

Lecture 27

Numerical Differentiation

Approximating derivatives from data

Suppose that a variable y depends on another variable x , i.e. $y = f(x)$, but we only know the values of f at a finite set of points, e.g., as data from an experiment or a simulation:

$$(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n).$$

Suppose then that we need information about the derivative of $f(x)$. One obvious idea would be to approximate $f'(x_i)$ by the **Forward Difference**

$$f'(x_i) = y'_i \approx \frac{y_{i+1} - y_i}{x_{i+1} - x_i}.$$

This formula follows directly from the definition of the derivative in calculus. An alternative would be to use a **Backward Difference**

$$f'(x_i) \approx \frac{y_i - y_{i-1}}{x_i - x_{i-1}}.$$

Since the errors for the forward difference and backward difference tend to have opposite signs, it would seem likely that averaging the two methods would give a better result than either alone. If the points are evenly spaced, i.e. $x_{i+1} - x_i = x_i - x_{i-1} = h$, then averaging the forward and backward differences leads to a symmetric expression called the **Central Difference**

$$f'(x_i) = y'_i \approx \frac{y_{i+1} - y_{i-1}}{2h}.$$

Errors of approximation

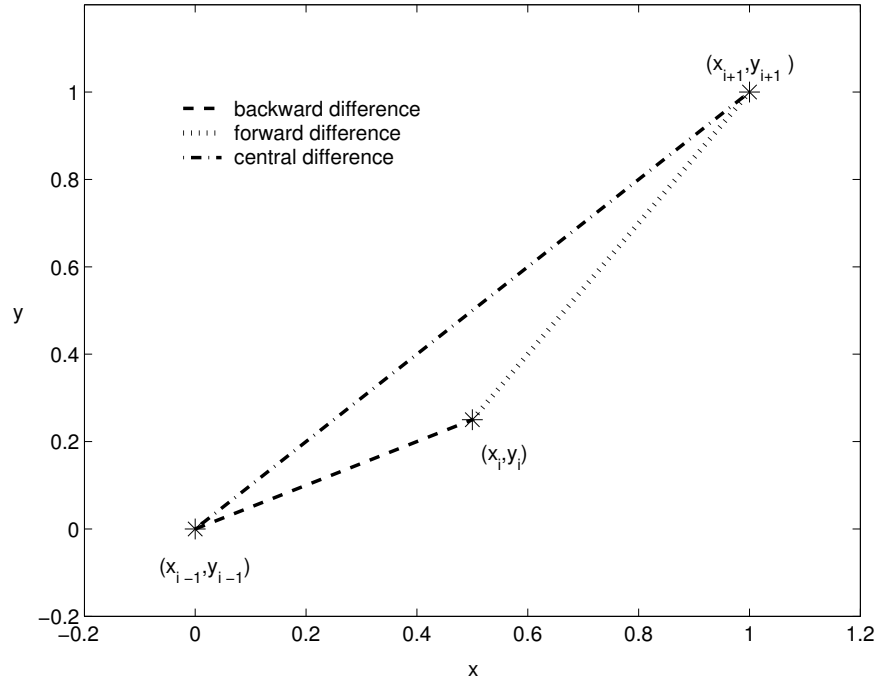
We can use Taylor polynomials to derive the accuracy of the forward, backward and central difference formulas. For example the usual form of the Taylor polynomial with remainder (sometimes called Taylor's Theorem) is

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(c),$$

where c is some (unknown) number between x and $x+h$. Letting $x = x_i$, $x+h = x_{i+1}$ and solving for $f'(x_i)$ leads to

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{h}{2}f''(c).$$

Notice that the quotient in this equation is exactly the forward difference formula. Thus the error of the forward difference is $-(h/2)f''(c)$ which means it is $O(h)$. Replacing h in the above calculation by $-h$ gives

Figure 27.1: The three difference approximations of y'_i .

the error for the backward difference formula; it is also $O(h)$. For the central difference, the error can be found from the third degree Taylor polynomials with remainder

$$\begin{aligned} f(x_{i+1}) &= f(x_i + h) = f(x_i) + hf'(x_i) + \frac{h^2}{2}f''(x_i) + \frac{h^3}{3!}f'''(c_1) \quad \text{and} \\ f(x_{i-1}) &= f(x_i - h) = f(x_i) - hf'(x_i) + \frac{h^2}{2}f''(x_i) - \frac{h^3}{3!}f'''(c_2), \end{aligned}$$

where $x_i \leq c_1 \leq x_{i+1}$ and $x_{i-1} \leq c_2 \leq x_i$. Subtracting these two equations and solving for $f'(x_i)$ leads to

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1}))}{2h} - \frac{h^2}{3!} \frac{f'''(c_1) + f'''(c_2)}{2}.$$

This shows that the error for the central difference formula is $O(h^2)$. Thus, central differences are significantly better and so: **It is best to use central differences whenever possible.**

There are also central difference formulas for higher order derivatives. These all have error of order $O(h^2)$:

$$\begin{aligned} f''(x_i) &= y''_i \approx \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2}, \\ f'''(x_i) &= y'''_i \approx \frac{1}{2h^3} [y_{i+2} - 2y_{i+1} + 2y_{i-1} - y_{i-2}], \quad \text{and} \\ f^{(4)}(x_i) &= y^{(4)}_i \approx \frac{1}{h^4} [y_{i+2} - 4y_{i+1} + 6y_i - 4y_{i-1} + y_{i-2}]. \end{aligned}$$

Partial Derivatives

Suppose $u = u(x, y)$ is a function of two variables that we only know at grid points (x_i, y_j) . We will use the notation

$$u_{i,j} = u(x_i, y_j)$$

frequently throughout the rest of the lectures. We can suppose that the grid points are evenly spaced, with an increment of h in the x direction and k in the y direction. The central difference formulas for the partial derivatives would be

$$\begin{aligned} u_x(x_i, y_j) &\approx \frac{1}{2h} (u_{i+1,j} - u_{i-1,j}) \quad \text{and} \\ u_y(x_i, y_j) &\approx \frac{1}{2k} (u_{i,j+1} - u_{i,j-1}). \end{aligned}$$

The second partial derivatives are

$$\begin{aligned} u_{xx}(x_i, y_j) &\approx \frac{1}{h^2} (u_{i+1,j} - 2u_{i,j} + u_{i-1,j}) \quad \text{and} \\ u_{yy}(x_i, y_j) &\approx \frac{1}{k^2} (u_{i,j+1} - 2u_{i,j} + u_{i,j-1}), \end{aligned}$$

and the mixed partial derivative is

$$u_{xy}(x_i, y_j) \approx \frac{1}{4hk} (u_{i+1,j+1} - u_{i+1,j-1} - u_{i-1,j+1} + u_{i-1,j-1}).$$

Caution: Notice that we have indexed u_{ij} so that as a matrix each row represents the values of u at a certain x_i and each column contains values at y_j . The arrangement in the matrix does not coincide with the usual orientation of the xy -plane.

Let's consider an example. Let the values of u at (x_i, y_j) be recorded in the matrix

$$(u_{ij}) = \begin{pmatrix} 5.1 & 6.5 & 7.5 & 8.1 & 8.4 \\ 5.5 & 6.8 & 7.8 & 8.3 & 8.9 \\ 5.5 & 6.9 & 9.0 & 8.4 & 9.1 \\ 5.4 & 9.6 & 9.1 & 8.6 & 9.4 \end{pmatrix} \quad (27.1)$$

Assume the indices begin at 1, i is the index for rows and j the index for columns. Suppose that $h = .5$ and $k = .2$. Then $u_y(x_2, y_4)$ would be approximated by the central difference

$$u_y(x_2, y_4) \approx \frac{u_{2,5} - u_{2,3}}{2k} \approx \frac{8.9 - 7.8}{2 \cdot 0.2} = 2.75.$$

The partial derivative $u_{xy}(x_2, y_4)$ is approximated by

$$u_{xy}(x_2, y_4) \approx \frac{u_{3,5} - u_{3,3} - u_{1,5} + u_{1,3}}{4hk} \approx \frac{9.1 - 9.0 - 8.4 + 7.5}{4 \cdot .5 \cdot .2} = -2.$$

Exercises

27.1 Suppose you are given the data in the following table.

t	0	.5	1.0	1.5	2.0
y	0	.19	.26	.29	.31

- a. Give the forward, backward and central difference approximations of $f'(1)$.
- b. Give the central difference approximations for $f''(1)$, $f'''(1)$ and $f^{(4)}(1)$.

27.2 Suppose values of $u(x, y)$ at points (x_i, y_j) are given in the matrix (27.1). Suppose that $h = .1$ and $k = .5$. Approximate the following derivatives by central differences:

- a. $u_x(x_3, y_4)$
- b. $u_{xx}(x_4, y_2)$
- c. $u_{yy}(x_3, y_4)$
- d. $u_{xy}(x_3, y_3)$