Computational Physics

Lecture-03

M. Reza Mozaffari

Physics Group, University of Qom

Contents

- Basis Concepts
- Numerical Differentiation

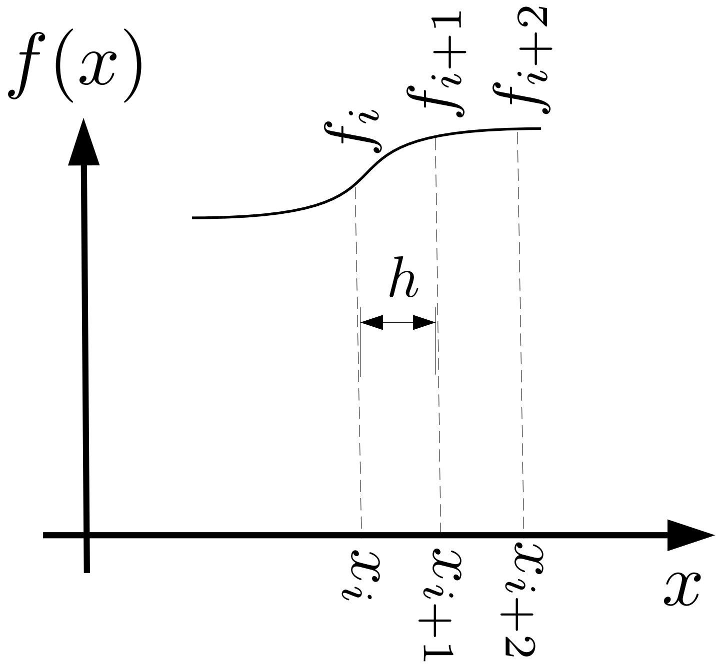
Numerical Differentiation

- Second order derivative (3-points)

$$f_{i+2} = f_i + \frac{f_i^{(1)}}{1!}(2h) + \frac{f_i^{(2)}}{2!}(2h)^2 + \frac{f_i^{(3)}}{3!}(2h)^3 + \cdots$$

$$f_{i+1} = f_i + \frac{f_i^{(1)}}{1!}h + \frac{f_i^{(2)}}{2!}h^2 + \frac{f_i^{(3)}}{3!}h^3 + \cdots$$

$+$



$$f_{i+2} - 2f_{i+1} = -f_i + f_i^{(2)}h^2 + f_i^{(3)}h^3 + \cdots$$

Truncate: $$f_{i+2} - 2f_{i+1} \approx -f_i + f_i^{(2)}h^2 + \mathrm{O}(h^3)$$

Numerical Differentiation

- Second order derivative (3-points)

$$f_{i+2} - 2f_{i+1} \approx -f_i + f_i^{(2)} h^2 + \mathrm{O}(h^3)$$

$$f_i^{(2)} \approx \frac{f_{i+2} - 2f_{i+1} + f_i}{h^2} + \mathrm{O}(h)$$

Forward

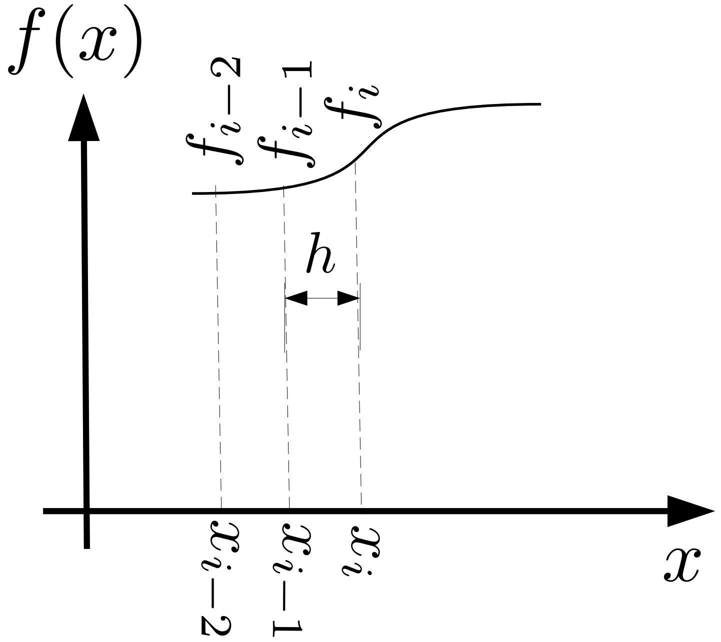
x	$f(x)$	$f^{(2)}(x)$
x_0	f_0	$f_0^{(2)}$
x_1	f_1	$f_1^{(2)}$
x_2	f_2	$f_2^{(2)}$
$\vdots$	$\vdots$	$\vdots$
x_{i-1}	f_{i-1}	$f_{i-1}^{(2)}$
x_i	f_i	$f_i^{(2)}$
x_{i+1}	f_{i+1}	$f_{i+1}^{(2)}$
$\vdots$	$\vdots$	$\vdots$
x_{N-1}	f_{N-1}	$f_{N-1}^{(2)}$
x_N	f_N	$f_N^{(2)}$

Numerical Differentiation

- Second order derivative (3-points)

$$f_{i-1} = f_i - \frac{f_i^{(1)}}{1!}h + \frac{f_i^{(2)}}{2!}h^2 - \frac{f_i^{(3)}}{3!}h^3 + \cdots$$

$$f_{i-2} = f_i - \frac{f_i^{(1)}}{1!}(2h) + \frac{f_i^{(2)}}{2!}(2h)^2 - \frac{f_i^{(3)}}{3!}(2h)^3 + \cdots$$



$$-f_{i-2} + 2f_{i-1} = f_i - f_i^{(2)}h^2 + f_i^{(3)}h^3 + \cdots$$

Truncate: $$-f_{i-2} + 2f_{i-1} = f_i - f_i^{(2)}h^2 + \mathrm{O}(h^3)$$

Numerical Differentiation

- Second order derivative (3-points)

$$-f_{i-2} + 2f_{i-1} = f_i - f_i^{(2)} h^2 + \mathrm{O}(h^3)$$

$$f_i^{(2)} \approx \frac{f_{i-2} - 2f_{i-1} + f_i}{h^2} + \mathrm{O}(h)$$

Backward

x	$f(x)$	$f^{(2)}(x)$
x_0	f_0	$f_0^{(2)}$
x_1	f_1	$f_1^{(2)}$
x_2	f_2	$f_2^{(2)}$
$\vdots$	$\vdots$	$\vdots$
x_{i-1}	f_{i-1}	$f_{i-1}^{(2)}$
x_i	f_i	$f_i^{(2)}$
x_{i+1}	f_{i+1}	$f_{i+1}^{(2)}$
$\vdots$	$\vdots$	$\vdots$
x_{N-1}	f_{N-1}	$f_{N-1}^{(2)}$
x_N	f_N	$f_N^{(2)}$

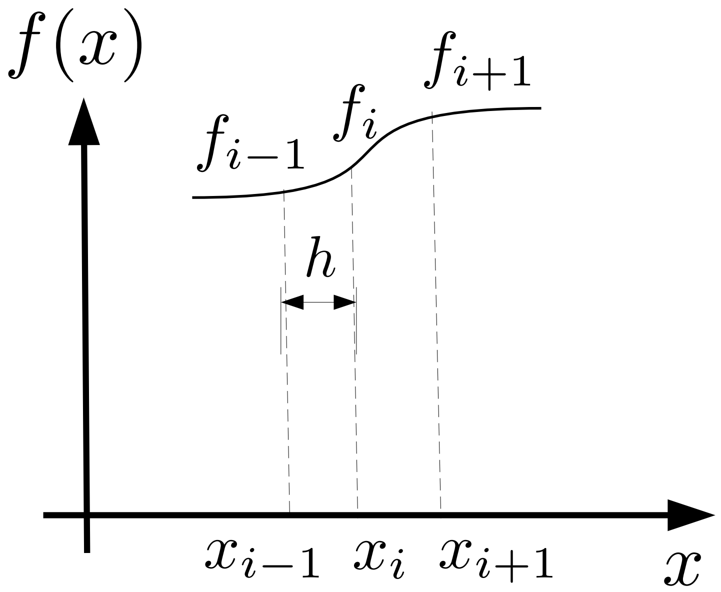
Numerical Differentiation

- Second order derivative (3-points)

$$f_{i+1} = f_i + \frac{f_i^{(1)}}{1!}h + \frac{f_i^{(2)}}{2!}h^2 + \frac{f_i^{(3)}}{3!}h^3 + \cdots$$

$$f_{i-1} = f_i - \frac{f_i^{(1)}}{1!}h + \frac{f_i^{(2)}}{2!}h^2 - \frac{f_i^{(3)}}{3!}h^3 + \cdots \quad +$$

$$f_{i+1} + f_{i-1} = 2f_i + f_i^{(2)}h^2 + \frac{1}{12}f_i^{(4)}h^4 + \cdots$$



Truncate: $f_{i+1} + f_{i-1} \approx 2f_i + f_i^{(2)}h^2 + \mathrm{O}(h^4)$

Numerical Differentiation

- Second order derivative (3-points)

$$f_{i+1} + f_{i-1} \approx 2f_i + f_i^{(2)} h^2 + \mathrm{O}(h^4)$$

$$f_i^{(2)} \approx \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} + \mathrm{O}(h^2)$$

Central

x	$f(x)$	$f^{(2)}(x)$
x_0	f_0	$f_0^{(2)}$
x_1	f_1	$f_1^{(2)}$
x_2	f_2	$f_2^{(2)}$
$\vdots$	$\vdots$	$\vdots$
x_{i-1}	f_{i-1}	$f_{i-1}^{(2)}$
x_i	f_i	$f_i^{(2)}$
x_{i+1}	f_{i+1}	$f_{i+1}^{(2)}$
$\vdots$	$\vdots$	$\vdots$
x_{N-1}	f_{N-1}	$f_{N-1}^{(2)}$
x_N	f_N	$f_N^{(2)}$

Numerical Differentiation

- Second order derivative

$$f_i^{(2)} \approx \frac{f_{i+2} - 2f_{i+1} + f_i}{h^2} + \mathrm{O}(h)$$

Forward

$$f_i^{(2)} \approx \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} + \mathrm{O}(h^2)$$

Central

$$f_i^{(2)} \approx \frac{f_{i-2} - 2f_{i-1} + f_i}{h^2} + \mathrm{O}(h)$$

Backward

x	$f(x)$	$f^{(1)}(x)$
x_0	f_0	$f_0^{(1)}$
x_1	f_1	$f_1^{(1)}$
x_2	f_2	$f_2^{(1)}$
$\vdots$	$\vdots$	$\vdots$
x_{i-1}	f_{i-1}	$f_{i-1}^{(1)}$
x_i	f_i	$f_i^{(1)}$
x_{i+1}	f_{i+1}	$f_{i+1}^{(1)}$
$\vdots$	$\vdots$	$\vdots$
x_{N-1}	f_{N-1}	$f_{N-1}^{(1)}$
x_N	f_N	$f_N^{(1)}$

Numerical Differentiation

- First order derivative

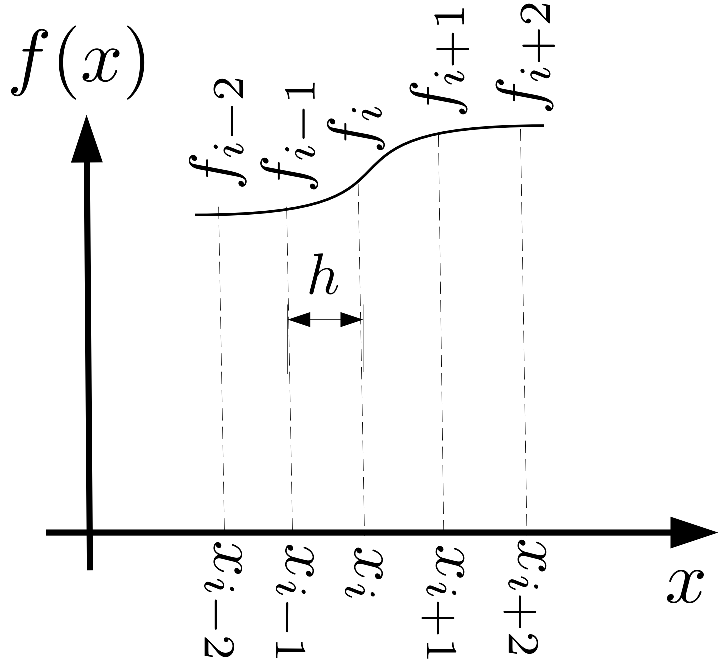
Asymmetry

$$f_i^{(2)} \approx \frac{f_{i+2} - 2f_{i+1} + f_i}{h^2} + \underline{\underline{O(h)}} \quad \text{Forward}$$

$$f_i^{(2)} \approx \frac{f_{i-2} - 2f_{i-1} + f_i}{h^2} + \underline{\underline{O(h)}} \quad \text{Backward}$$

Symmetry

$$f_i^{(2)} \approx \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} + \underline{\underline{O(h^2)}} \quad \text{Central}$$



Numerical Differentiation

- Second order derivative

$$\vdots$$

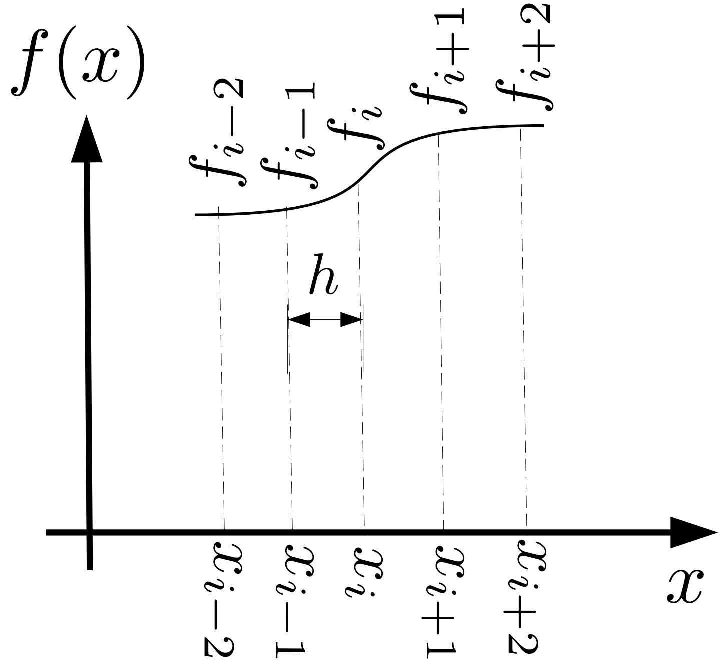
$$f_{i-2} = f_i - \frac{f_i^{(1)}}{1!}(2h) + \frac{f_i^{(2)}}{2!}(2h)^2 - \frac{f_i^{(3)}}{3!}(2h)^3 + \cdots$$

$$f_{i-1} = f_i - \frac{f_i^{(1)}}{1!}h + \frac{f_i^{(2)}}{2!}h^2 - \frac{f_i^{(3)}}{3!}h^3 + \cdots$$

$$f_{i+1} = f_i + \frac{f_i^{(1)}}{1!}h + \frac{f_i^{(2)}}{2!}h^2 + \frac{f_i^{(3)}}{3!}h^3 + \cdots$$

$$f_{i+2} = f_i + \frac{f_i^{(1)}}{1!}(2h) + \frac{f_i^{(2)}}{2!}(2h)^2 + \frac{f_i^{(3)}}{3!}(2h)^3 + \cdots$$

$$\vdots$$



Numerical Differentiation

- Second order derivative

Asymmetry

$$f_i^{(2)} \approx \frac{-f_{i+3} + 4f_{i+2} - 5f_{i+1} + 2f_i}{h^2} + \mathrm{O}(h^2)$$

$$f_i^{(2)} \approx \frac{-f_{i-3} + 4f_{i-2} - 5f_{i-1} + 2f_i}{h^2} + \mathrm{O}(h^2)$$

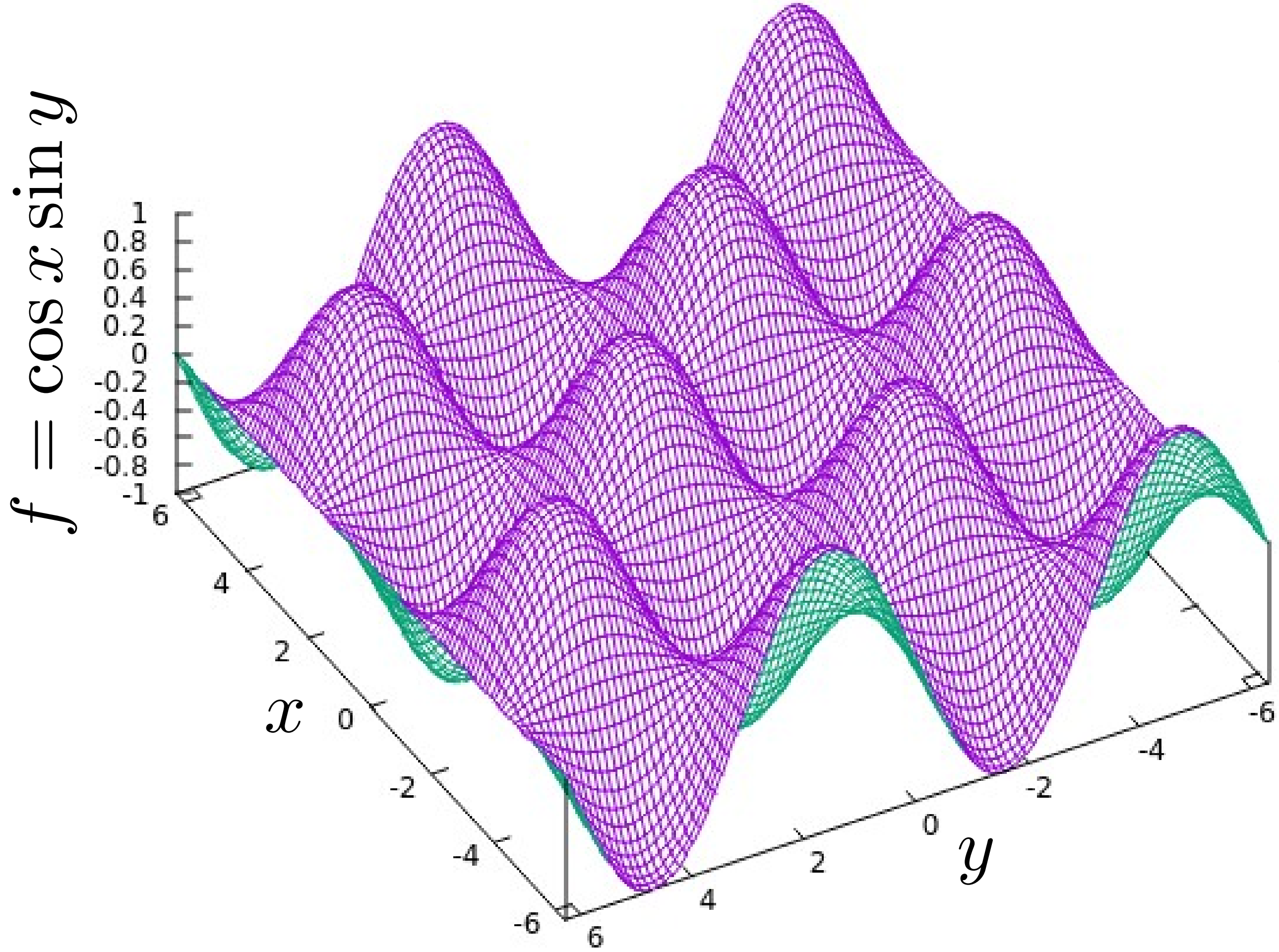
Symmetry

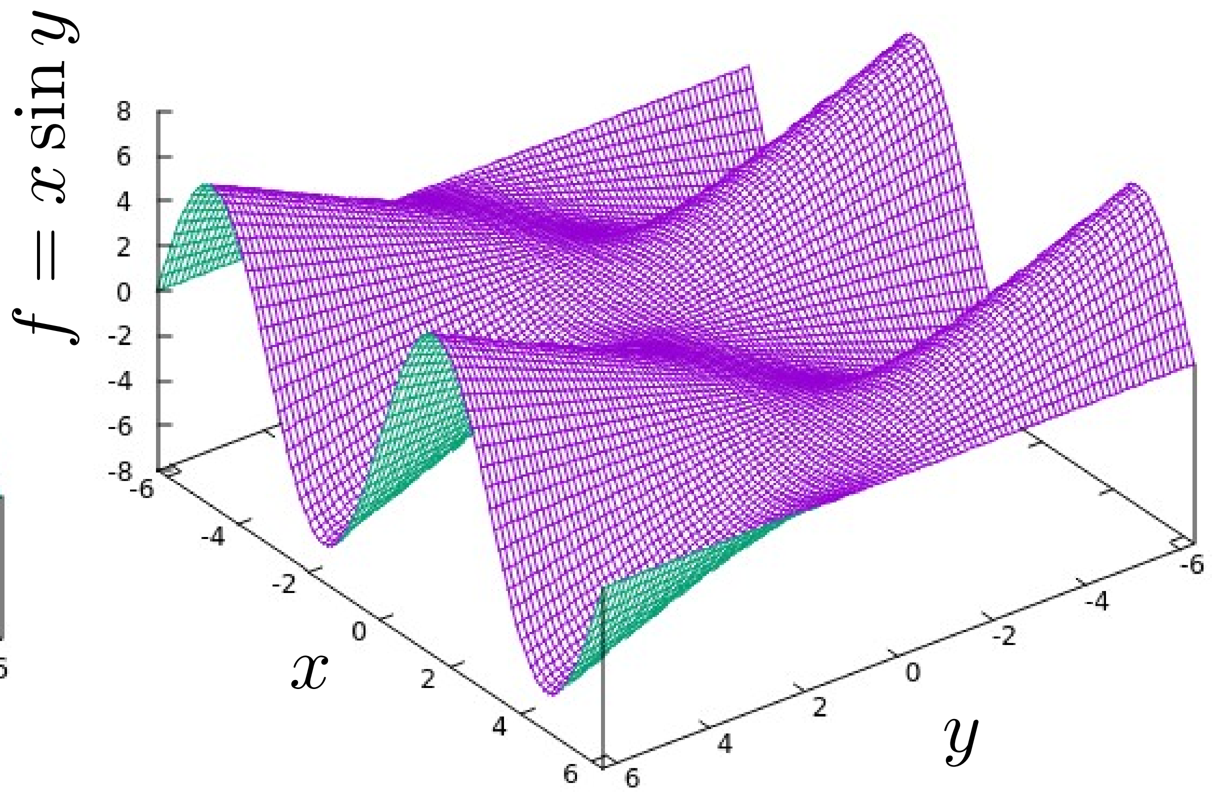
$$f_i^{(2)} \approx \frac{-f_{i+2} + 16f_{i+1} - 30f_i + 16f_{i-1} - f_{i-2}}{12h^2} + \mathrm{O}(h^4)$$

x	$f(x)$	$f^{(2)}(x)$
x_0	f_0	$f_0^{(2)}$
x_1	f_1	$f_1^{(2)}$
x_2	f_2	$f_2^{(2)}$
$\vdots$	$\vdots$	$\vdots$
x_{i-1}	f_{i-1}	$f_{i-1}^{(2)}$
x_i	f_i	$f_i^{(2)}$
x_{i+1}	f_{i+1}	$f_{i+1}^{(2)}$
$\vdots$	$\vdots$	$\vdots$
x_{N-1}	f_{N-1}	$f_{N-1}^{(2)}$
x_N	f_N	$f_N^{(2)}$

Numerical Differentiation

- Two dimensional finite difference





Numerical Differentiation

- Two dimensional finite difference

$$f = f(x, y)$$

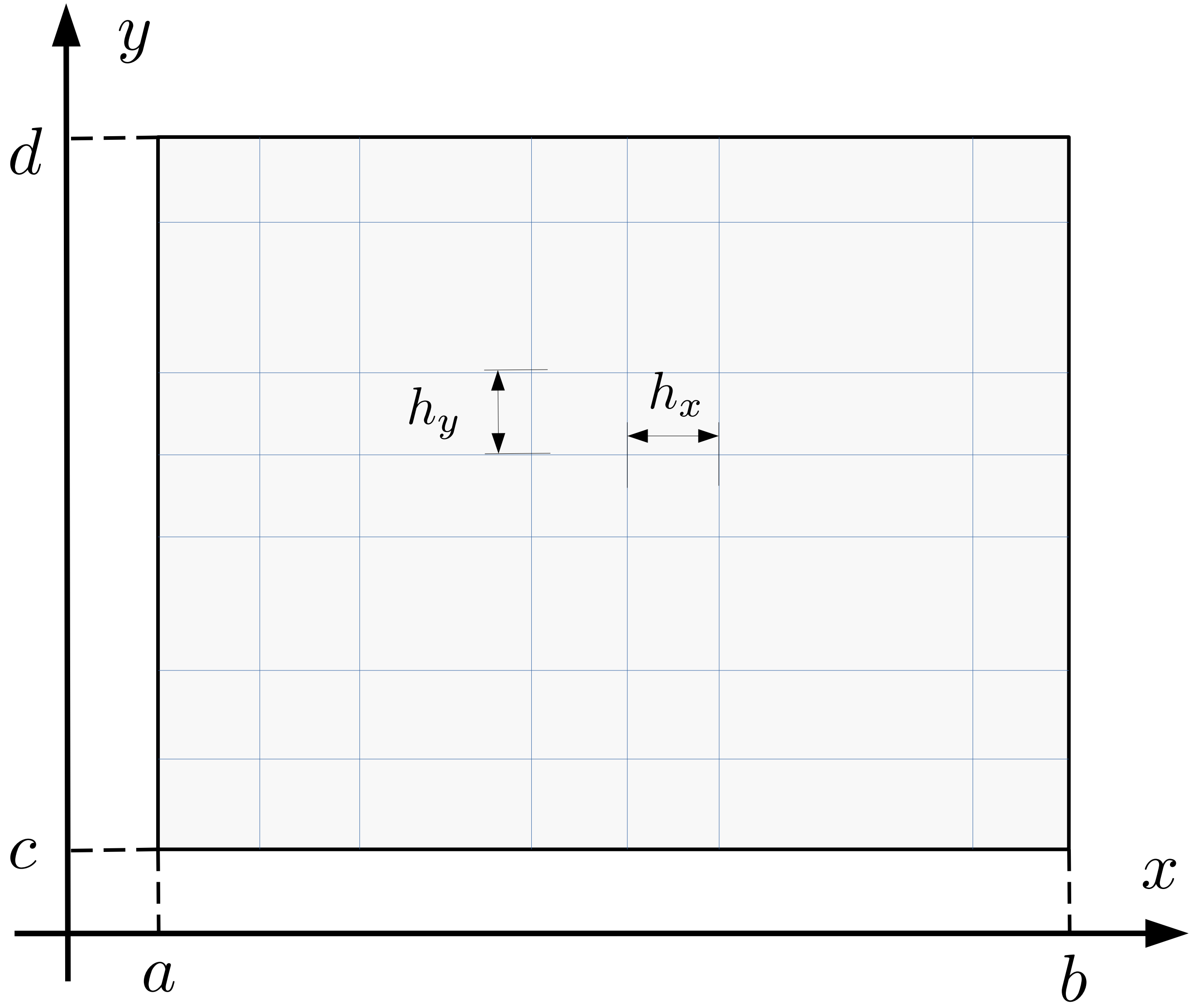
$$a \leq x \leq b$$

$$c \leq y \leq d$$

$$h_x = \frac{b-a}{N_x} \qquad h_y = \frac{d-c}{N_y}$$

$$x_i = a + ih_x \qquad y_j = c + jh_y$$

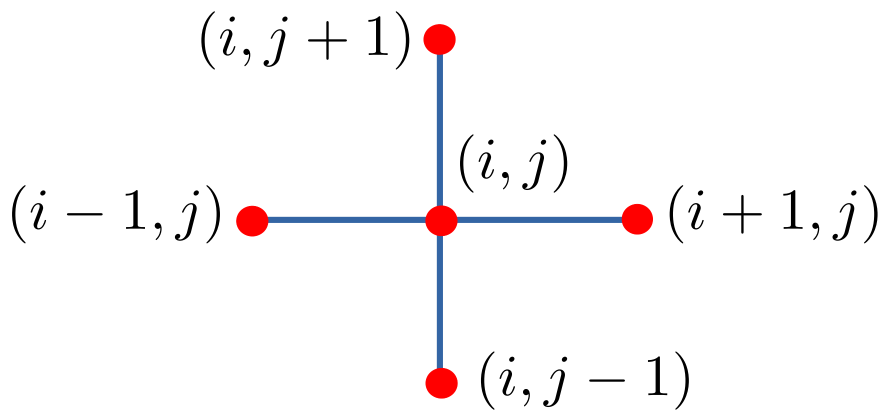
$$i = 0, 1, 2, \cdots, N_x \qquad j = 0, 1, 2, \cdots, N_y$$



Numerical Differentiation

$$f = f(x, y) \qquad a \le x \le b \qquad c \le y \le d$$

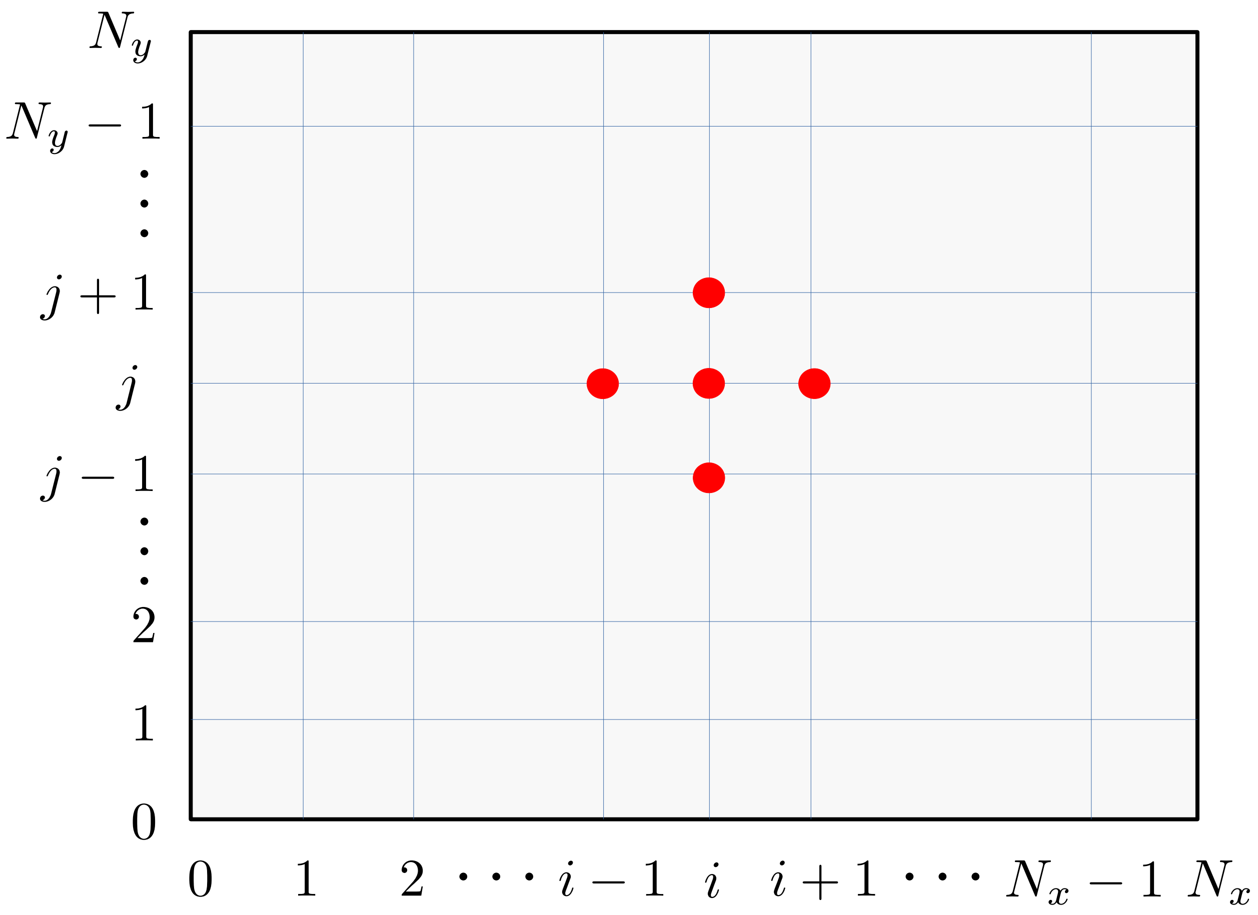
- Two dimensional finite difference



$$(i, j) = (x_i, y_j)$$

$$(i \pm 1, j) = (x_i \pm h_x, y_j)$$

$$(i, j \pm 1) = (x_i, y_j \pm h_y)$$



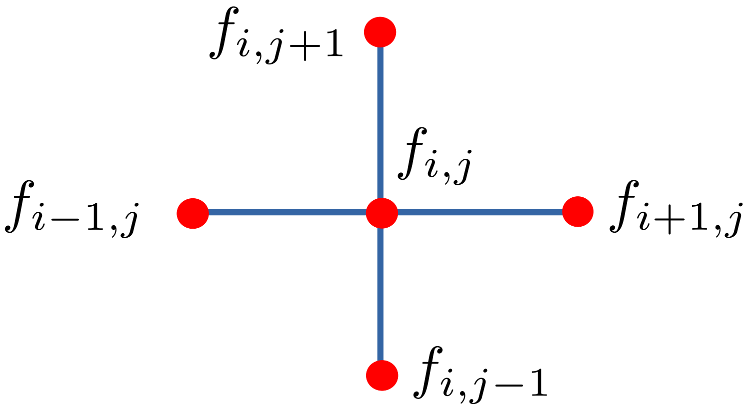
Numerical Differentiation

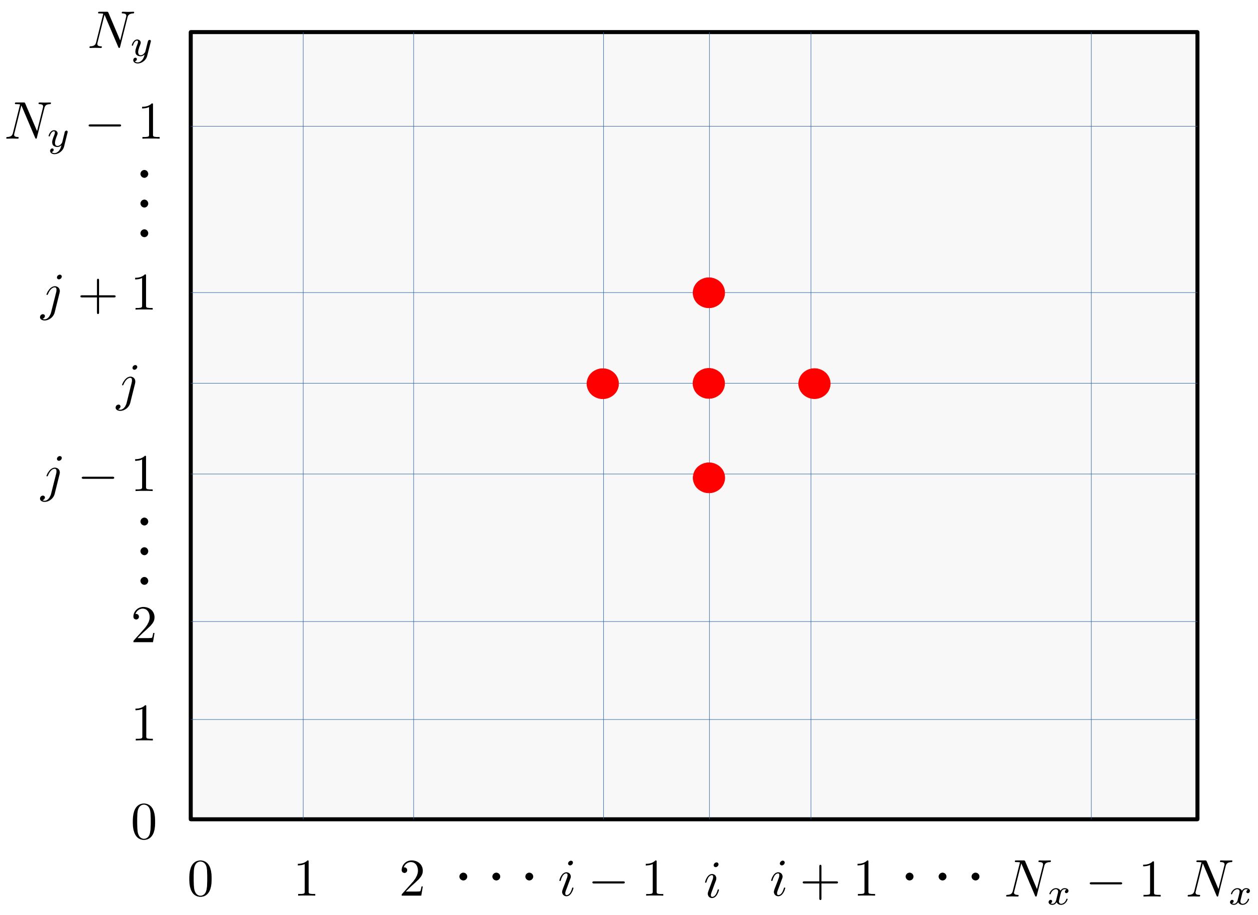
$$f = f(x, y)$$

$$a \leq x \leq b$$

$$c \leq y \leq d$$

- Two dimensional finite difference





$$f_{i,j} = f(x_i, y_j)$$

$$f_{i\pm1,j} = f(x_i \pm h_x, y_j)$$

$$f_{i,j\pm1} = f(x_i, y_j \pm h_y)$$

Numerical Differentiation

- Taylor expansion

$$f_{i+1,j+1} = f_{i,j} + f^{x}_{i,j} h_x + f^{y}_{i,j} h_y + \frac{1}{2}\left(f^{xx}_{i,j} h_x^2 + 2 f^{xy}_{i,j} h_x h_y + f^{yy}_{i,j} h_y^2 \right) + \cdots$$

$$f^{x}_{i,j} = \left(\frac{\partial f}{\partial x}\right)_{i,j}, \qquad f^{y}_{i,j} = \left(\frac{\partial f}{\partial y}\right)_{i,j}$$

$$f^{xx}_{i,j} = \left(\frac{\partial^2 f}{\partial x^2}\right)_{i,j}, \qquad f^{xy}_{i,j} = \left(\frac{\partial^2 f}{\partial x \partial y}\right)_{i,j} = \left(\frac{\partial^2 f}{\partial y \partial x}\right)_{i,j}, \qquad f^{yy}_{i,j} = \left(\frac{\partial^2 f}{\partial y^2}\right)_{i,j}$$

Numerical Differentiation

- First order derivative

x-axis

$$f_{i+1,j} = f_{i,j} + f^{x}_{i,j} h_x + \frac{1}{2} f^{xx}_{i,j} h_x^2 + \cdots$$

$$f_{i+1,j} \approx f_{i,j} + f^{x}_{i,j} h_x + \mathrm{O}(h_x^2)$$

$$f^{x}_{i,j} \approx \frac{f_{i+1,j} - f_{i,j}}{h_x} + \mathrm{O}(h_x)$$

$$f_{i-1,j} = f_{i,j} - f^{x}_{i,j} h_x + \frac{1}{2} f^{xx}_{i,j} h_x^2 + \cdots$$

$$f_{i-1,j} \approx f_{i,j} - f^{x}_{i,j} h_x + \mathrm{O}(h_x^2)$$

$$f^{x}_{i,j} \approx \frac{f_{i,j} - f_{i-1,j}}{h_x} + \mathrm{O}(h_x)$$

Numerical Differentiation

- First order derivative

y-axis

$$f_{i,j+1} = f_{i,j} + f^{y}_{i,j} h_y + \frac{1}{2} f^{yy}_{i,j} h_y^2 + \cdots$$

$$f_{i,j+1} \approx f_{i,j} + f^{y}_{i,j} h_y + \mathrm{O}(h_y^2)$$

$$f^{y}_{i,j} \approx \frac{f_{i,j+1} - f_{i,j}}{h_y} + \mathrm{O}(h_y)$$

$$f_{i,j-1} = f_{i,j} - f^{y}_{i,j} h_y + \frac{1}{2} f^{yy}_{i,j} h_y^2 + \cdots$$

$$f_{i,j-1} \approx f_{i,j} - f^{y}_{i,j} h_y + \mathrm{O}(h_y^2)$$

$$f^{y}_{i,j} \approx \frac{f_{i,j} - f_{i,j-1}}{h_y} + \mathrm{O}(h_y)$$

Numerical Differentiation

- First order derivative

x-axis

$$f_{i+1,j} = f_{i,j} + f^{x}_{i,j} h_x + \frac{1}{2} f^{xx}_{i,j} h_x^2 + \cdots$$

$$f_{i-1,j} = f_{i,j} - f^{x}_{i,j} h_x + \frac{1}{2} f^{xx}_{i,j} h_x^2 + \cdots$$

$$f_{i+1,j} - f_{i-1,j} \approx 2 f^{x}_{i,j} h_x + \mathrm{O}(h_x^3)$$

$$f^{x}_{i,j} \approx \frac{f_{i+1,j} - f_{i-1,j}}{2h_x} + \mathrm{O}(h_x^2)$$

y-axis

$$f_{i,j+1} = f_{i,j} + f^{y}_{i,j} h_y + \frac{1}{2} f^{yy}_{i,j} h_y^2 + \cdots$$

$$f_{i,j-1} = f_{i,j} - f^{y}_{i,j} h_y + \frac{1}{2} f^{yy}_{i,j} h_y^2 + \cdots$$

$$f_{i,j+1} - f_{i,j-1} \approx 2 f^{y}_{i,j} h_y + \mathrm{O}(h_y^3)$$

$$f^{y}_{i,j} \approx \frac{f_{i,j+1} - f_{i,j-1}}{2h_y} + \mathrm{O}(h_y^2)$$

Numerical Differentiation

- Second order derivative

x-axis

$$f_{i+1,j} = f_{i,j} + f^{x}_{i,j} h_x + \frac{1}{2} f^{xx}_{i,j} h_x^2 + \cdots$$

$$f_{i-1,j} = f_{i,j} - f^{x}_{i,j} h_x + \frac{1}{2} f^{xx}_{i,j} h_x^2 + \cdots$$

$$f_{i+1,j} + f_{i-1,j} \approx 2 f_{i,j} + f^{xx}_{i,j} h_x^2 + \mathrm{O}(h_x^4)$$

$$f^{xx}_{i,j} \approx \frac{f_{i+1,j} - 2 f_{i,j} + f_{i-1,j}}{h_x^2} + \mathrm{O}(h_x^2)$$

y-axis

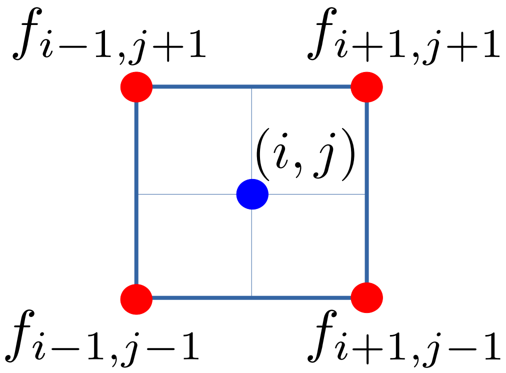
$$f_{i,j+1} = f_{i,j} + f^{y}_{i,j} h_y + \frac{1}{2} f^{yy}_{i,j} h_y^2 + \cdots$$

$$f_{i,j-1} = f_{i,j} - f^{y}_{i,j} h_y + \frac{1}{2} f^{yy}_{i,j} h_y^2 + \cdots$$

$$f_{i,j+1} + f_{i,j-1} \approx 2 f_{i,j} + f^{yy}_{i,j} h_y^2 + \mathrm{O}(h_y^4)$$

$$f^{yy}_{i,j} \approx \frac{f_{i,j+1} - 2 f_{i,j} + f_{i,j-1}}{h_y^2} + \mathrm{O}(h_y^2)$$

Numerical Differentiation



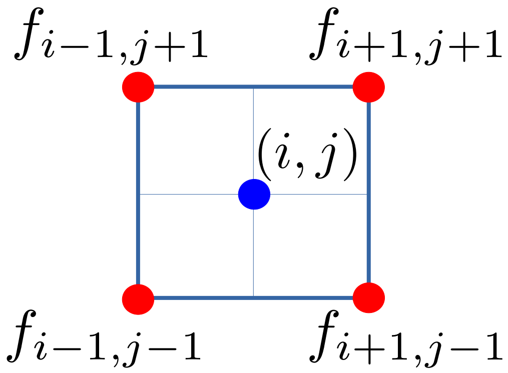
- Second order derivative

$$f_{i+1,j+1} = f_{i,j} + f_{i,j}^{x} h_x + f_{i,j}^{y} h_y + \frac{1}{2}\left(f_{i,j}^{xx} h_x^2 + 2 f_{i,j}^{xy} h_x h_y + f_{i,j}^{yy} h_y^2\right)$$
$$+\frac{1}{6}\left(f_{i,j}^{xxx} h_x^3 + 3 f_{i,j}^{xxy} h_x^2 h_y + 3 f_{i,j}^{xyy} h_x h_y^2 + f_{i,j}^{yyy} h_y^3\right) + \cdots$$

$$f_{i-1,j+1} = f_{i,j} - f_{i,j}^{x} h_x + f_{i,j}^{y} h_y + \frac{1}{2}\left(f_{i,j}^{xx} h_x^2 - 2 f_{i,j}^{xy} h_x h_y + f_{i,j}^{yy} h_y^2\right)$$
$$+\frac{1}{6}\left(-f_{i,j}^{xxx} h_x^3 + 3 f_{i,j}^{xxy} h_x^2 h_y - 3 f_{i,j}^{xyy} h_x h_y^2 + f_{i,j}^{yyy} h_y^3\right) + \cdots$$

$$f_{i+1,j-1} = f_{i,j} + f_{i,j}^{x} h_x - f_{i,j}^{y} h_y + \frac{1}{2}\left(f_{i,j}^{xx} h_x^2 - 2 f_{i,j}^{xy} h_x h_y + f_{i,j}^{yy} h_y^2\right)$$
$$+\frac{1}{6}\left(f_{i,j}^{xxx} h_x^3 - 3 f_{i,j}^{xxy} h_x^2 h_y + 3 f_{i,j}^{xyy} h_x h_y^2 - f_{i,j}^{yyy} h_y^3\right) + \cdots$$

Numerical Differentiation



- Second order derivative

$$f_{i-1,j-1} = f_{i,j} - f_{i,j}^{x} h_x - f_{i,j}^{y} h_y + \frac{1}{2}\left(f_{i,j}^{xx} h_x^2 - 2 f_{i,j}^{xy} h_x h_y - f_{i,j}^{yy} h_y^2\right)$$
$$+\frac{1}{6}\left(-f_{i,j}^{xxx} h_x^3 - 3 f_{i,j}^{xxy} h_x^2 h_y - 3 f_{i,j}^{xyy} h_x h_y^2 - f_{i,j}^{yyy} h_y^3\right) + \cdots$$

$$f_{i+1,j+1} - f_{i-1,j+1} - f_{i+1,j-1} + f_{i-1,j-1} = 4 h_x h_y f_{i,j}^{xy}$$
$$+\frac{2}{3} h_x h_y \left(f_{i,j}^{xxxy} h_x^2 + f_{i,j}^{xyyy} h_y^2\right) + \cdots$$

Truncate: $f_{i+1,j+1} - f_{i-1,j+1} - f_{i+1,j-1} + f_{i-1,j-1} \approx 4 h_x h_y f_{i,j}^{xy} + \mathrm{O}(h_x^3 h_y, h_x h_y^3)$

$$f_{i,j}^{xy} \approx \frac{f_{i+1,j+1} - f_{i-1,j+1} - f_{i+1,j-1} + f_{i-1,j-1}}{4 h_x h_y} + \mathrm{O}(h_x^2, h_y^2)$$