Using the TI83+ to perform a linear regression and graph the results

Marc R. Roussel
Department of Chemistry and Biochemistry
University of Lethbridge

February 23, 2016

In this document, I will walk you through the use of your TI83+ calculator to solve a problem in which you need to carry out a linear regression and plot the results. Specifically, we will work through example 8.12 from my textbook, *A Life Scientist's Guide to Physical Chemistry*

1. First, you need to be clear as to what you are hoping to accomplish. In this case, we will get the slope of a graph of $\ln K$ vs T^{-1} in order to obtain the enthalpy of reaction, using equation (8.12).

2. I suggest you start by clearing all lists, so that you're starting with your calculator in a reasonably clean state. For this, hit 2nd MEM 4 and then ENTER.

3. My first step is usually to enter the data directly as provided in the problem. This makes various kinds of errors much less likely. On the TI83+, press the STAT key, then hit ENTER to edit the data table. Go to `L1` and enter the temperatures (in °C, as given) in this column, then enter the K values in `L2`.

4. We need T^{-1}, with T in Kelvin. You can do this in one or two steps. I'm going to do it in one step, but you should be able to adapt this method to do it in two steps if you like. Move the cursor to highlight `L3` in the table heading. At the bottom of the screen, it should say

```
L3 =
```

You can type a formula to calculate L3. Here is the formula you want, as it will appear at the bottom of the screen:

```
L3 = (L1+273.15)^-1
```

To get L1, type [2nd] [LIST], and use the cursor to select L1, then hit [ENTER].

5. Using the same technique, calculate $\ln K$ for all your data, storing the result in L4.

6. While you're here, note the minimum and maximum values of T^{-1} and of $\ln K$. You will need these for graphing later. In this case, T^{-1} goes from 0.00341 to 0.0036, and $\ln K$ goes from -1.347 to -0.357.

7. It's now time to do the linear regression. The values you want to plot on your x axis are the T^{-1} values in L3. The y values are the $\ln K$ values in L4. Hit [STAT], use the cursors to highlight CALC, then choose 4:LinReg(ax+b) and hit [ENTER]. You will see

```
LinReg(ax+b)
```

and a blinking cursor on your screen. You now have to tell this function where your x and y values are. Using [2nd] [LIST], enter

```
LinReg(ax+b) L3,L4
```

then hit [ENTER]. Note that there is a [,] key. When you do this, the following should appear on your screen:

```
LinReg
y=ax+b
a=-5425.338634
b=18.21521875
```

The value of a is the slope, while b is the intercept.

8. We're going to want to plot the line of best fit, so we want to store its equation. Hit the [Y=] key. Make sure that `Plot1` is selected at the top of the screen. (You can always use another plot, but you have to adjust some of the other instructions below if you do.) If there is anything next to `\Y1=`, then hit the [CLEAR] key. Then hit [VARS] and choose `5:Statistics`. Use the cursor keys to select `EQ` at the top of the screen, then select `1:RegEQ` and hit [ENTER].

9. It's time to set up the plot. Press [2nd] [STAT PLOT]. Select `1:Plot1` and press [ENTER]. Make sure that `On` is selected, as well as the first type of plot. Set `Xlist` to `L3` and `Ylist` to `L4` using [2nd] [LIST]... Make sure the `Mark` is set to something visible (not the tiny dot).

10. Now we need to set up the visible window. Press the [WINDOW] key. We previously determined that the x (T^{-1}) values run from 0.00341 to 0.0036. A reasonable plotting range would therefore be 0.0033 to 0.0037, with tic marks every 0.0001. This is of course not the only sensible choice, but you do need to make sure your points are visible inside the plotting area, so don't set the window too tight. Set `Xmin=0.0033`, `Xmax=0.0037` and `Xscl=0.0001`. Similarly, set `Ymin=-1.5`, `Ymax=0` and `Yscl=0.5`.

11. If you now press the [GRAPH] key, you should get your graph. The tic marks set above will help you figure out the scale.

12. Once you have used the graph (e.g. copying it reasonably carefully into an exam paper), you may want to get the slope or intercept and to do some arithmetic with them. In this case, we want to calculate

$$\Delta_r H^\circ_m = -R(\text{slope}).$$

The slope can be retrieved by pressing [VARS], then choosing `5:Statistics`, selecting `EQ`, and then `2:a`. This will print the character `a` on your screen which you can then multiply by $-R$ in the usual way to get the enthalpy of (in this case) the transfer process. Note that the `a` obtained through the statistics variables is different from the memory `A` that you access by [ALPHA] [A].