Tutorial to run LEP nonlinear regression code

Step 1: Open chapter 7 and click on LEP-7-3.pol to view Polymath code for Example 7-3

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odules s omputer	Example 7-3 Use of Regression to Find the Rate Law Parameters	<u>(Nonlinear</u> Regression Tutorial)	<u>LEP-</u> <u>7-3.zip</u>	<u>LEP-7-</u> <u>3.cdf</u>
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Step 2: The following page will open. We will carry out regression for first part of the problem where you need to determine both a and k. Copy the data of t and Ca as shown below

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150	0.02	256			
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Model:		Print	Ctrl+P	I .	
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a=2.0	k=0.	1			
# Part	b				
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Model:					
t = ((.05^(1	-2))-Ca^(1-2))/(k*(1-2))			
Guess	value:				
A-0.1					

Step 3: Open Polymath. If you don't have it then refer to the installation instruction present on http://www.umich.edu/~elements/5e/software/polymath.html

When you open, the following window will appear. Click on Program tab and select "REG Regression". The shortcut button for REG is also available on menu bar as shown below by red circle

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Step 4: A blank spreadsheet will open. Right click on cell corresponding to row 01, column C01 and paste the data. Your spreadsheet should look like this. For a detailed tutorial on nonlinear regression, refer to http://umich.edu/~elements/5e/software/polymath.html

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Step 5: Change the column name of C01 to t. To change the column name of C01, double click on the column name "C01" or right click on C01 and select "Column Name..." A dialog box will appear where column name can be changed. Enter t in the column name and click OK



Similarly, change the column name of C02 to Ca

Step 6: Now go back to Polymath code page on website (**Step 1**) and select the equation for t as shown below

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#Examp # Part	ple 7-3 t a	Use of Regression to Fin	d Rate Law Parameters			
t 50 100 150 200 250 300 Model	Ca 0.03 0.03 0.02 0.02 0.01 0.01	8 06 56 22 95 74				
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a=2.0	k=0.	1	Print	Ctrl+P		
# Part t 50 100 150 200 250 300 Model: t = ()	Ca 0.03 0.03 0.02 0.02 0.01 0.01 : (.05^(1	8 06 56 22 95 74 -2))-Ca^(1-2))/(k*(1-2))	Inspect	Ctrl+Shift+I		
Guess k=0.1	Value:					

Step 7: Go back to your Polymath software and click on Nonlinear (red circle). Place the cursor in the rectangular box below "Model:" and paste your equation (blue rectangle). Click on the refresh button (green circle) to update the page.

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Step 8: Now you need to enter the guess value of the model parameters. The model parameters are a and k. Go back to the Polymath code (Step 1) and you will find that guess value is already given. Guess value given for a is 2 and for k it is 0.1. Enter the guess value under "Model Parameters Initial Guess" section.

If it displays Ca also in the model parameter list, then click on f(x) button. It will remove Ca from the parameter list.

You can also choose your own guess value (Note: The solution Polymath provides may be very sensitive to the initial value guesses, so if the first regression solution is not very good, you may want to change the initial guesses and rerun the regression).

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Step 9: When you are done, click on pink arrow \Rightarrow to have Polymath perform the regression. You will see a screen like this that details the results from the regression analysis. You can see that $R^2 = 0.999$ which indicates a very good fit

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Step 10: Now, you can go back to Step 1 and repeat the Step 2-9 to do the second part of Example 7-3