Math 4543: Numerical Methods

Lecture 17 — Numerical Differentiation

Syed Rifat Raiyan
Lecturer
Department of Computer Science & Engineering
Islamic University of Technology, Dhaka, Bangladesh
Email: rifatraiyan@iut-dhaka.edu

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

Forward Difference:

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

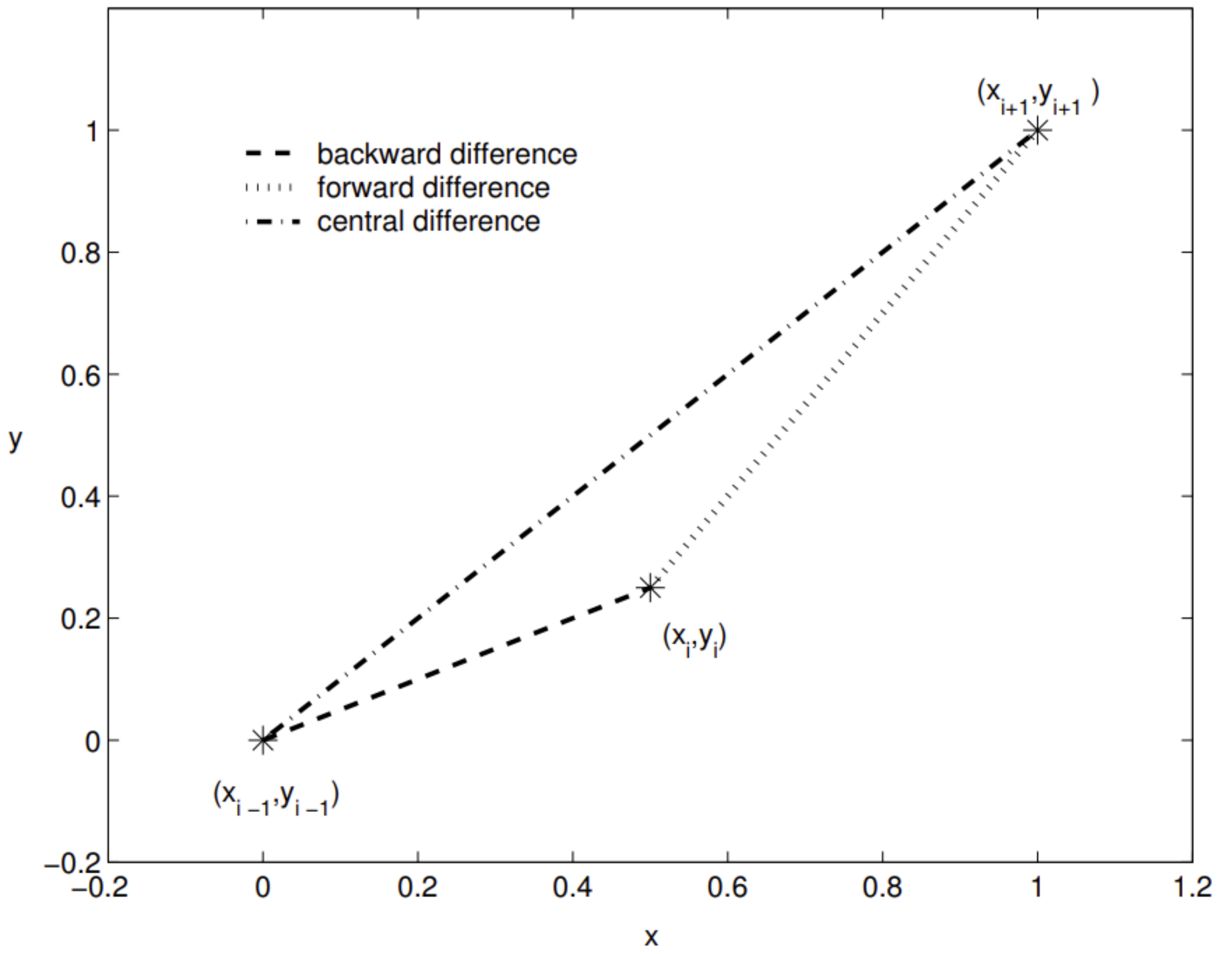
Backward Difference:

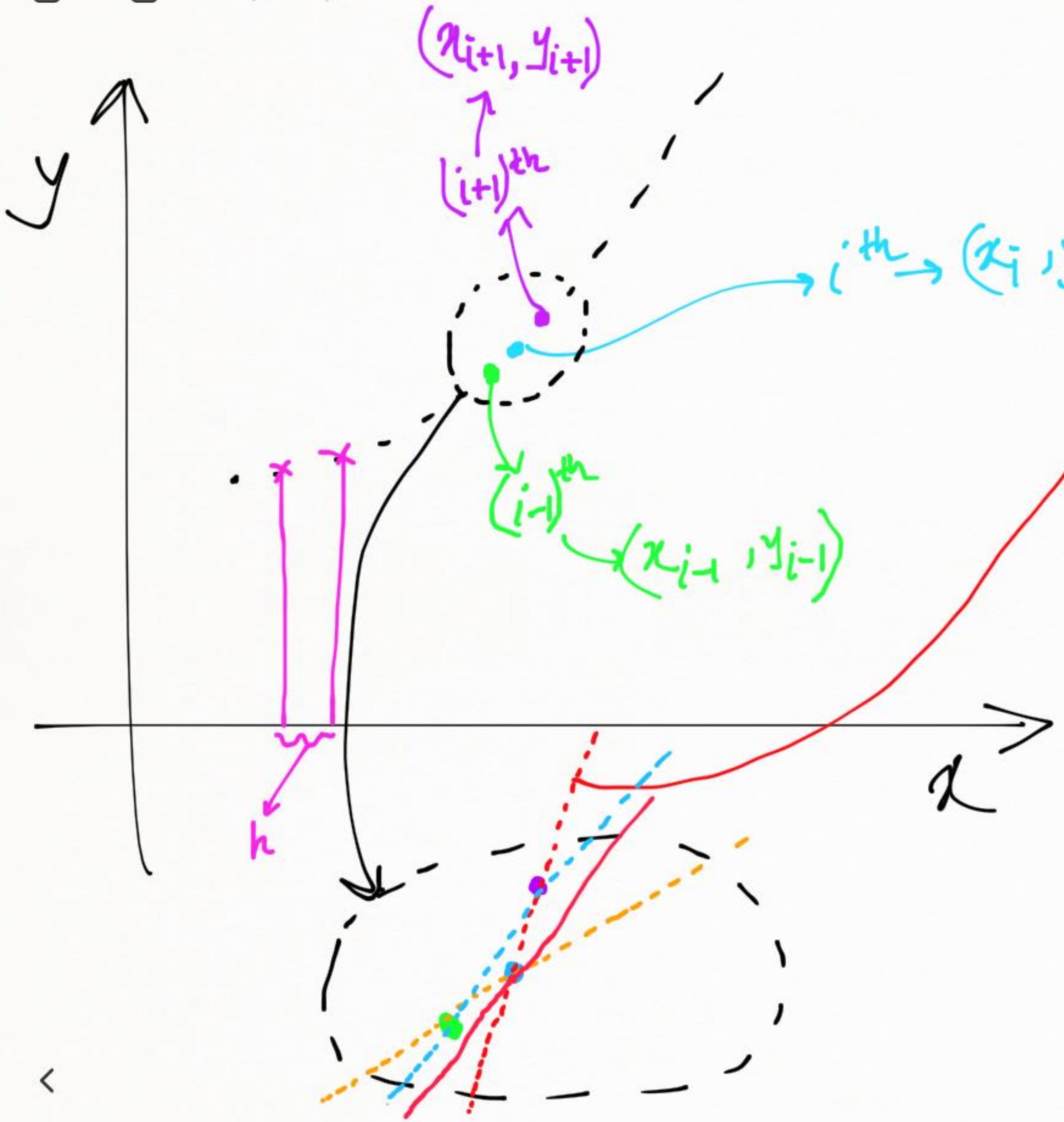
$$\boxed{f'(x_i) \approx \frac{y_i - y_{i-1}}{x_i - x_{i-1}}}$$

Central Difference:

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

$$x_{i+1} - x_i = x_i - x_{i-1} = h$$





fwd:

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

Bckd:

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

CD:

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

Errors of Approximation

Using the Taylor polynomial

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

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

$x < c < x + h$

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

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

Forward Difference formula with +ve *h*

Backward Difference formula with -ve *h*

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

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

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

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

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

Central Difference formula

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

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

$x_i < c_1 < x_i + h$

$x_i - h < c_2 < x_i$

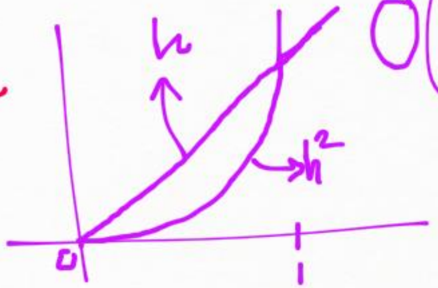
$$f(x_{i+1}) - f(x_{i-1}) = 2h f'(x_i) + \frac{h^3}{3!} f'''(c_1) + \frac{h^3}{3!} f'''(c_2)$$

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

$O(h) \to FD, BD$

$$\Rightarrow f'(x_i) = \underbrace{\frac{f(x_{i+1}) - f(x_{i-1})}{2h}}_{CD} - \boxed{\frac{h^2}{3!} \times \frac{f'''(c_1) + f'''(c_2)}{2}}$$

$O(h^2) \to CD$



Errors of Approximation

Using the Taylor polynomial

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

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

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

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

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,

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

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

The second partial derivatives are,

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

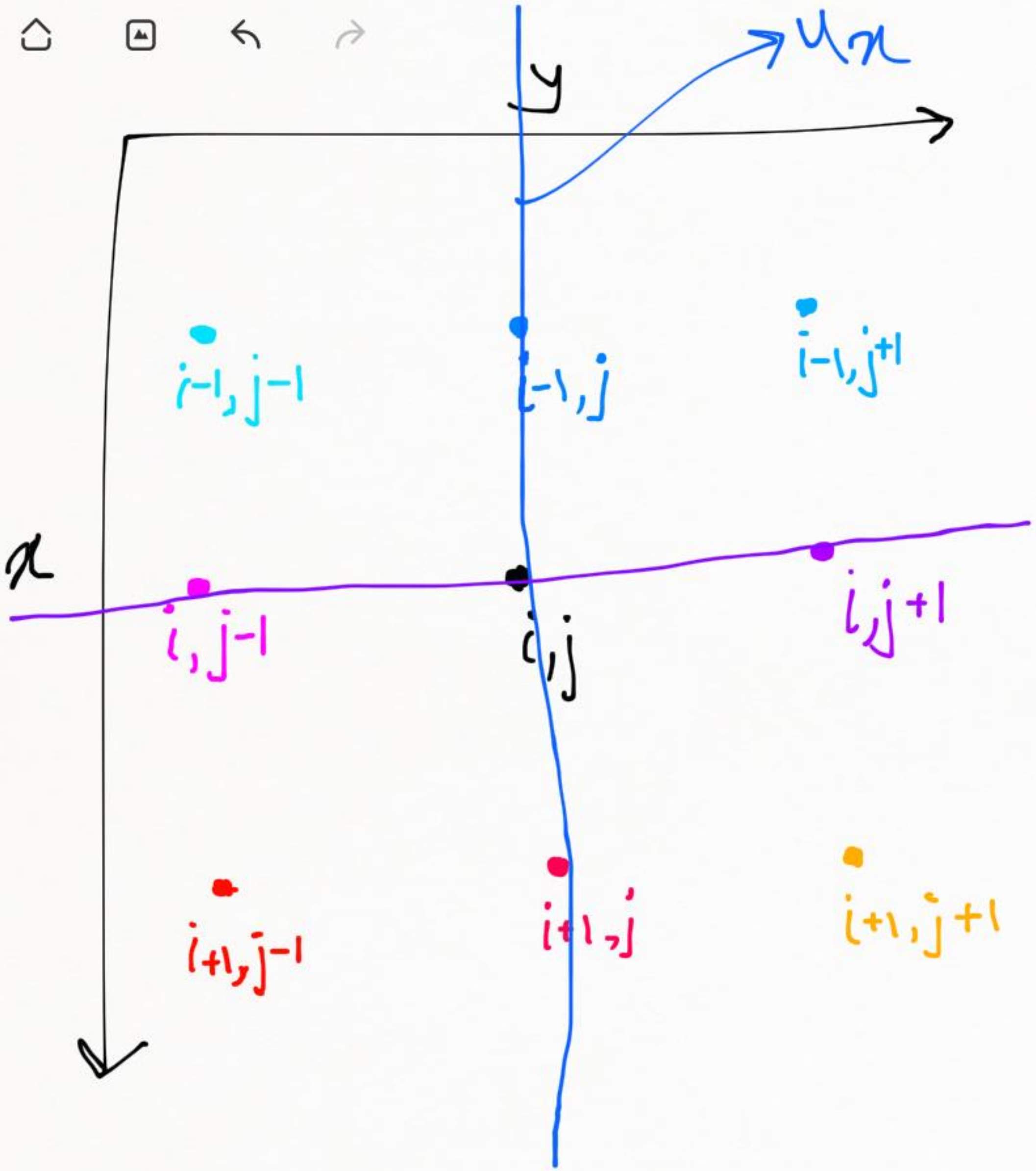
$$\boxed{u_{yy}(x_i, y_j) \approx \frac{1}{k^2}\left(u_{i,j+1} - 2u_{i,j} + u_{i,j-1}\right)}$$

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

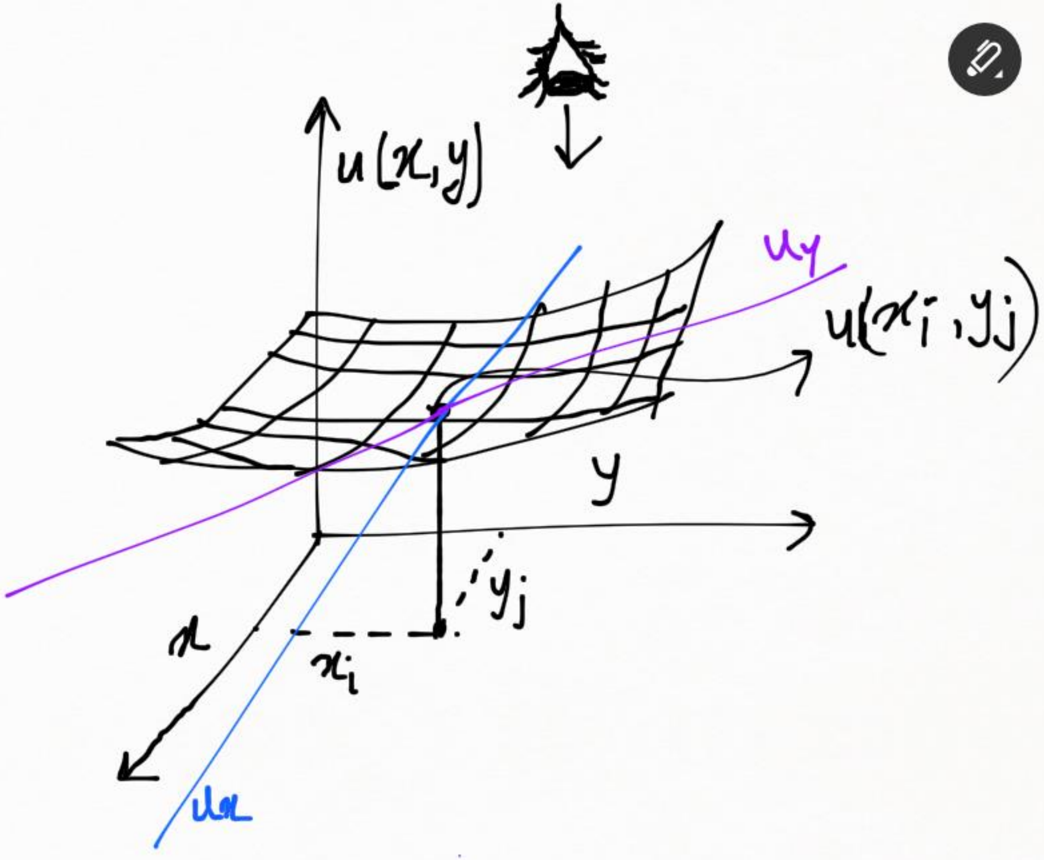
$$u_x(x_i, y_j) = \left.\frac{\partial u}{\partial x}\right|_{x_i, y_j}$$

$$u_{xx}(x_i, y_j) = \left.\frac{\partial^2 u}{\partial x^2}\right|_{x_i, y_j}$$

$$u_{xy}(x_i, y_j) = \left.\frac{\partial}{\partial x}\left(\frac{\partial u}{\partial y}\right)\right|_{x_i, y_j} = \left.\frac{\partial}{\partial y}\left(\frac{\partial u}{\partial x}\right)\right|_{x_i, y_j}$$



ux
y
i-1, j-1
i-1, j
i-1, j+1
x
i, j-1
i, j
i, j+1
i+1, j-1
i+1, j
i+1, j+1



u(x, y)
uy
u(xi , yj)
y
yj
x
xi
ux

$$u_{xy}(x_i, y_j) \approx \frac{u_y(x_{i+1}, y_j) - u_y(x_{i-1}, y_j)}{2h}$$

$$= \frac{\dfrac{u_{i+1,j+1} - u_{i+1,j-1}}{2k} - \dfrac{u_{i-1,j+1} - u_{i-1,j-1}}{2k}}{2h}$$

$$= \boxed{\frac{u_{i+1,j+1} - u_{i+1,j-1} - u_{i-1,j+1} + u_{i-1,j-1}}{4hk}}$$

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

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