



Math 4543: Numerical Methods

Lecture 17 — Numerical Differentiation

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Lecture Plan

The agenda for today

- Approximate derivatives from functional values at discrete points
- Error analysis of the approximation approaches
- Approximate partial derivatives of bivariate functional values at discrete grid points

Derivative Approximation

How do we estimate them from discrete points?

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

Forward Difference:

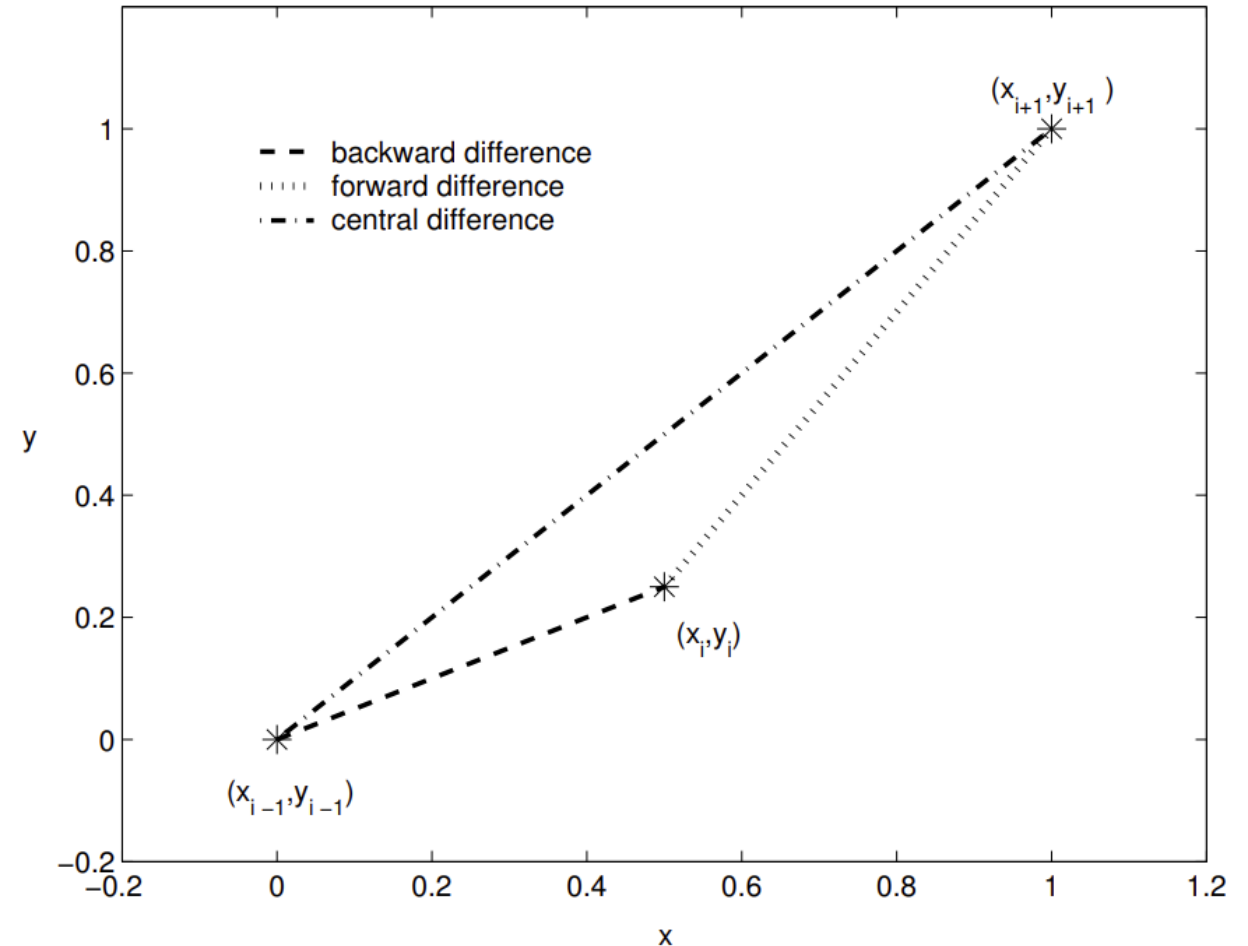
$$f'(x_i) = y'_i \approx \frac{y_{i+1} - y_i}{x_{i+1} - x_i}$$

Backward Difference:

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

Central Difference:

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



Errors of Approximation

Using the Taylor polynomial

The usual form of the Taylor polynomial with remainder (sometimes called Taylor's Theorem) is

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

$x < c < x+h$

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

Error for both FD and BD = $\mathcal{O}(h)$

Forward Difference
formula with +ve h

Backward Difference
formula with -ve h

$$\left. \begin{aligned} f(x_{i+1}) &= f(x_i + h) = f(x_i) + hf'(x_i) + \frac{h^2}{2}f''(x_i) + \frac{h^3}{3!}f'''(c_1) \\ f(x_{i-1}) &= f(x_i - h) = f(x_i) - hf'(x_i) + \frac{h^2}{2}f''(x_i) - \frac{h^3}{3!}f'''(c_2) \end{aligned} \right\} \rightarrow f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} - \frac{h^2}{3!} \frac{f'''(c_1) + f'''(c_2)}{2}$$

Error for both CD = $\mathcal{O}(h^2)$

$x_i \leq c_1 \leq x_{i+1}$ and $x_{i-1} \leq c_2 \leq x_i$

Central Difference formula

Errors of Approximation

Using the Taylor polynomial

And for all higher order derivatives, we see an Central Difference error of order $O(h^2)$.

$$f''(x_i) = y_i'' \approx \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2},$$

$$f'''(x_i) = y_i''' \approx \frac{1}{2h^3} [y_{i+2} - 2y_{i+1} + 2y_{i-1} - y_{i-2}], \quad \text{and}$$

$$f^{(4)}(x_i) = y_i^{(4)} \approx \frac{1}{h^4} [y_{i+2} - 4y_{i+1} + 6y_i - 4y_{i-1} + y_{i-2}].$$

Partial Derivative Approximation

How do we estimate them from discrete grid points?

Suppose $u = u(x, y)$ is a function of two variables that we only know at discrete grid points

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

Assume that the grid points are evenly spaced, with a step size of h along the x -direction and k along the y -direction. The central difference formulae for partial derivatives would be,

$$u_x(x_i, y_j) \approx \frac{1}{2h} (u_{i+1,j} - u_{i-1,j}) \quad \text{and}$$

$$u_y(x_i, y_j) \approx \frac{1}{2k} (u_{i,j+1} - u_{i,j-1}).$$

The second partial derivatives are,

$$u_{xx}(x_i, y_j) \approx \frac{1}{h^2} (u_{i+1,j} - 2u_{i,j} + u_{i-1,j})$$

$$u_{yy}(x_i, y_j) \approx \frac{1}{k^2} (u_{i,j+1} - 2u_{i,j} + u_{i,j-1})$$

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

Partial Derivative Approximation

Some examples

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

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

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

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

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

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