CHAPTER

15 Numerical Differentiation Using Excel

Objectives

After reading this chapter, you will know

- How to calculate derivative values from a data set by using finite differences
- How to use Excel's Data Analysis package to filter noisy data
- How to calculate derivative values from a data set by using curve fitting

15.1 INTRODUCTION

One of the basic data manipulations is *differentiation*—it can also be one of the more problematic if there is noise in the data. This chapter presents two methods for numerical differentiation: using finite differences on the data values themselves and using *curve fitting* to obtain a best-fit equation through the data. It is then possible to take the derivative of the equation. Curve fitting is one way to handle differentiation of noisy data; another is *filtering*. Data-filtering methods are also presented in this chapter.

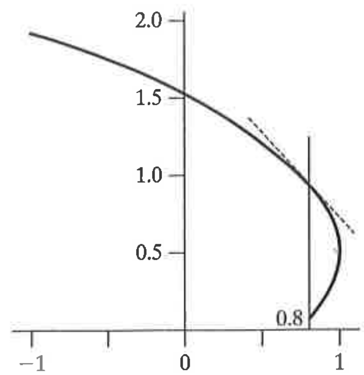
15.2 FINITE DIFFERENCES

Finite differences are simply algebraic approximations of derivatives and are used to calculate approximate derivative values from data sets. These may be used directly or as a first step in integrating a differential equation. However, some care should be taken when calculating derivatives from data, because noise in the data can have a significant impact on the derivative values, even to the extent of making them meaningless.

15.2.1 Derivatives as Slopes

In Figure 15.1, a tangent line has been drawn to the curve at $x = 0.8$:

Figure 15.1
Evaluating the slope at $x = 0.8$.



The slope of the tangent line is the value of the *derivative* of the function (a parabola) evaluated at $x = 0.8$. When you have a continuous curve, the tangent line is fairly easy to draw, and the slope can be calculated.

Because the plotted function is a parabola, described by the equation

$$y = 0.5 + \sqrt{(1-x)}, \tag{15.1}$$

it is possible to take the derivative of the function,

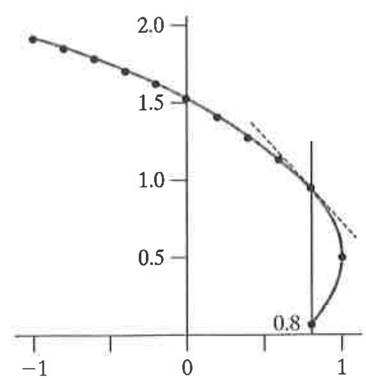
$$\frac{dy}{dx} = -\frac{1}{2}(1-x)^{-1/2}, \tag{15.2}$$

and evaluate the derivative at $x = 0.8$:

$$\left.\frac{dy}{dx}\right|_{x=0.8} = -\frac{1}{2}(1-0.8)^{-1/2} = -1.118. \tag{15.3}$$

But when the function is represented by a series of data points (Figure 15.2) instead of a continuous curve, how do you calculate the slope at $x = 0.8$?

Figure 15.2
How do you obtain the slope at $x = 0.8$ with discrete data?



The usual method for estimating the slope at $x = 0.8$ is to use the x and y values at adjacent points and calculate the slope, using

$$\text{slope} \approx \frac{\Delta y}{\Delta x}. \tag{15.4}$$

The "approximately equal to" symbol is a reminder that the deltas in the equation make this a *finite-difference* approximation of the slope and will give the true value of the slope only in the limit as Δx goes to zero. There are several options for using adjacent points to estimate the slope at $x = 0.8$.

- You could use the points at $x = 0.6$ and $x = 0.8$. This is called a *backward difference* (technically, a "backward finite difference approximation of a first derivative"; see Figure 15.3).

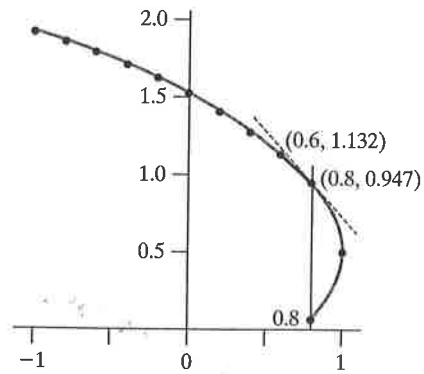


Figure 15.3
Estimating slope with a backward finite difference.

$$\text{slope}_B \approx \frac{\Delta y}{\Delta x} = \frac{0.947 - 1.132}{0.8 - 0.6} = -0.925. \tag{15.5}$$

- You could use the points at $x = 0.8$ and $x = 1.0$ to estimate the slope at $x = 0.8$. This is called a *forward-difference* approximation (Figure 15.4).

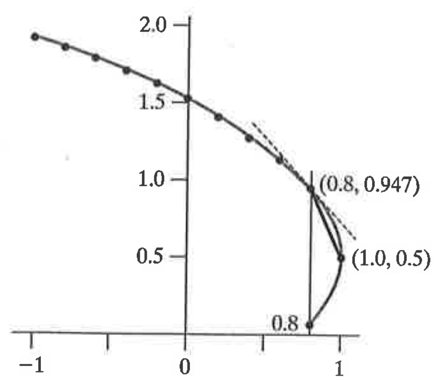


Figure 15.4
Estimating slope with a forward finite difference.

$$\text{slope}_F \approx \frac{\Delta y}{\Delta x} = \frac{0.5 - 0.947}{1.0 - 0.8} = -2.235. \tag{15.6}$$

- You could use the points around $x = 0.8$: $x = 0.6$ and $x = 1.0$. This is called a *central difference* approximation (Figure 15.5).

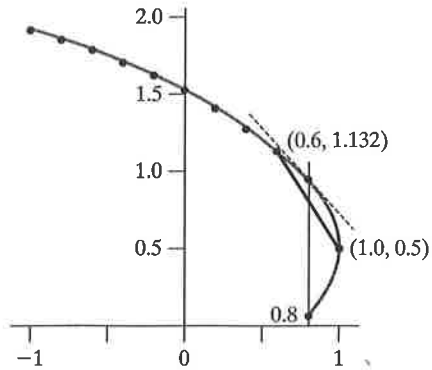


Figure 15.5
Estimating slope with a central finite difference.

$$\text{slope}_C \approx \frac{\Delta y}{\Delta x} = \frac{0.5 - 1.132}{1.0 - 0.6} = -1.58. \qquad (15.7)$$

Which is the correct way to calculate the slope at $x = 0.8$? Well, all three finite differences are approximations, so none is actually "correct." But all three methods can be and are used. Central difference approximations are the most commonly used.

In this case, none of the methods gives a particularly good approximation, because the points are widely spaced and the curvature (slope) changes dramatically between the points. These finite-difference approximations will give better results if the points are closer together (and approximate the true slope as Δx goes to zero).

15.2.2 Caution on Using Finite Differences with Noisy Data

Finite-difference calculations can give very poor results with *noisy data.* For example, if a thermocouple is left in a pot of boiling water, you would expect the temperature to remain constant over time, as shown in Figure 15.6. If the thermocouple measures precisely, the temperature vs. time plot would be a horizontal line, and the slope calculated using any finite-difference approximation would be zero:

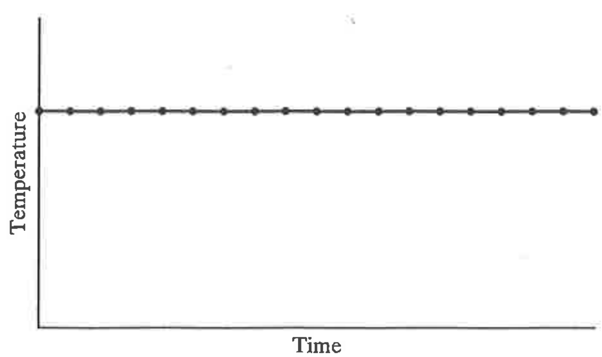


Figure 15.6
Ideal temperature vs. time graph for a constant temperature source.

But if the thermocouple is returning a noisy signal because of corrosion, or loose connections, or because the thermocouple is bouncing in and out of the water, the data might look more like the points plotted in Figure 15.7.

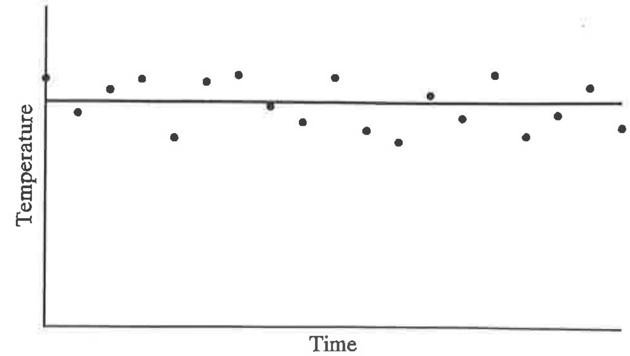


Figure 15.7
Constant temperature source, but noisy data.

If you try to use finite-difference approximations on adjacent points to estimate the derivative with data like these, you will get all sorts of values, but none is likely to be correct. If you have noisy data, your options are as follows:

- Try to clean up the data as they are being taken (fix the equipment or filter the signal electronically)
- Try to clean up the data after they have been taken (numerical filtering of the data)
- Fit a curve to the data and then differentiate the equation of the curve

Some of these options will be discussed here.

15.2.3 Common Finite-Difference Forms

We've already seen three equations for common finite-difference forms for first derivatives. Now let's write them in standard mathematical form. If you want to evaluate the derivative at point i, the adjacent points can be identified as points $i-1$ (to the left) and $i+1$ (to the right), as illustrated in Figure 15.8.

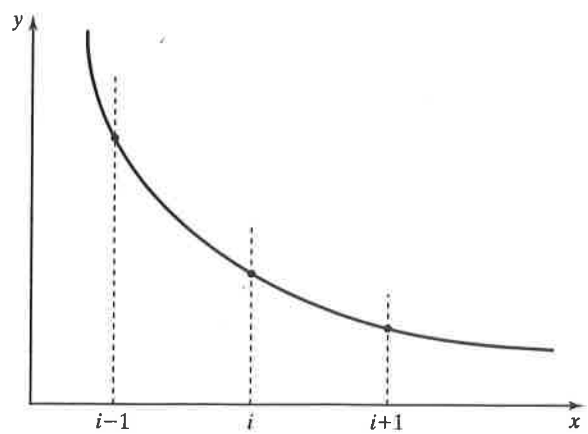
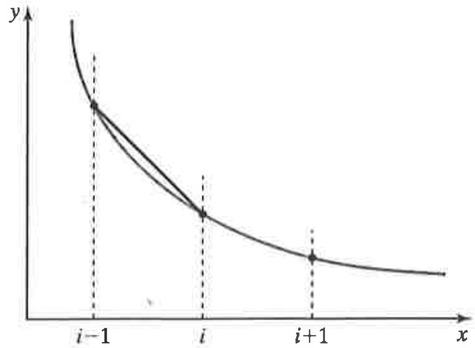


Figure 15.8
Nomenclature using in defining finite differences.

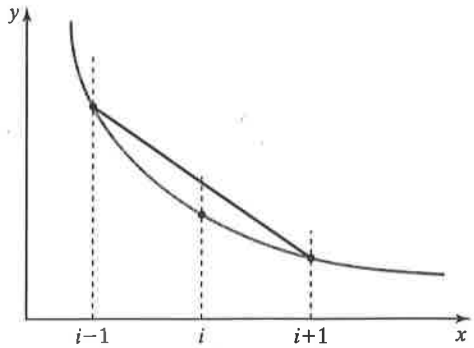
The finite-difference equations can then be written in terms of these generic points and applied wherever needed. The most commonly used finite-difference approximations for first derivatives are listed in Table 15.1.

Table 15.1 First-derivative finite-difference approximations

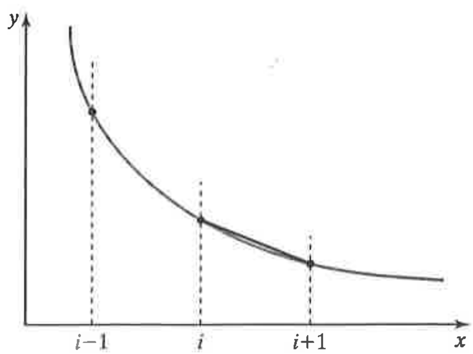
Backward difference $\left.\dfrac{dy}{dx}\right|_i \approx \dfrac{y_i - y_{i-1}}{x_i - x_{i-1}}$



Central difference $\left.\dfrac{dy}{dx}\right|_i \approx \dfrac{y_{i+1} - y_{i-1}}{x_{i+1} - x_{i-1}}$



Forward difference $\left.\dfrac{dy}{dx}\right|_i \approx \dfrac{y_{i+1} - y_i}{x_{i+1} - x_i}$



Finite-difference approximations involving more points are sometimes used to obtain better approximations of derivatives. These multipoint approximations are called *higher order approximations.* A few higher order approximations for first derivatives are listed in Table 15.2.

Table 15.2 Higher order finite-difference approximations for first derivatives

Asymmetric	$\left.\dfrac{dy}{dx}\right\|_i \approx \dfrac{-y_{i-2} + 4y_{i-1} - 3y_i}{2\Delta x}$
Asymmetric	$\left.\dfrac{dy}{dx}\right\|_i \approx \dfrac{-3y_i + 4y_{i+1} - y_{i+2}}{2\Delta x}$
Central	$\left.\dfrac{dy}{dx}\right\|_i \approx \dfrac{-y_{i-2} + 8y_{i-1} - 8y_{i+1} + y_{i+2}}{12\,\Delta x}$