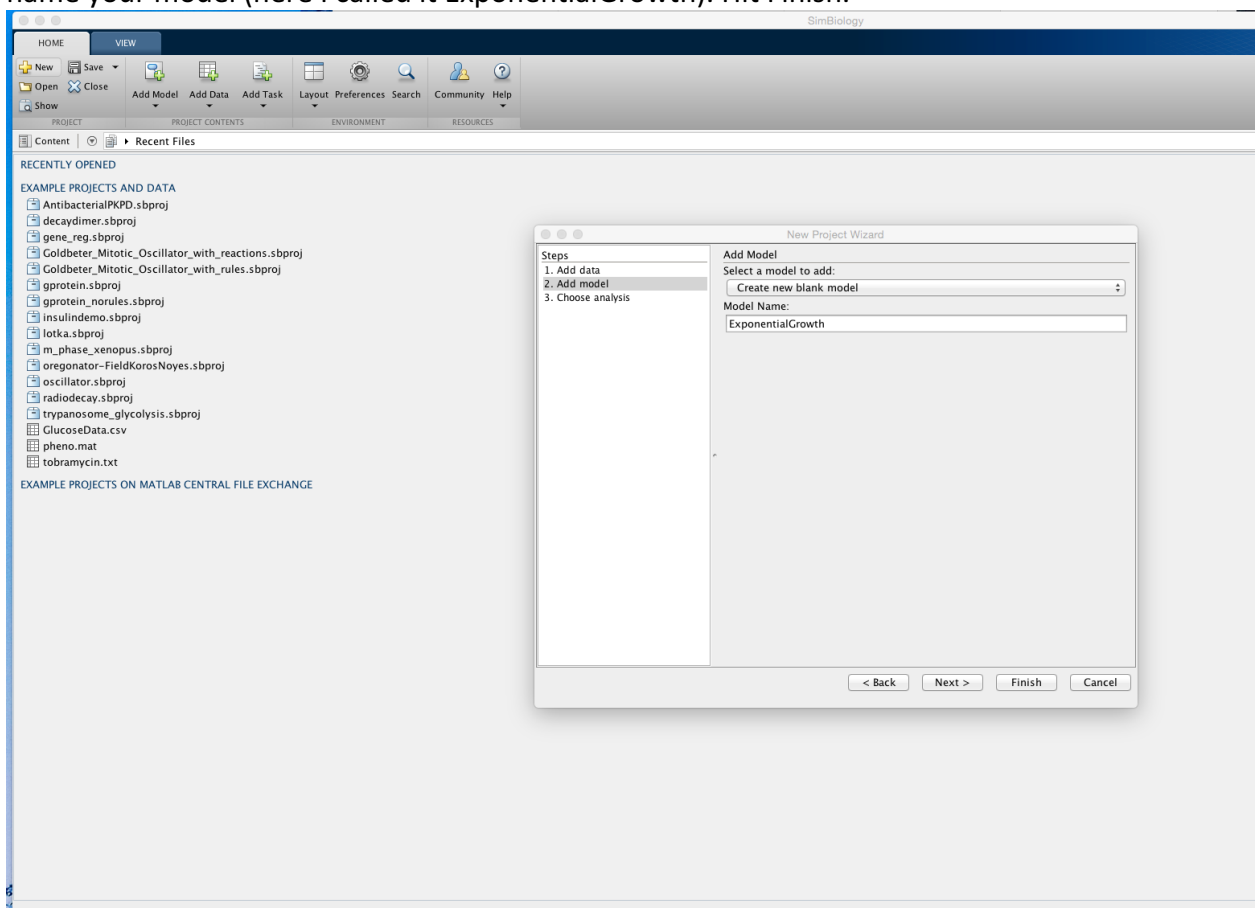
MA 331: Differential Equations for the Life Sciences Simbiology Tutorial

Objective

In this exercise, we will use simbiology to perform an inverse problem to estimate the growth parameter for exponential growth, using US population data from 1950-1960. We will also examine the sensitivities.

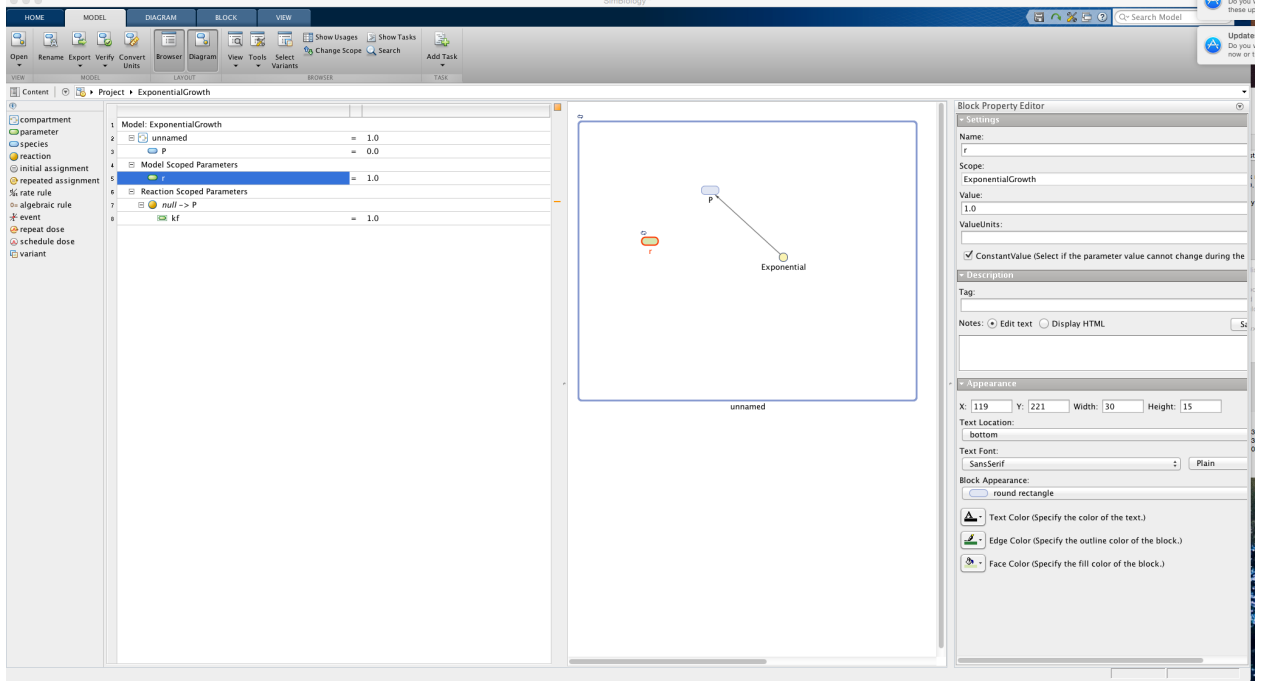
Steps

1. Open MATLAB
2. Type “simbiology” into the command line and hit enter
3. In the “Home” tab, click “Add Model” button and select “Create New Blank Model” and name your model (here I called it ExponentialGrowth). Hit Finish.

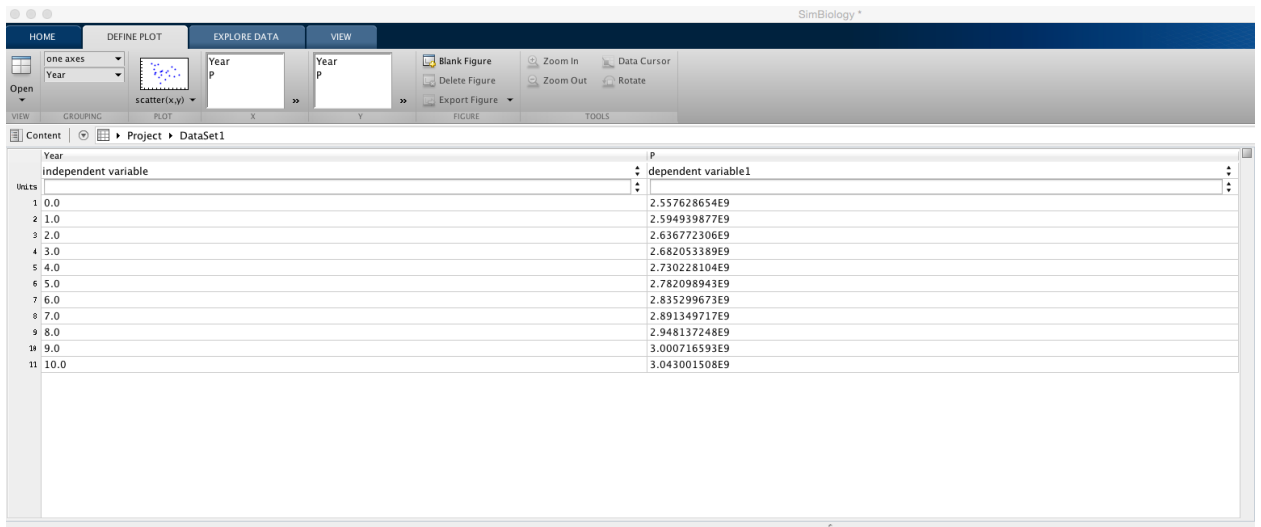


4. Click “diagram” or open diagram in order to create your model
5. Drag one species and one reaction into the “unnamed” rectangular space
6. Double click on “species_1”, and enter a new name (here I called mine P for population). In the initial condition box list an initial condition (in my case 2557628654 – the initial population)
7. Double click on “reaction_1” and rename it (here I named it exponential – if you did logistic you could call it ‘logistic’)

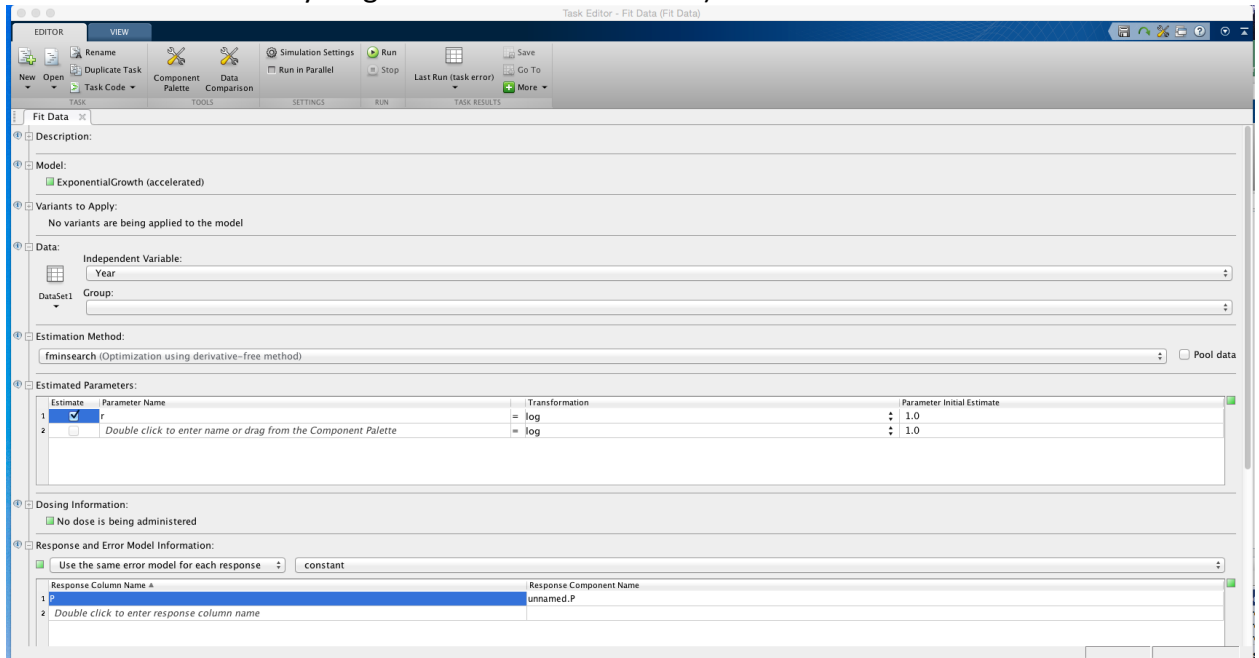
8. In the "ReactionRate" box, type in your reaction rate (here it is $r \cdot P$ because I am assuming exponential growth)
9. Option-click-drag an arrow from growth reaction to your species (**NOTE: you must drag from the reaction to the species!!!**)
10. Add a parameter (or however many you need for your reaction) and give it the corresponding name (here I named mine 'r' because my reaction rate is $r \cdot P$)



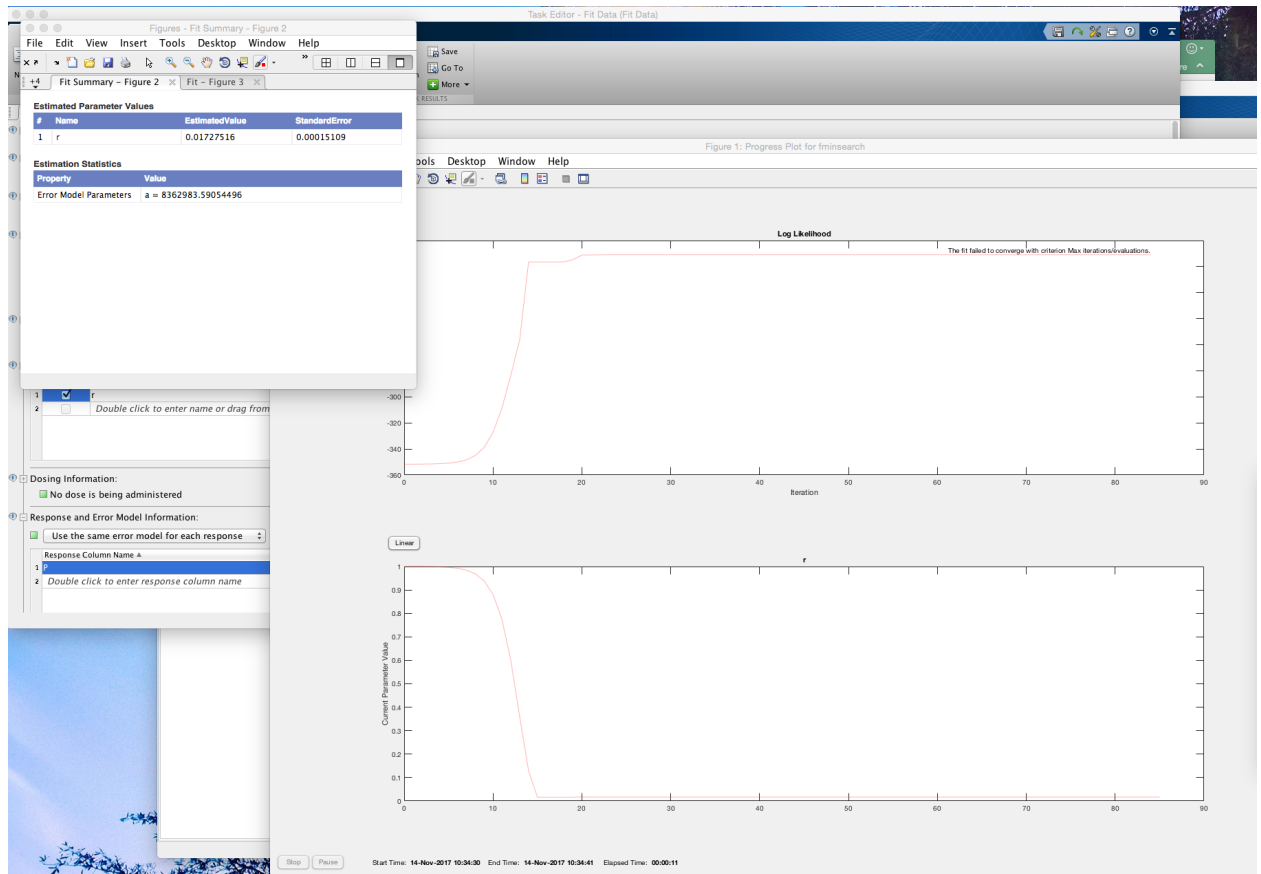
11. Click Add Task -> Fit Data
12. Click the '+' under Data. Then Click to Select Data and choose "Load Data from File". Select your file and hit 'OK'. Note the names of your column labels. Under 'Independent Variable' select, the name of your independent variable (here it is Year). Do not fill in anything for 'Group'. Go back to your main menu. Double click on Project -> Dataset1. Set Year to be 'independent variable' and P to be 'dependent variable'. Go back to your fit data window.



13. Click the '+' under Estimation Method and change the estimation method to 'fminsearch'
14. Under Estimated Parameters, enter the parameters you wish to estimate. As you double click and add them, it should autofill them for you. Make sure to give them the same name as you did when you defined your model. Here I put in 'r'. I let the transformation be log. Here you can set an initial guess for your parameter value. I just put it as 1. Make sure to check the box for estimate.
15. Under Response and Error Model Information. Response Column name should be the name of your data for the dependent variable (here P). Response Component name should be the name of your dependent variable in your model (here P, it changes to unnamed.P because my diagram was called unnamed)



16. Click Simulation settings (in the Editor tab at the top). Make sure that your StopTime matches the end of your data time. Here it is 10 years so StopTime = 10. You may change the Absolute and or Relative Tolerances if you are getting jagged answers (lower them)
17. Click 'Run' This should then pop up a window where you can track the parameter value as well as the log likelihood. When it is finished, more windows will pop up with the estimates for your parameters, residuals and fits.



Here are some links to help with Simbiology:

<https://www.mathworks.com/help/simbio/index.html>

<https://www.mathworks.com/help/simbio/gs/simbiology-desktop-overview.html>

Common Problems and Their Solutions

1. Fit Error: "The variable name ** cannot appear in the right-hand side of the responseMap input argument because it is the group variable or the independent variable of the data"
 - a. **Solution 1:** Make sure that in your task editor, under 'Data' you did not select Group: P. Group should be left blank. Independent variable should be Year
 - b. **Solution 2:** Make sure you followed step 12: . Go back to your main menu. Double click on Project -> Dataset1. Set Year to be 'independent variable' and P to be 'dependent variable'. Go back to your fit data window.

2. The parameters are a flat line and the log likelihood never changed! **Solution:** make sure you initialized P in step 6: In the initial condition box list an initial condition (in my case 2557628654 – the initial population)