Finding the Derivative of Experimental Data

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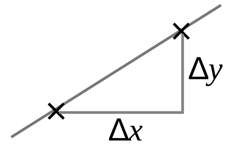
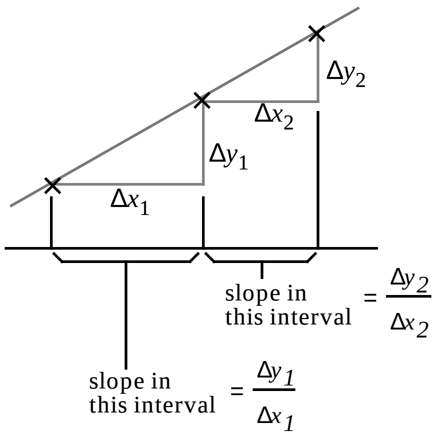
Derivatives can be used to express how fast a value is changing, and are therefore related, mathematically, to the slope of a line. If you understand how to find the slope of a line, you possess the knowledge needed to understand derivatives. Recall that the slope of a line is simply the change in *y* divided by the change in *x*.

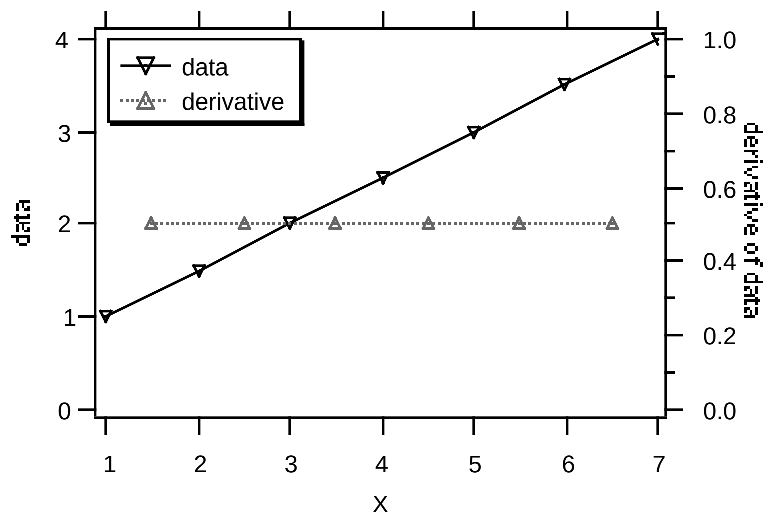


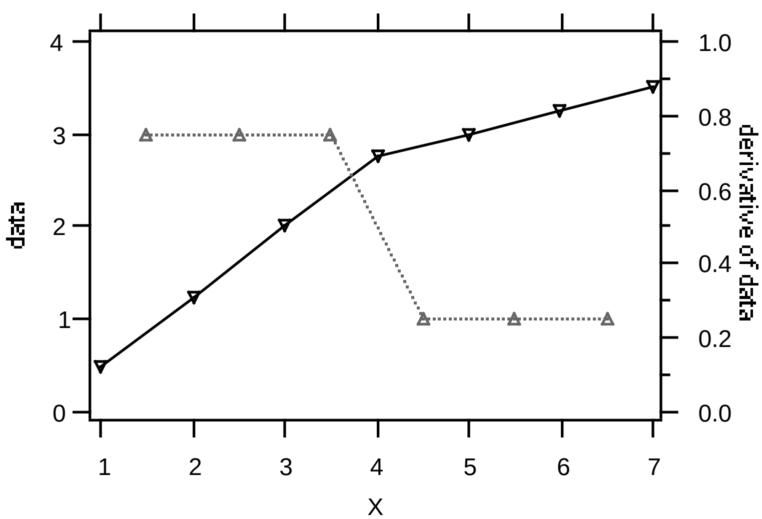
$$slope = \frac{\Delta y}{\Delta x}$$



When you plot a series of data points, you can join each pair of adjacent points with a straight line and a slope can be associated with each such line segment. One way to calculate the derivative (actually, an approximation of the derivative) is to associate the slope of each line segment with the *x*-value of its midpoint.

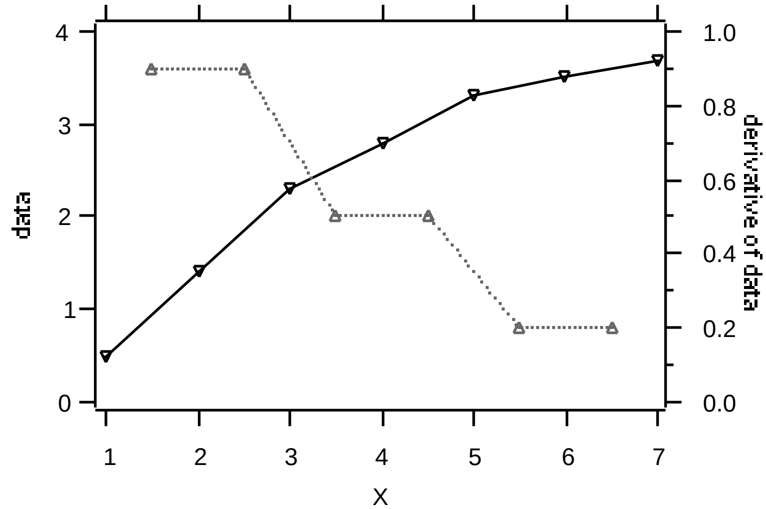
Consider first the case when all of the data points lie on a single straight line. In this instance, the slopes of the individual line segments are all the same, and so the derivative has the same value at all values of *x*. (Note also that the derivative has one fewer points than there are data; this is because, if there are *N* data points, there are (*N*-1) line segments joining them.)

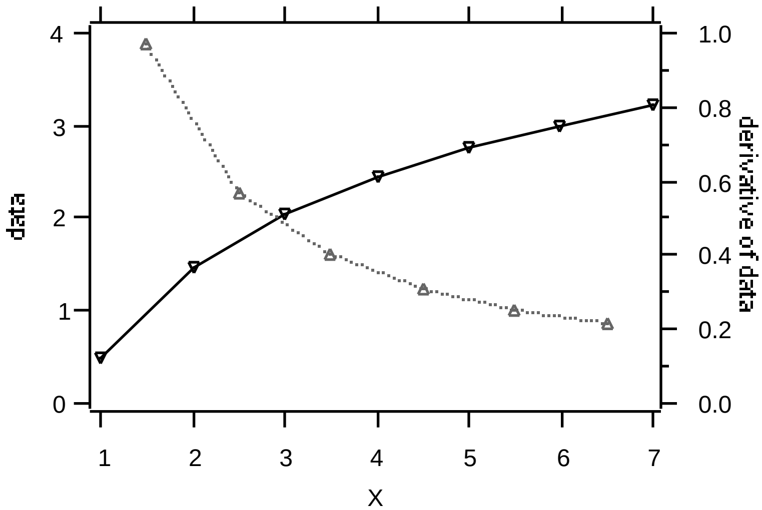




Now consider what happens if there is a "bend" in the plot of the data. For values of *x* less than 4, the slope of the data plot is 0.75; for values of *x* greater than 4, the slope is 0.25. The derivative should, therefore, have a value of 0.75 when *x* is less than 4 and 0.25 when *x* is greater than 4. Rather than jumping suddenly from 0.75 to 0.25 right at *x*=4 the way it should, however, the derivative plot varies linearly between *x*=3.5 and *x*=4.5. Remember that this method *approximates* the derivative. Can you see that the approximation gets better as the data become more closely spaced in the *x*-direction?

This time the plot of the data has two "bends". Does it make sense that the derivative is a measure of how fast *y* is changing with respect to *x*?





Finally, we have the case where the data vary smoothly from *x*=1 to *x*=7. That is, every line segment has a different slope. Note that the slope of the data plot starts steep at small *x* and flattens out (approaches zero) as *x* increases. The derivative, as you would expect, starts with a large value at the left of the plot, and smoothly approaches zero as *x* increases.

To summarize, connect each pair of adjacent data points with a straight line segment and find the slope of that line segment. Next, calculate the *x*-value of the midpoint of each line segment. Finally, the first derivative of the data can be estimated by plotting the slopes of the line segments versus the *x*-values of the midpoints of the line segments. (You might imagine applying this same method to the derivative itself. The result, giving the slope of the derivative at each point, is called the *second* derivative. And so on.)

The last plot above includes seven data points, collected at intervals of *x*=1. What would happen if, instead of seven data points, seven *hundred* data points had been collected at intervals of *x*=0.01? Clearly, each individual line segment joining pairs of data points would be shorter, and the data plot would be smoother. Can you see that the derivative plot would also be smoother? The real derivative (not an estimate thereof) results when the *x*-spacing between adjacent data points becomes arbitrarily small. Therefore, the closer together in the *x*-direction your data points fall, the more closely the method described above estimates the derivative of the data.

One place where this technique becomes useful is in the analysis of titration data. To find the equivalence point of the titration, you want to find the point on the plot of the titration data where the slope is a maximum. Trying to do this with just the titration data can be difficult, but plotting the first derivative of the data makes it very clear where the maximum slope occurs: