

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

Chapter 7: Collection and Analysis of Rate Data

Living Example Problems

The following examples can be accessed with Polymath™, MATLAB™, or Wolfram CDF Player™.

Living Example Problem	Polymath™ Code	Matlab Code	Wolfram CDF Code *
Example 7-3 Use of Regression to Find the Rate Law Parameters	LEP-7-3.pol (Nonlinear Regression Tutorial) (LEP Tutorial for nonlinear regression)	LEP-7-3.zip	LEP-7-3.cdf
Regression tool to fit experimental C(t) vs t data to Polynomial equation of form $C(t)=a_0+a_1 t+a_2 t^2+a_3 t^3+\dots$	Complete Tutorial	---	---

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

```
#Example 7-3 Use of Regression to Find Rate Law Parameters
# Part a
t      Ca
50     0.038
100    0.0306
150    0.0256
200    0.0222
250    0.0195
300    0.0174

Model:
t = ((.05^(1-2))-Ca^(1-2))/(k*(1-2))

Guess Value:
a=2.0 k=0.1

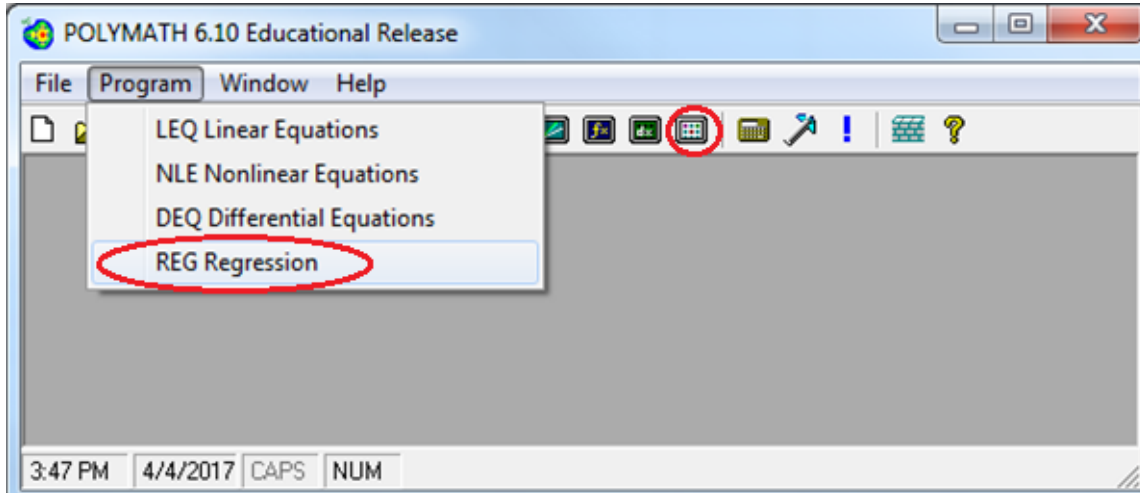
# Part b
t      Ca
50     0.038
100    0.0306
150    0.0256
200    0.0222
250    0.0195
300    0.0174

Model:
t = ((.05^(1-2))-Ca^(1-2))/(k*(1-2))

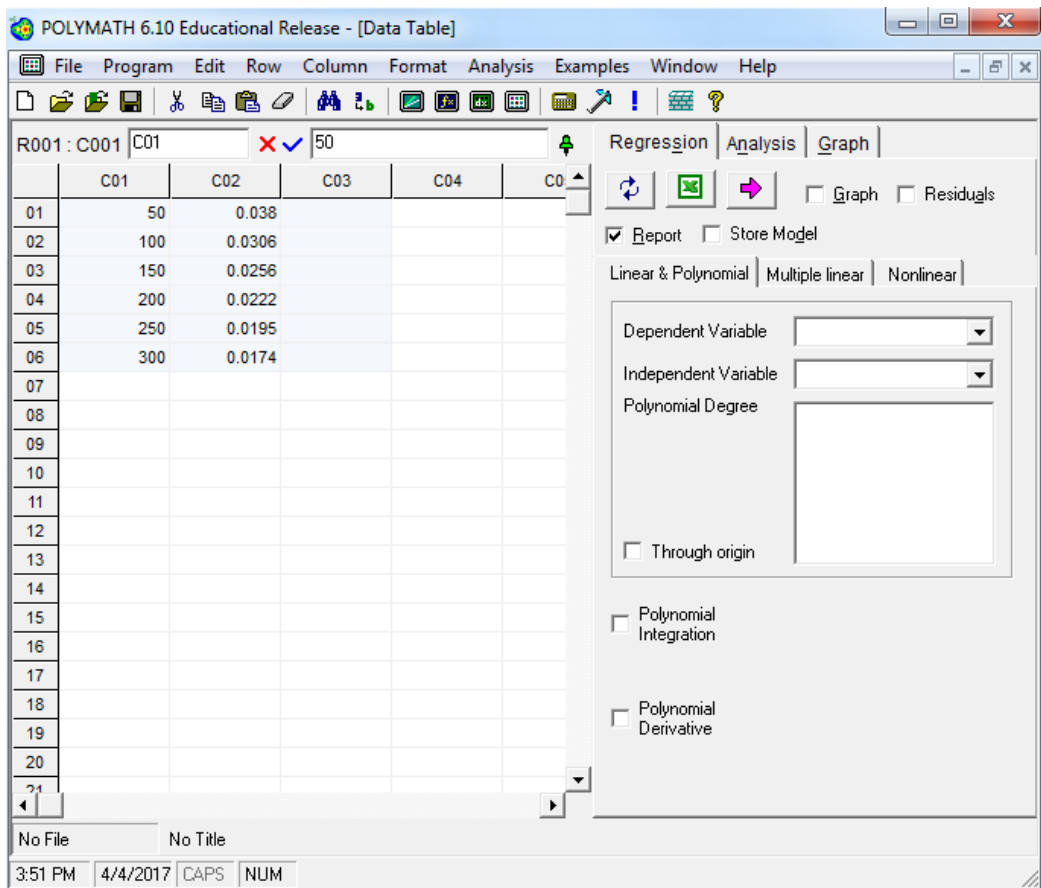
Guess Value:
k=0.1
```

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>

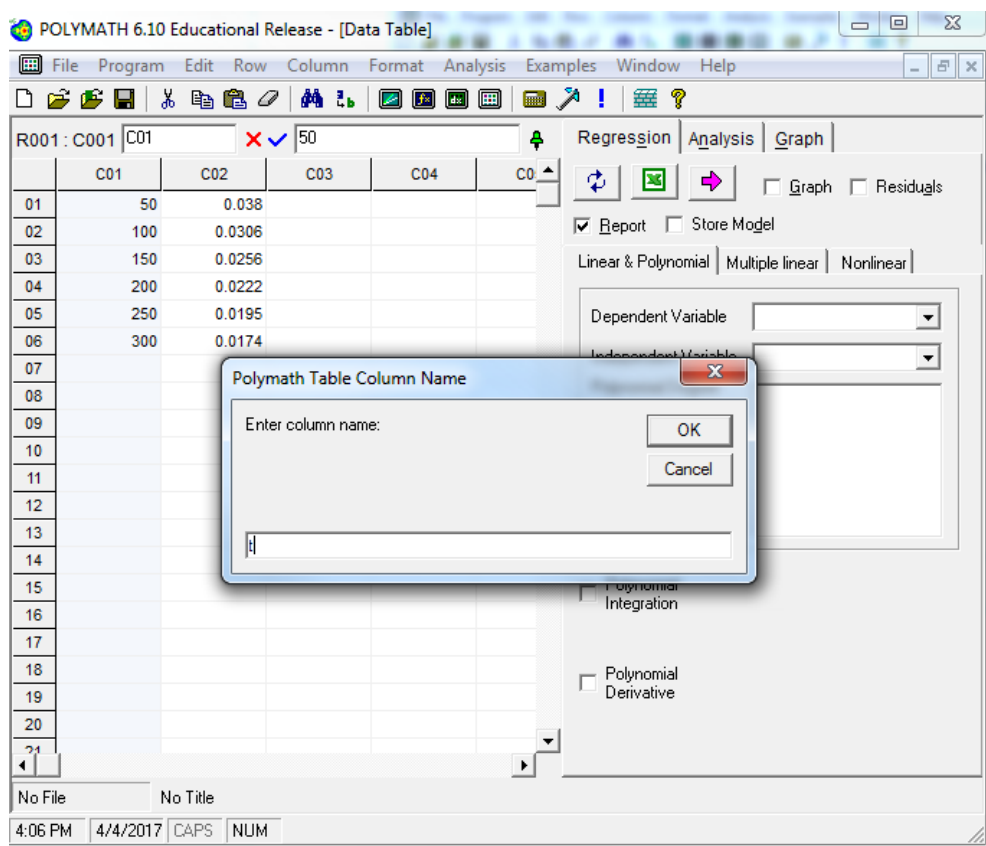
When you open, the following window will appear. Click on Program tab and select "REG Regression". The shortcut button for REG is also available on menu bar as shown below by red circle



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>

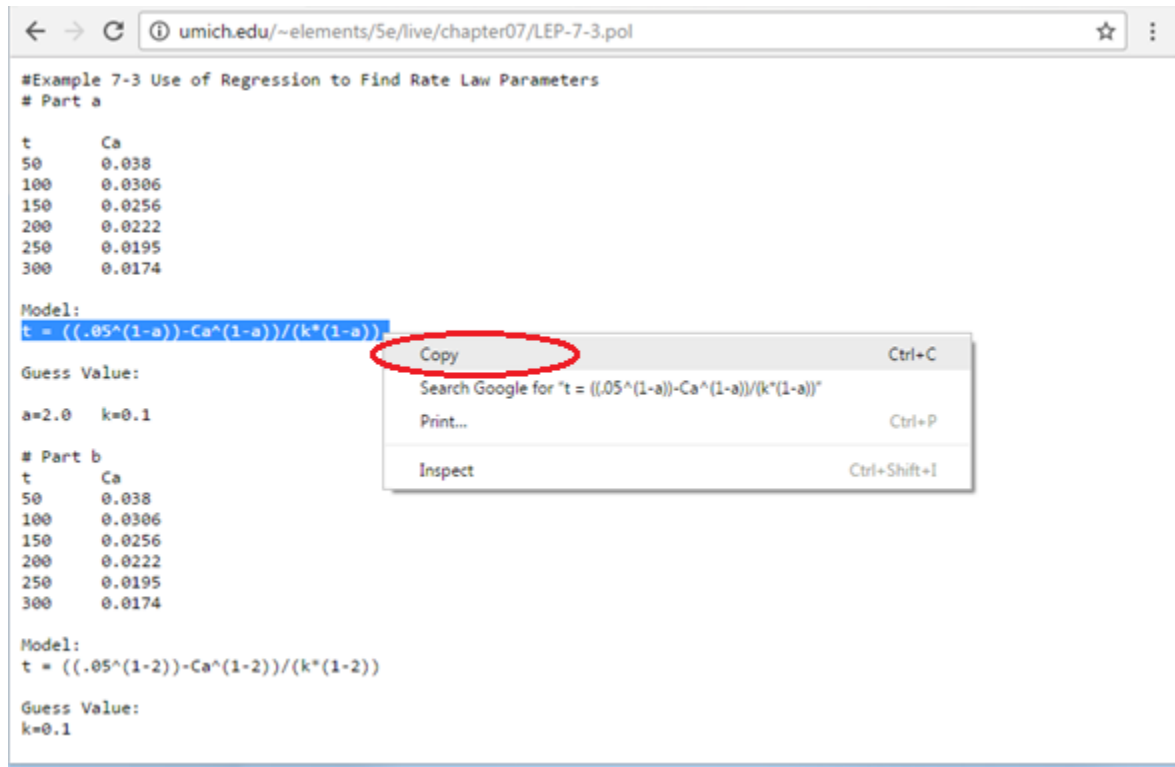


Step 5: Change the column name of C01 to t. To change the column name of C01, double click on the column name “C01” or right click on C01 and select “Column Name...” A dialog box will appear where column name can be changed. Enter t in the column name and click OK



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



← → ↻ umich.edu/~elements/5e/live/chapter07/LEP-7-3.pol ☆ ⋮

```
#Example 7-3 Use of Regression to Find Rate Law Parameters
# Part a
t      Ca
50     0.038
100    0.0306
150    0.0256
200    0.0222
250    0.0195
300    0.0174

Model:
t = ((.05^(1-a))-Ca^(1-a))/(k*(1-a))

Guess Value:
a=2.0  k=0.1

# Part b
t      Ca
50     0.038
100    0.0306
150    0.0256
200    0.0222
250    0.0195
300    0.0174

Model:
t = ((.05^(1-2))-Ca^(1-2))/(k*(1-2))

Guess Value:
k=0.1
```

Context menu options:

- Copy (Ctrl+C)
- Search Google for "t = ((.05^(1-a))-Ca^(1-a))/(k*(1-a))"
- Print... (Ctrl+P)
- Inspect (Ctrl+Shift+I)

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.

POLYMATH 6.10 Educational Release - [Data Table]

File Program Edit Row Column Format Analysis Examples Window Help

R001 : C002 Ca 0.038

	t	Ca	C03	C04	C05
01	50	0.038			
02	100	0.0306			
03	150	0.0256			
04	200	0.0222			
05	250	0.0195			
06	300	0.0174			
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Regression Analysis Graph

Report Store Model

Linear & Polynomial Multiple linear **Nonlinear**

Model: $t = \frac{(.05^{1-a}) - Ca^{1-a}}{k^{1-a}}$

e.g. $y = 2^x A + B$

Model Parameters Initial Guess:

a	
Ca	
k	

Dependent Variable: t
 Independent Variable/s: unknown
 Model Variable/s: a, Ca, k
 Available Variables: unknown

No File No Title

4:18 PM 4/4/2017 CAPS NUM

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).


The screenshot shows the POLYMATH 6.10 Educational Release interface. The main window displays a data table with columns for time (t) and concentration (Ca). The regression settings panel on the right is open, showing the model equation and initial guess values for parameters a and k.

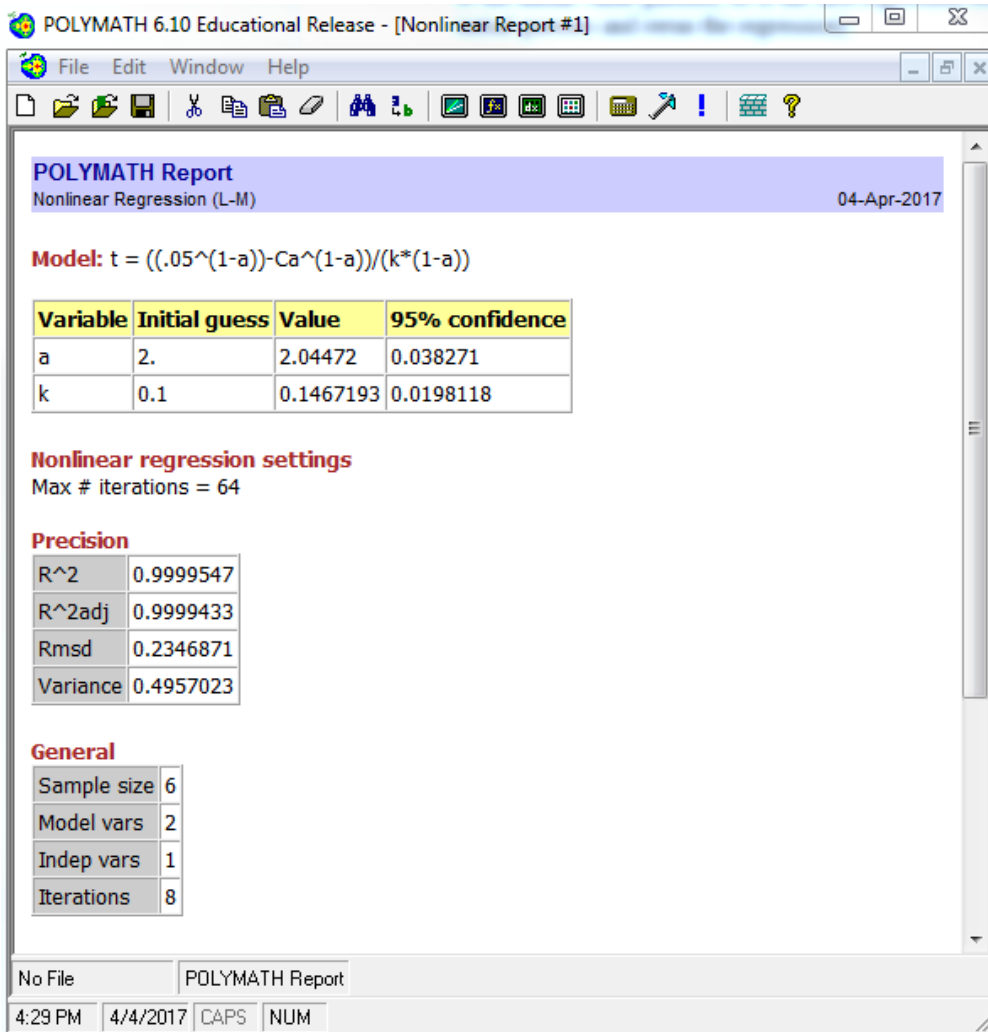
	t	Ca	C03	C04	C0
01	50	0.038			
02	100	0.0306			
03	150	0.0256			
04	200	0.0222			
05	250	0.0195			
06	300	0.0174			
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Regression Settings:

- Model: $t = \frac{[(0.05^{1-a}) - Ca^{1-a}]/k^{1-a}}$
- Model Parameters Initial Guess:

Model parm	Initial guess
a	2
k	0.1
- Dependent Variable: t
- Independent Variable/s: Ca
- Model Variable/s: a, k
- Available Variables: Ca, t

Step 9: When you are done, click on pink arrow  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



From the above report

a = 2.044
k = 0.1467

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