

## Derivatives and rates of change

For physical systems that are changing in some way, for example with time or through space, it is very natural to ask how rapid this change is. The appropriate mathematical construct is the **derivative**. One simple way of visualizing its meaning is that the derivative of a function at a given point gives the slope of a graph of that function. You know how to calculate derivatives analytically by algebraic manipulation; but how can we calculate the derivative using only the numerical values of the function? For example, suppose we were given the *positions* of a particle at some sequence of times; how should we go about finding the particle's *speed* from this information?

In this exercise, you will study two so-called *finite-difference approximations* to the rate of change of a function  $f(x)$ . These are

$$\Delta_1 = \frac{f(x + dx) - f(x)}{dx}; \quad \Delta_2 = \frac{f(x + dx) - f(x - dx)}{2dx}.$$

In the limit that  $dx \rightarrow 0$ , both these finite-difference approximations reduce to the derivative. However in a digital computer, how small should  $dx$  be for the numerical calculation to be within some tolerance of the analytical value? Are both approximations equally accurate? How far can we trust them?

To test this, create a spreadsheet which evaluates  $\Delta_1$  and  $\Delta_2$  for two different functions:

- $f(x) = (x + a)^4$ , and initially choose  $x = 2.5$ ,  $a = 1$ ,
- $f(x) = \sin(x)$  with  $x = 0.8$ .

Your spreadsheet should calculate  $\Delta_1$  and  $\Delta_2$  for both functions, using a range of successively smaller differences  $dx$ , starting from 1.0, then reducing by powers of 10 as far as  $10^{-7}$ .

In these examples you can, of course, calculate the true value of the derivative analytically. Your spreadsheet

- should evaluate the difference between the approximate expressions  $\Delta_1$  and  $\Delta_2$  and the exact derivative in each case.
- test whether the differences are smaller than a tolerance of  $10^{-4}$ . You can do this using Excel's IF and ABS functions. Look up the summaries of the IF and ABS functions provided by the Excel's function wizard if you are not sure.

The exact layout of the spreadsheet is up to you. The table below shows a suggestion for the first few rows.

function       $(x+a)^4$   
 x =                      2.5  
 a =                      1  
 Target error        0.0001  
 derivative            171.5

dx	$?_1[(x+a)^4]$	Abs(Difference)	Converged?	$?_2[(x+a)^4]$	Abs(Difference)	Converged
1	260	88.5	Not Converged	185.5	14	Not Converged
0.1	178.991	7.491	Not Converged	171.64	0.14	Not Converged
0.01	172.236401	0.736401	Not Converged	171.5014	0.0014	Not Converged

You should see from your table which approximation converges more quickly. To make this more quantitative, you obviously should plot a graph showing the differences for  $\Delta_1$  and  $\Delta_2$  as a function of  $dx$ . Because of the large range in the values of  $dx$  - seven orders of magnitude - you will need to take logarithms to base 10 of both quantities; Abs(Difference) and  $dx$ . Fit a trendline to the data points for the five largest values of  $dx$ . (The mathematically inclined student should be able to show that the slopes of the lines are expected to have approximately the values given by the trendline fit.)

For the very smallest values of  $dx$  the accuracy of the finite-difference approximations may start to get worse. Try calculating the quantities for  $dx = 10^{-8}, 10^{-9}$ , or even smaller values. How do you account for the fact that the numerical approximation to the derivative appears firstly to improve but then gets worse as  $dx \rightarrow 0$ ?

Save the spreadsheet as “username-derivatives.xls”.