

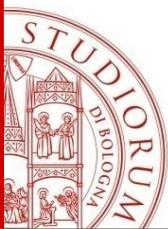
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# Numerical Differentiation

## ***PROBLEM***

Estimate the derivatives (slope, curvature, etc.) of a function, given a set of function values at a discrete set of points.

→ **Finite Difference Formulas**



# Numerical Differentiation

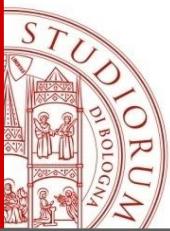
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The simplest way to numerically compute a derivative is to mimic the formal definition:

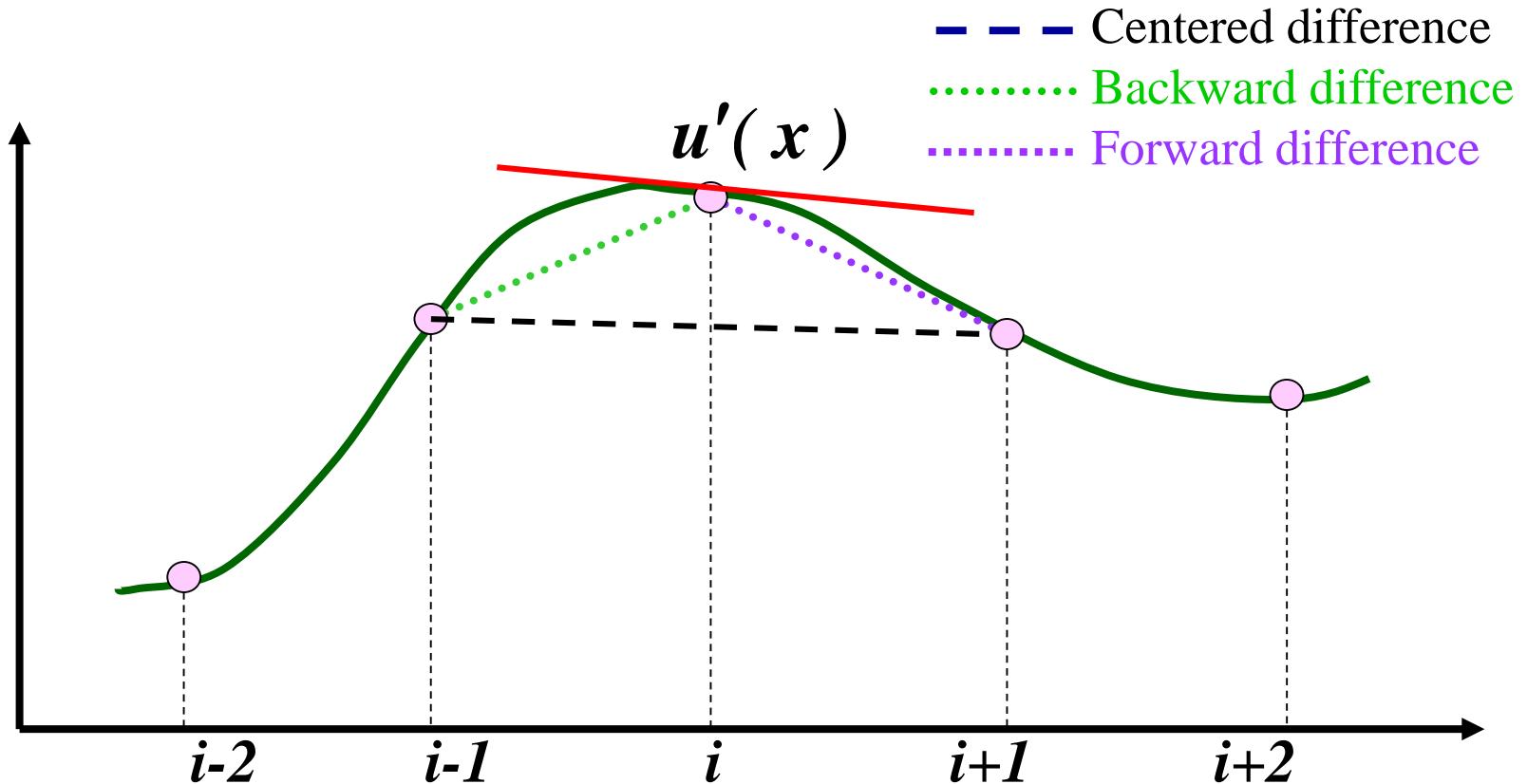
$$u'(x) = \lim_{\Delta x \rightarrow 0} \frac{u(x + \Delta x) - u(x)}{\Delta x}$$

$$u'(x) \approx \frac{u(x + \Delta x) - u(x)}{\Delta x}$$

For a linear function  $u(x)=ax+b$  the formula is exact.



# First Derivative at a point: finite difference schemes



# First Derivative

Centered difference

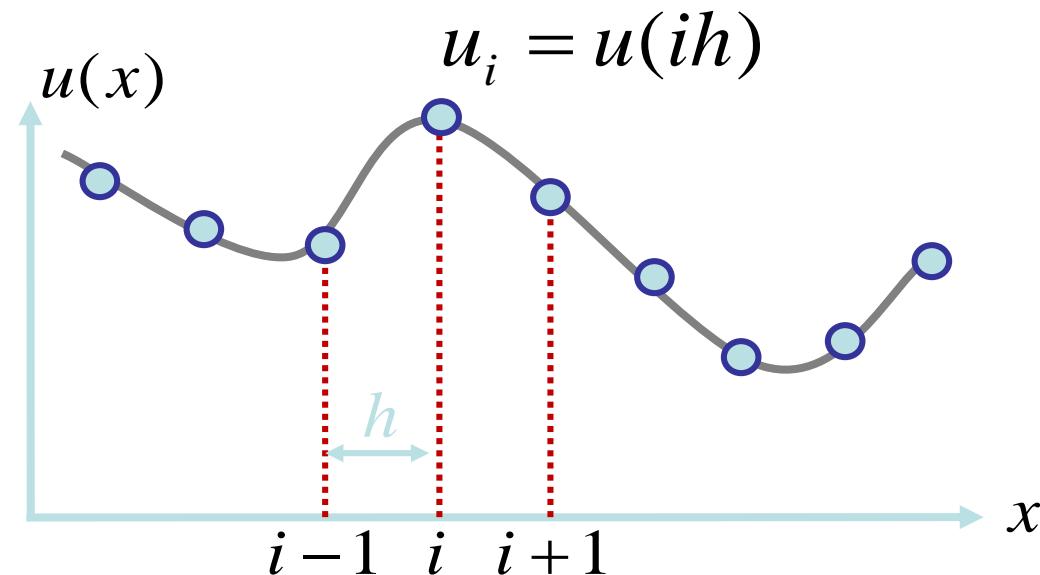
$$D_x u \equiv \frac{u_{i+1} - u_{i-1}}{2h}$$

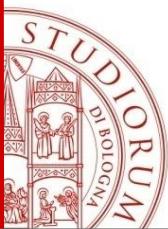
Forward difference

$$D_x^+ u \equiv \frac{u_{i+1} - u_i}{h}$$

Backward difference

$$D_x^- u \equiv \frac{u_i - u_{i-1}}{h}$$





# Local Truncation Error

We write a Taylor expansion of  $u(x)$  about  $x=ih$

$$u_{i+1} = u(ih + h) = u(ih) + hu'(ih) + \frac{1}{2!}h^2u''(ih) + O(h^3)$$

$$u_{i-1} = u(ih - h) = u(ih) - hu'(ih) + \frac{1}{2!}h^2u''(ih) + O(h^3)$$

Second order error term

$$D_x u_i = u'(ih) + O(h^2)$$



First order error terms

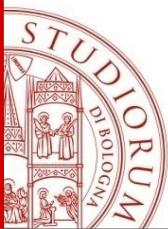
$$D_x^+ u_i = u'(ih) + O(h)$$



$$D_x^- u_i = u'(ih) + O(h)$$



Stencils



# Local Truncation Error

$$D_x u_i = u'(ih) + O(h^2)$$

*Proof*

$$u_{i+1} = u(ih + h) = u(ih) + hu'(ih) + \frac{1}{2!}h^2u''(ih) + \frac{1}{3!}h^3u'''(ih) + O(h^4)$$

$$u_{i-1} = u(ih - h) = u(ih) - hu'(ih) + \frac{1}{2!}h^2u''(ih) - \frac{1}{3!}h^3u'''(ih) + O(h^4)$$

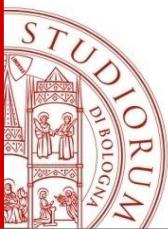
Subtracting these two eqs:

$$u(ih + h) - u(ih - h) = 2hu'(ih) + 2\frac{h^3}{3!}u'''(ih) + O(h^4)$$

$$u'(ih) = \left( \frac{u(ih + h) - u(ih - h)}{2h} \right) + \frac{1}{3!}h^2u''(ih) + O(h^3)$$

Second order error term  $\uparrow$

As the distance  $h$  tends to zero, we expect the approximation to improve.



# Consistency

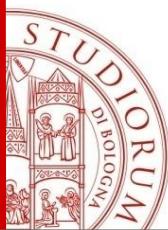
For  $h \rightarrow 0$       LTE approaches to zero

The “speed” in which the error goes to zero as  $h \rightarrow 0$  is called the **rate of convergence**.

When the truncation error is of the order of  $O(h)$ , we say that the method is a first order method. We refer to a method as a **pth-order method** if the truncation error is of the order of  $O(h^p)$

Order of **CONSISTENCY**  $O(h^p)$

Centered scheme ( $O(h^2)$ ) is a more accurate formula than forward or backward ( $O(h)$ ), that is the LTE decreases more rapidly.



# Second Derivative

approximation of the second derivative by  
**Centered Difference formula**

$$D_{xx} u_i = u''(ih) + O(h^2)$$

$$D_{xx} u \equiv \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2}$$

Second order error term

**Proof**

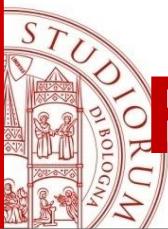
$$u_{i+1} = u(ih + h) = u(ih) + hu'(ih) + \frac{1}{2!}h^2u''(ih) + \frac{1}{3!}h^3u'''(ih) + O(h^4)$$

$$u_{i-1} = u(ih - h) = u(ih) - hu'(ih) + \frac{1}{2!}h^2u''(ih) - \frac{1}{3!}h^3u'''(ih) + O(h^4)$$

Sum of these two eqns:

$$u(ih + h) + u(ih - h) = 2u(ih) + 2\left(\frac{h^2}{2!}u''(ih)\right) + 2\frac{h^4}{4!}u^{iv}(ih) + \dots$$

$$u''(ih) = \left( \frac{u(ih + h) - 2u(ih) + u(ih - h)}{h^2} \right) - \frac{1}{12}h^2u^{(iv)}(ih) + \dots$$



# Finite Difference Formulas for $k>1$

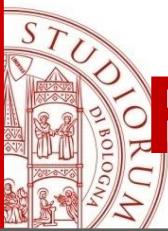
## *Linear Operators*

$$\Delta^1 u(x) = u(ih + h) - u(ih) \quad \text{Forward linear operator}$$

$$\nabla^1 u(x) = u(ih) - u(ih - h) \quad \text{Backward linear operator}$$

$$\delta^1 u(x) = u(ih + \frac{h}{2}) - u(ih - \frac{h}{2}) \quad \text{Centered linear operator}$$

$$\Delta^1 u_i = u_{i+1} - u_i \quad \nabla^1 u_i = u_i - u_{i-1} \quad \delta^1 u_i = u_{i+\frac{1}{2}} - u_{i-\frac{1}{2}}$$



# Finite Difference Formulas for $k>1$

*We define the linear operators of order  $k$  at  $x_i = ih$  as*

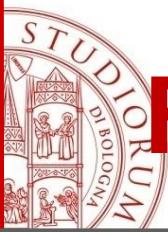
$$\Delta^k u_i = \Delta(\Delta^{k-1} u_i) = \Delta^{k-1} u_{i+1} - \Delta^{k-1} u_i$$

$$\nabla^k u_i = \nabla(\nabla^{k-1} u_i) = \nabla^{k-1} u_i - \nabla^{k-1} u_{i-1}$$

$$\delta^k u_i = \delta(\delta^{k-1} u_i) = \delta^{k-1} u_{i+\frac{1}{2}} - \delta^{k-1} u_{i-\frac{1}{2}}$$

Computing second order centered finite differencing

$$\begin{aligned} D_{xx} u_i &= D^+ D^- u_i \\ &= D^- D^+ u_i \\ &= D_{1/2} D_{1/2} u_i \end{aligned}$$



# Finite Difference Formulas for $k>1$

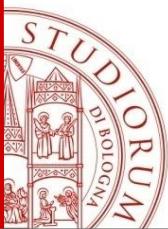
*Theorem*

**Let  $u(x) \in C^k [x_0, x_n]$ ,  $h > 0$ ,  $x_i = x_0 + ih$ ,**  
**then  $\exists \eta \in [x_i, x_i + h]$**

$$u^k(\eta) = \frac{\Delta^k u_i}{h^k}$$

Compute...

$$\delta^4 u_i = u_{i+2} - 4u_{i+1} + 6u_i - 4u_{i-1} + u_{i-2}$$
$$\Rightarrow u^{iv}(x_i) \approx \frac{u(x_{i+2}) - 4u(x_{i+1}) + 6u(x_i) - 4u(x_{i-1}) + u(x_{i-2})}{(h)^4}$$



# Numerical problems

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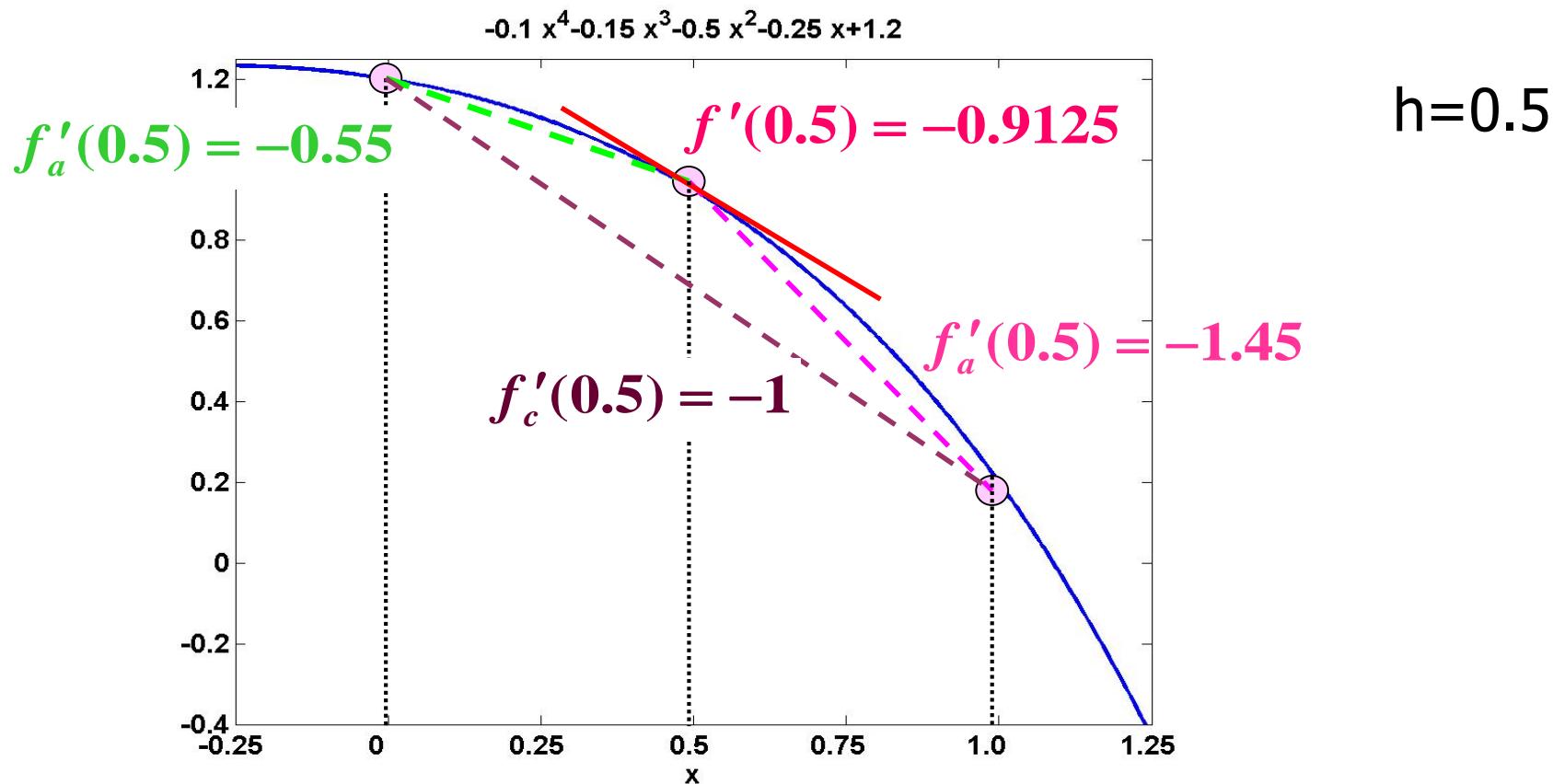
- **Truncation Error:**  
error due to the truncation of the Taylor expansion
- **Rounding error:**  
approximation error in finite arithmetic

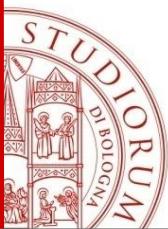
In finite arithmetic a numerical evaluation which uses an arbitrarily small value of  $h$  does not lead to a reduction of total error.

# Example

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

Estimate the first derivative with backward, forward and centered differences at point  $x = 0.5$  (with  $h = 0.5$  and 0.25)





# Example, $h=0.5$

## Forward Difference

$$h = 0.5, f'(0.5) = \frac{f(1) - f(0.5)}{1 - 0.5} = \frac{0.2 - 0.925}{0.5} = -1.45$$

$$\text{relative error } \frac{-1.45 + 0.91250}{-0.91250} = 0.58904$$

## Backward Difference

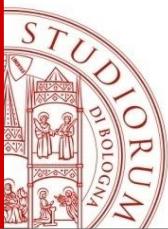
$$h = 0.5, f'(0.5) = \frac{f(0.5) - f(0)}{1 - 0.5} = \frac{0.925 - 1.2}{0.5} = -0.55$$

$$\text{relative error } \frac{-0.55 + 0.91250}{-0.91250} = -0.39726$$

## Centered Difference

$$h = 0.5, f'(0.5) = \frac{f(1) - f(0)}{1 - 0} = \frac{0.2 - 1.2}{1} = -1.0$$

$$\text{relative error } \frac{-1 + 0.91250}{-0.91250} = 0.09589$$



# Example, h=0.25

## Forward Difference

$$f'_a(0.5) = \frac{f(0.75) - f(0.5)}{0.75 - 0.5} = \frac{0.63632813 - 0.925}{0.25} = -1.1547,$$

relative error  $\frac{-1.1547 + 0.91250}{-0.91250} = 0.26541$

## Backward Difference

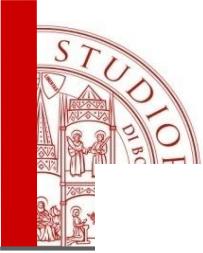
$$f'_i(0.5) = \frac{f(0.5) - f(0.25)}{0.75 - 0.5} = \frac{0.925 - 1.10351563}{0.25} = -0.71406$$

relative error  $\frac{-0.71406 + 0.91250}{-0.91250} = -0.21747$

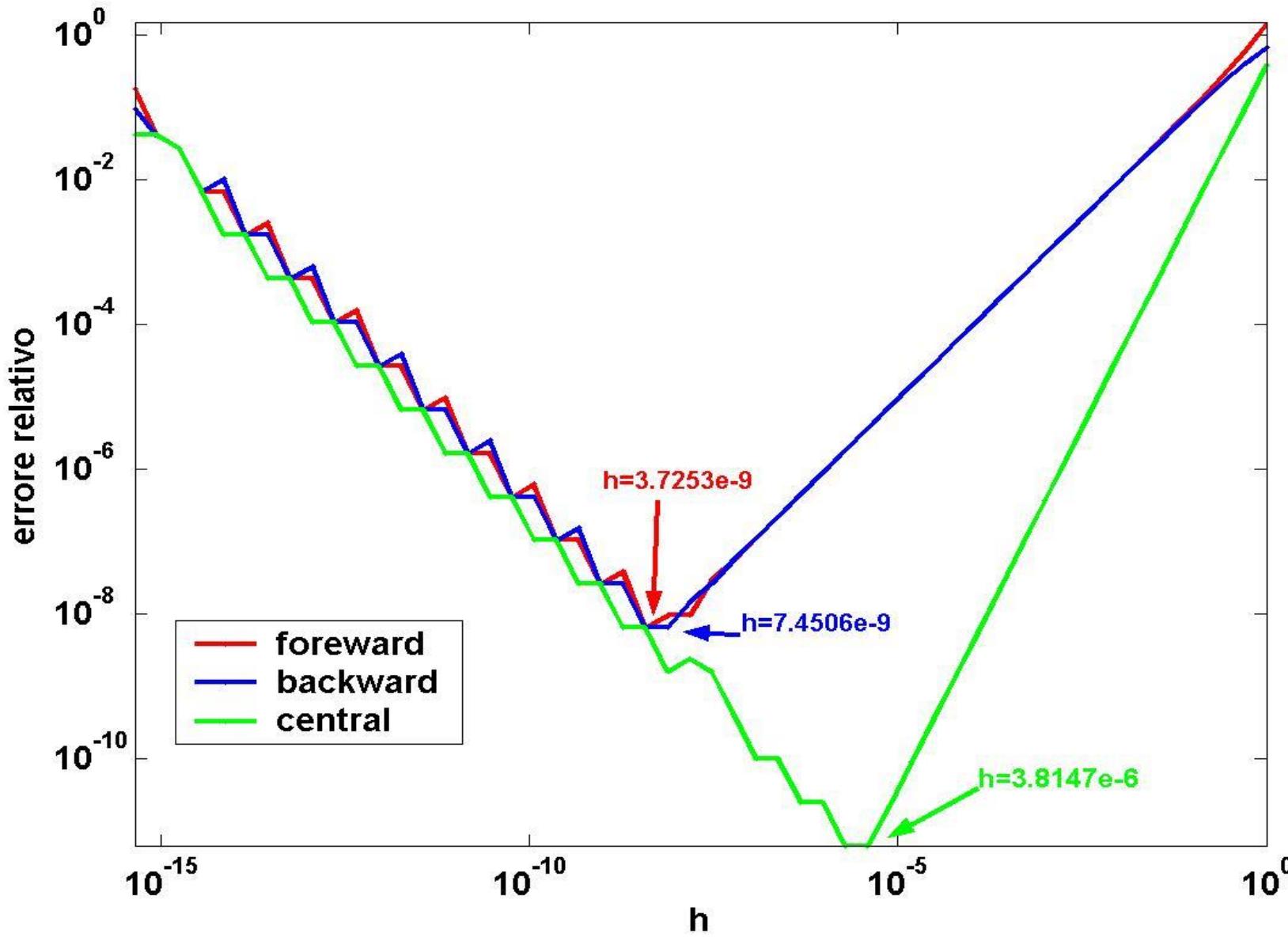
## Centered Difference

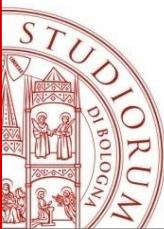
$$f'_c(0.5) = \frac{f(0.75) - f(0.25)}{0.75 - 0.25} = \frac{0.63632813 - 1.10351563}{0.5} = -0.93438$$

relative error  $\frac{-0.93438 + 0.91250}{-0.91250} = 0.023973$



# Relative errors as a function of h



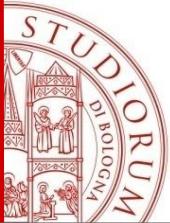


# Remarks

- Rounding errors cause deterioration of the approximation for small values of  $h$ .
- The value of  $h$  which allows a correct evaluation of the formulas depends on the accuracy of the machine.
- If the terms  $f(x_i \pm h)$  are calculated inaccurately then the errors are multiplied by a factor  $1 / h$ , which grows very quickly for small values of  $h$ .

$$\tilde{f}(x_i + h) = f(x_i + h) + \delta \rightarrow \hat{f}'_a(x_i) = \frac{\tilde{f}(x_i + h) - f(x_i)}{h} =$$

**Computed value**  $= \frac{f(x_i + h) - f(x_i)}{h} + \frac{\delta}{h} = f'_a(x_i) + \frac{\delta}{h}$



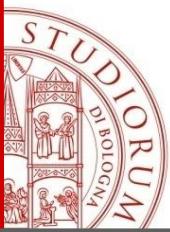
# Differentiation Via Polynomial Interpolation

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The first stage is to construct an interpolating polynomial from the data. An approximation of the derivative at any point can be then obtained by a direct differentiation of the interpolant.

**Example** The Lagrange form of the polynomial interpolation through 3 values  $(x_i, y_i)$  is:

$$\begin{aligned} p(x) &= L_1(x)y_1 + L_2(x)y_2 + L_3(x)y_3 \\ &= \frac{(x - x_2)(x - x_3)}{(x_1 - x_2)(x_1 - x_3)} y_1 + \frac{(x - x_1)(x - x_3)}{(x_2 - x_1)(x_2 - x_3)} y_2 + \frac{(x - x_1)(x - x_2)}{(x_3 - x_2)(x_3 - x_1)} y_3 \end{aligned}$$



## Differentiating the interpolant

$$p'(x) \equiv \frac{2x - x_2 - x_3}{(x_1 - x_2)(x_1 - x_3)} y_1 + \frac{2x - x_1 - x_3}{(x_2 - x_1)(x_2 - x_3)} y_2 + \frac{2x - x_1 - x_2}{(x_3 - x_2)(x_3 - x_1)} y_3$$

Assuming uniform x points

$$p'(x) = \frac{2x - x_2 - x_3}{2\Delta x^2} y_1 + \frac{2x - x_1 - x_3}{-\Delta x^2} y_2 + \frac{2x - x_1 - x_2}{2\Delta x^2} y_3$$

## First derivative of the Lagrange interpolant:

$$p'(x) = \frac{2x - x_2 - x_3}{2\Delta x^2} y_1 + \frac{2x - x_1 - x_3}{-\Delta x^2} y_2 + \frac{2x - x_1 - x_2}{2\Delta x^2} y_3$$

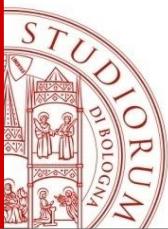
Evaluate the derivative at several points:

$$p'(x_1) = \frac{2x_1 - x_2 - x_3}{2\Delta x^2} y_1 + \frac{2x_1 - x_1 - x_3}{-\Delta x^2} y_2 + \frac{2x_1 - x_1 - x_2}{2\Delta x^2} y_3 = \frac{-3y_1 + 4y_2 - y_3}{2\Delta x}$$

$$p'(x_2) = \frac{2x_2 - x_2 - x_3}{2\Delta x^2} y_1 + \frac{2x_2 - x_1 - x_3}{-\Delta x^2} y_2 + \frac{2x_2 - x_1 - x_2}{2\Delta x^2} y_3 = \frac{y_3 - y_1}{2\Delta x} \quad \text{↗}$$

We get the centered difference formula

$$p'(x_3) = \frac{2x_3 - x_2 - x_3}{2\Delta x^2} y_1 + \frac{2x_3 - x_1 - x_3}{-\Delta x^2} y_2 + \frac{2x_3 - x_1 - x_2}{2\Delta x^2} y_3 = \frac{y_1 - 4y_2 + 3y_3}{2\Delta x}$$



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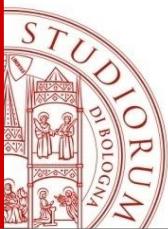
To calculate derivatives with higher order from the Lagrange interpolating polynomial,

$$p'(x) = \frac{2x - x_2 - x_3}{2\Delta x^2} y_1 + \frac{2x - x_1 - x_3}{-\Delta x^2} y_2 + \frac{2x - x_1 - x_2}{2\Delta x^2} y_3$$

differentiate

$$p''(x) = \frac{1}{\Delta x^2} y_1 + \frac{2}{-\Delta x^2} y_2 + \frac{1}{\Delta x^2} y_3 = \frac{y_1 - 2y_2 + y_3}{\Delta x^2}$$

To obtain derivatives of order n the interpolation polynomial must be of degree greater than or equal to n.



# Truncation Error

We know that the interpolation error is

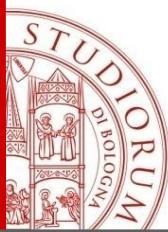
$$f(x) = p(x) + \frac{\Pi_k(x)}{(k+1)!} f^{(k+1)}(\xi) \quad ; \quad \Pi_k(x) = \prod_{i=0}^k (x - x_i)$$

$$f'(x) = p'(x) + \frac{\Pi'_k(x)}{(k+1)!} f^{(k+1)}(\xi) + \frac{\Pi_k(x)}{(k+1)!} \frac{d}{dx} f^{(k+1)}(\xi)$$

if  $x = x_i$  is one of the knots, then  $\Pi_k(x_i) = 0$ :

$$f'(x) = p'(x) + \frac{\Pi'_k(x_i)}{(k+1)!} f^{(k+1)}(\xi)$$

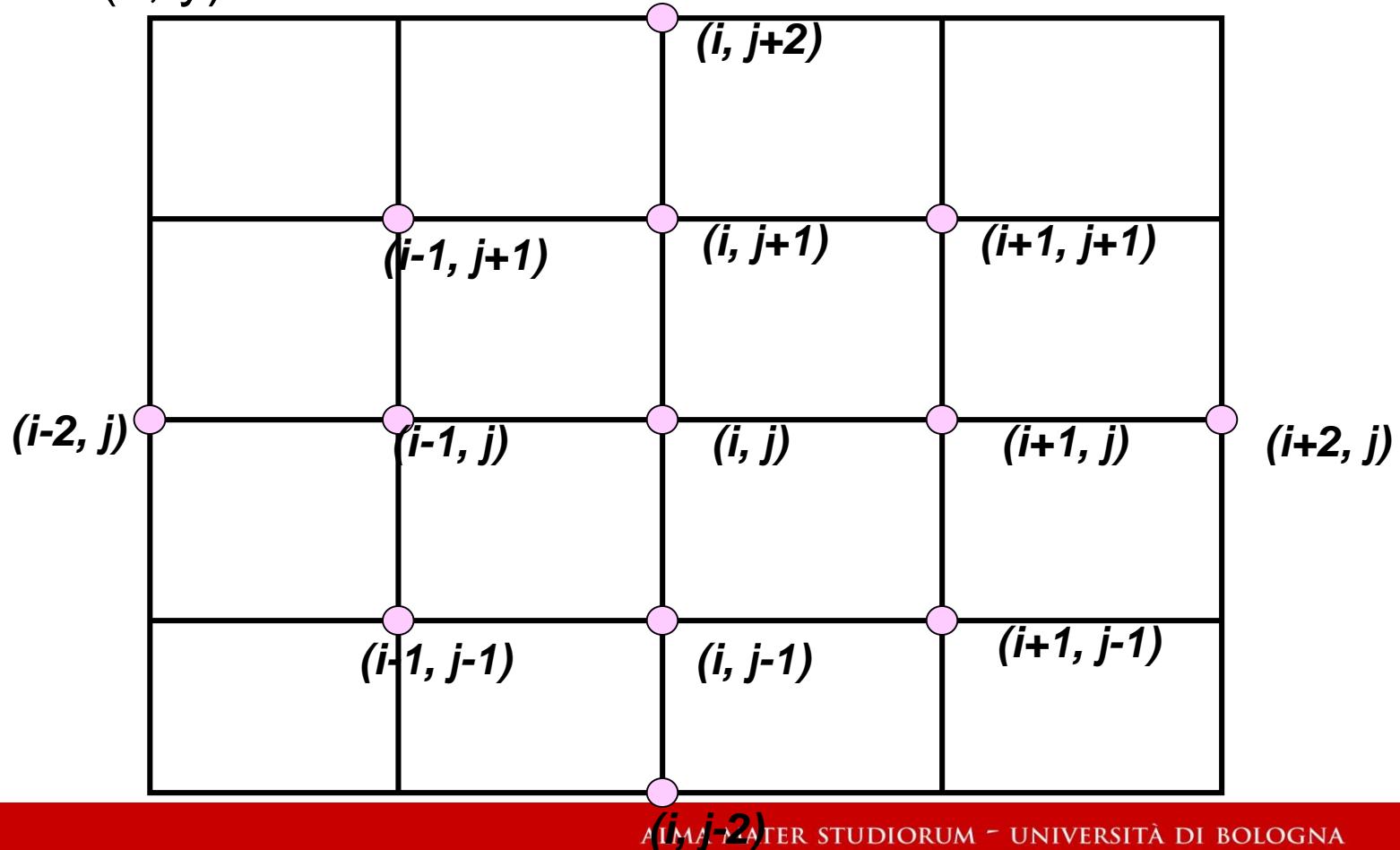
**Truncation Error**



# Partial Derivatives

Extension of the one-dimensional case:

Finite difference formula to approximate partial derivatives of function  $u(x, y)$



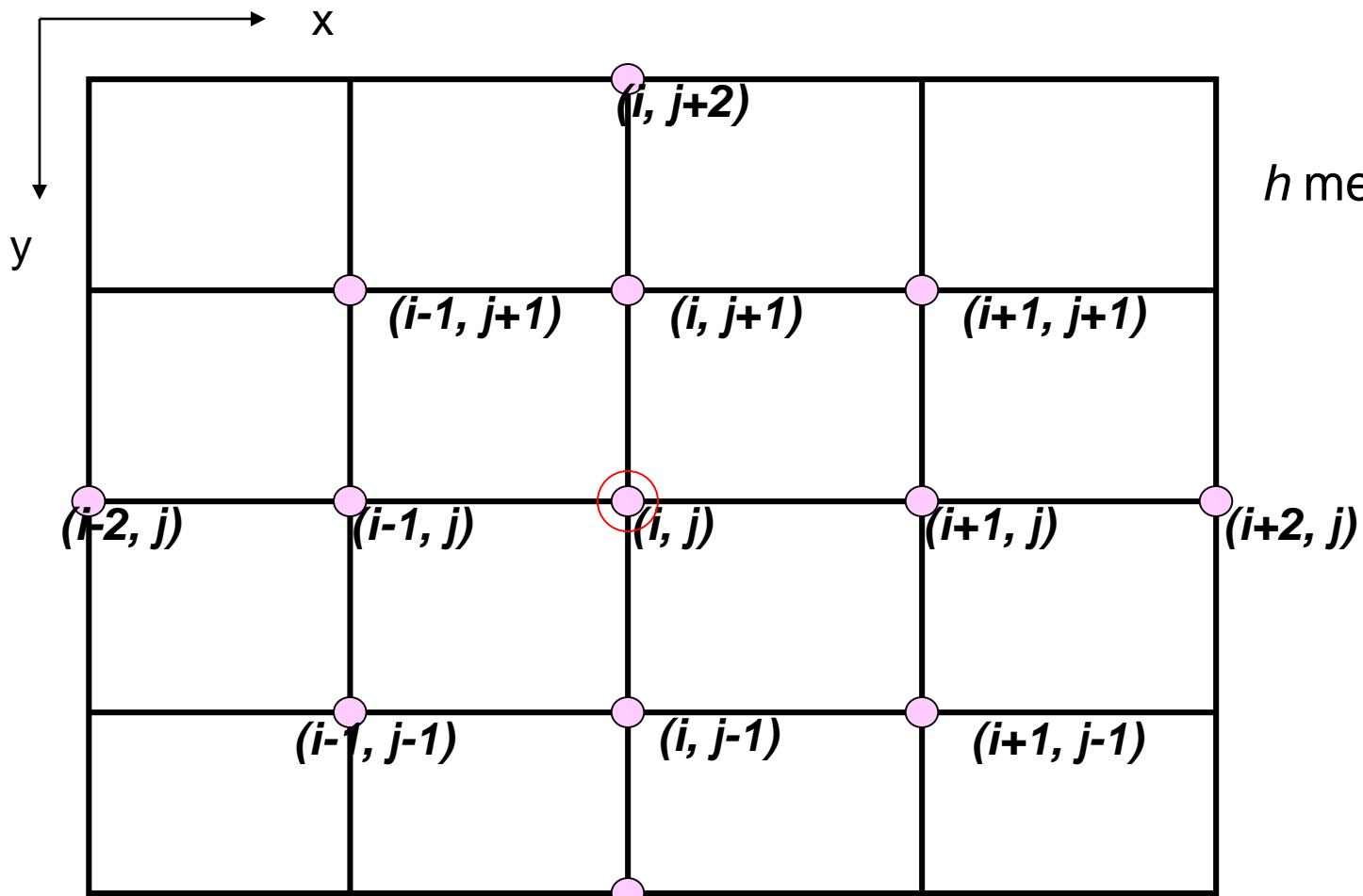
$$u_x = \frac{1}{2h} (-u(x_{i-1}, y_j) + u(x_{i+1}, y_j))$$

➡

$$D_{xx} u \equiv \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2}$$

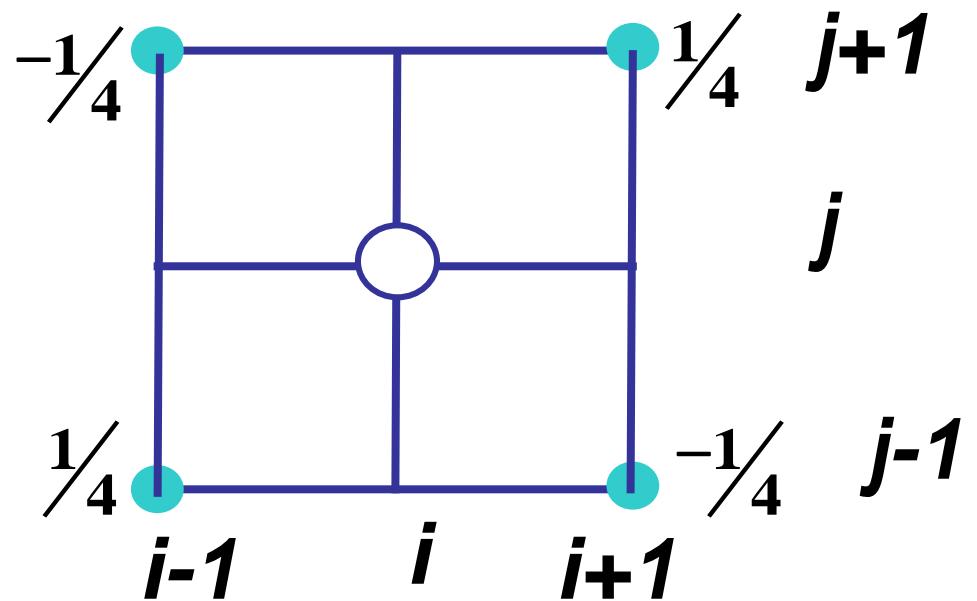
$$u_{xx} = \frac{1}{h^2} (u(x_{i-1}, y_j) - 2u(x_i, y_j) + u(x_{i+1}, y_j))$$

1      -2      1

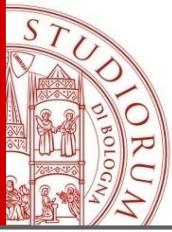


$$u_x = \frac{1}{2h} (u(x_{i+1}, y_j) - u(x_{i-1}, y_j))$$

$$u_{xy} = \frac{\partial}{\partial y} (u_x) = \frac{1}{4kh} (u(x_{i+1}, y_{j+1}) - u(x_{i+1}, y_{j-1}) - u(x_{i-1}, y_{j+1}) + u(x_{i-1}, y_{j-1}))$$

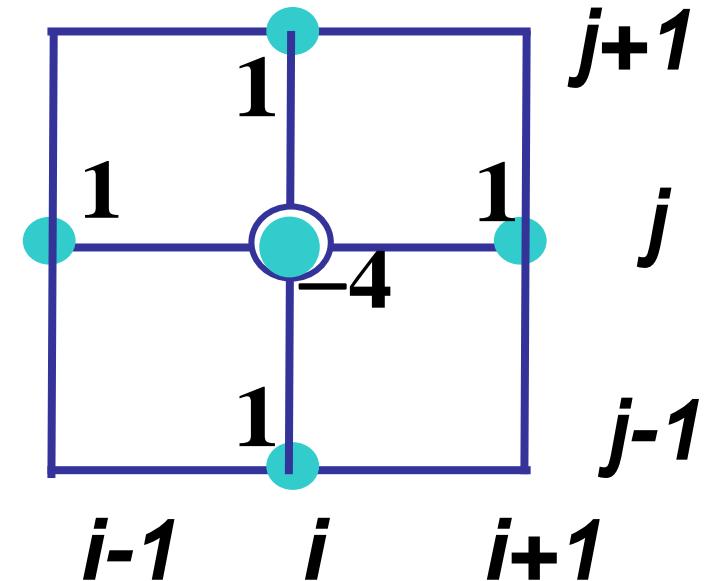


$$D_{xy} u \equiv \frac{u_{i+1,j+1} - u_{i-1,j+1} - u_{i+1,j-1} + u_{i-1,j-1}}{4h^2}$$

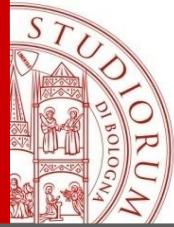


# Laplacian Operator (5-points)

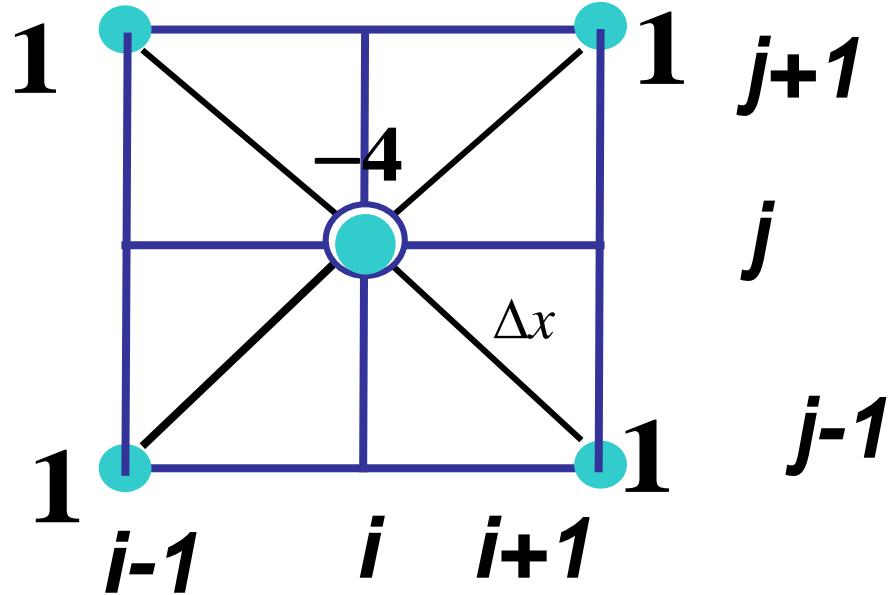
$$\begin{aligned}\nabla^2 u &= u_{xx} + u_{yy} = \\ \approx &\frac{u_{i+1,j} - 2u_{ij} + u_{i-1,j}}{h^2} + \frac{u_{i,j+1} - 2u_{ij} + u_{i,j-1}}{h^2} \\ \approx &\frac{u_{i+1,j} + u_{i,j+1} + u_{i-1,j} + u_{i,j-1}}{h^2} - 4\frac{u_{ij}}{h^2}\end{aligned}$$



*local truncation error O(  $h^2$  )*

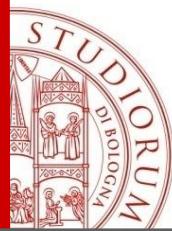


# Laplacian Operator (5-points)

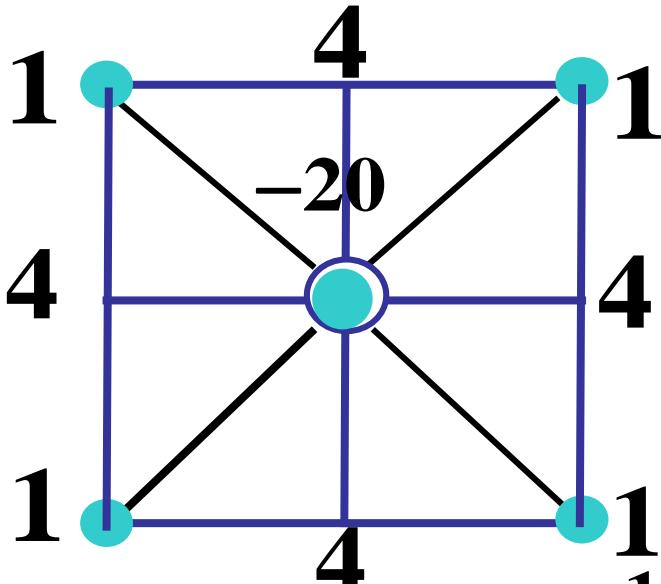


$$\nabla^2 u(x_i, y_j) \approx \frac{u_{i+1,j+1} + u_{i-1,j-1}}{2\Delta x^2} + \frac{u_{i+1,j-1} + u_{i-1,j+1}}{2\Delta x^2} - 4 \frac{u_{ij}}{2\Delta x^2}$$

The local Truncation error for both the approximations is  $O(h^2)$



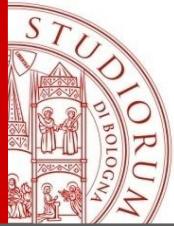
# Laplacian Operator (9-points)



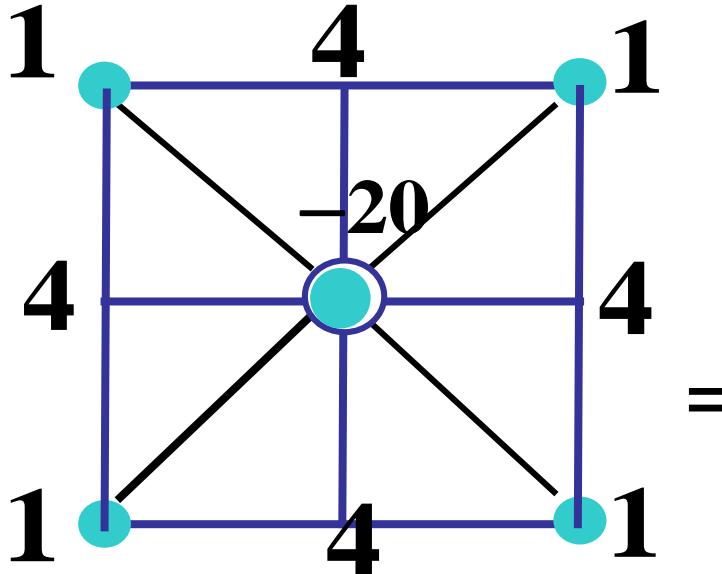
$$\nabla^2 u(x_i, y_j) \approx \frac{1}{6\Delta x^2} \left[ 4u_{i+1,j} + 4u_{i-1,j} + 4u_{i,j-1} + 4u_{i,j+1} + u_{i-1,j-1} + u_{i-1,j+1} + u_{i+1,j-1} + u_{i+1,j+1} - 20u_{ij} \right]$$

The local Truncation Error is  $O(h^2)$

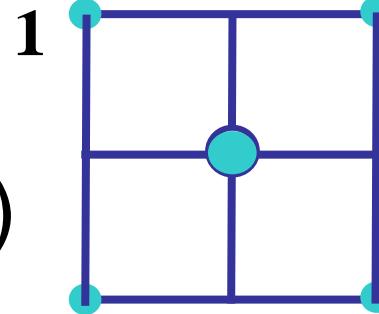
$$\nabla_9^2 u(x_i, y_j) \approx \nabla^2 u + \frac{h^2}{2} (u_{xxxx} + 2u_{xxyy} + u_{yyyy}) + O(h^4)$$



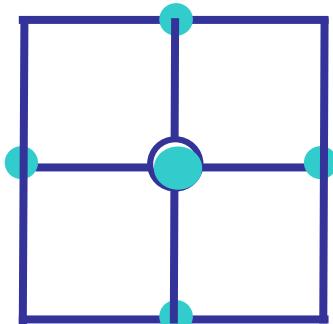
# Laplacian Operator (9-points)



$$= (1 - a)$$



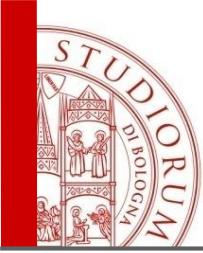
$$+ a/2$$



$a = 1/3$  is the only value of  $a$  which yields a higher order of accuracy for the Laplacian

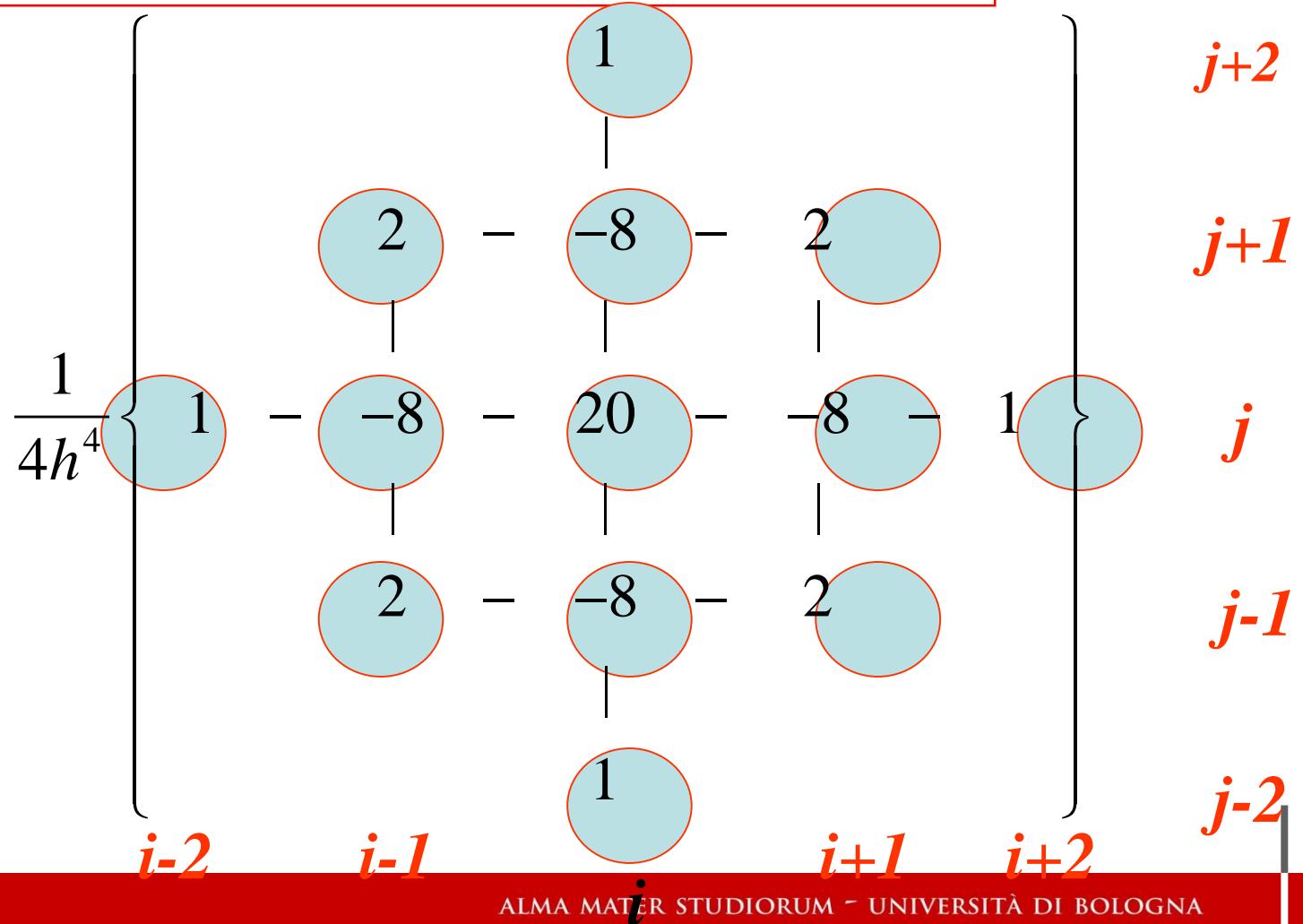
$$\begin{aligned} \nabla^2 u(x_i, y_j) \approx & \frac{1}{6\Delta x^2} \left[ 4u_{i+1,j} + 4u_{i-1,j} + 4u_{i,j-1} + 4u_{i,j+1} \right. \\ & \left. + u_{i-1,j-1} + u_{i-1,j+1} + u_{i+1,j-1} + u_{i+1,j+1} - 20u_{ij} \right] \end{aligned}$$

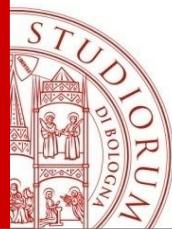
The local Truncation Error is  $O(h^2)$



# Biharmonic operator

$$\nabla^4 u = (\nabla^2 u)^2 = \frac{\partial^4 u}{\partial x^4} + 2 \frac{\partial^2 u}{\partial x^2 \partial y^2} + \frac{\partial^4 u}{\partial y^4} \approx$$





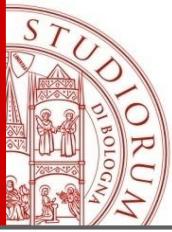
# Divergence Operator (1)

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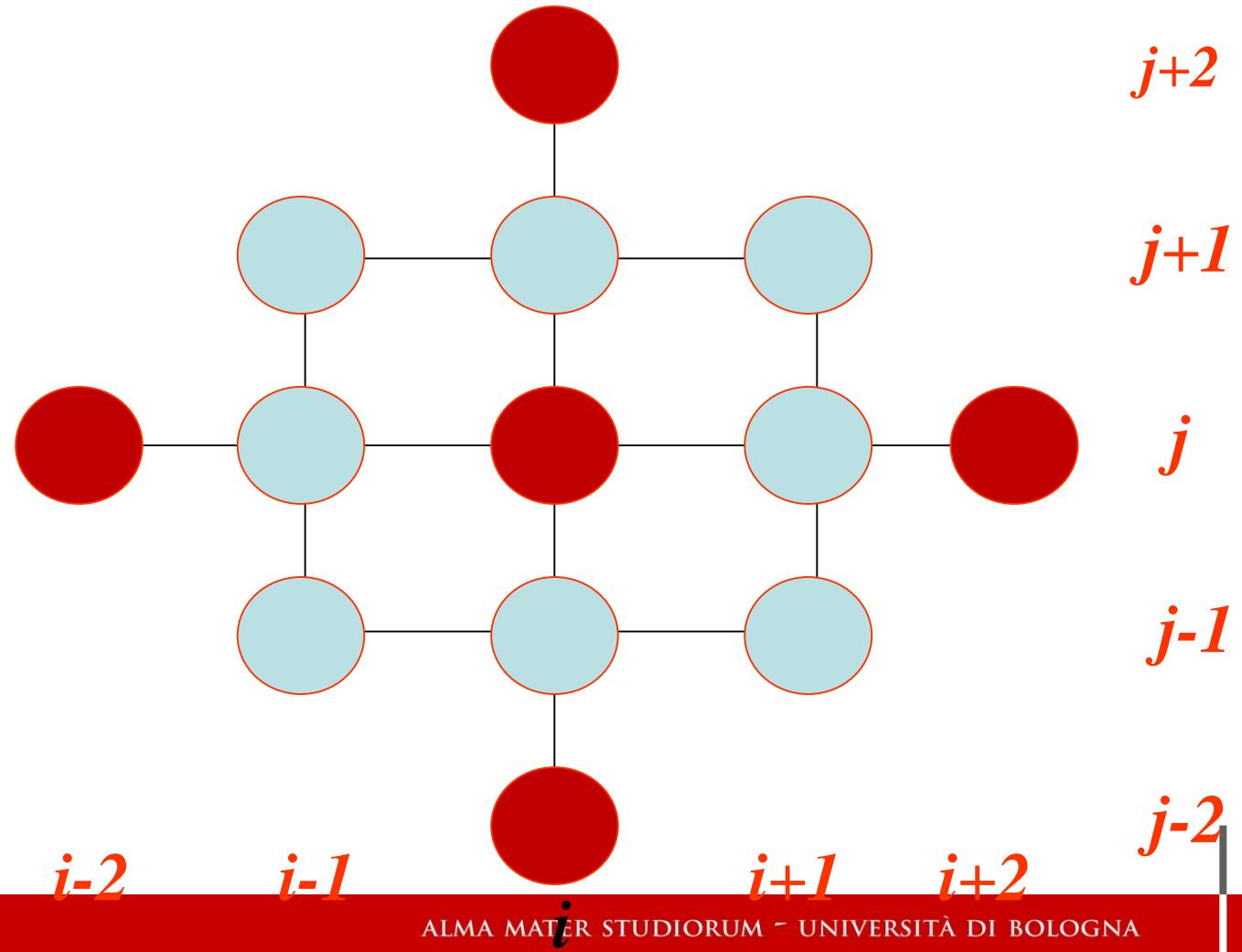
$$\operatorname{div}(b\nabla u) = \frac{\partial}{\partial x} \left( b \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left( b \frac{\partial u}{\partial y} \right)$$

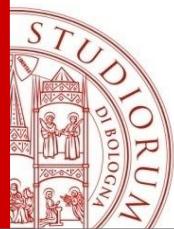
$$\operatorname{div}(b\nabla u) \approx \delta_x(b_{i,j}\delta_x u_{i,j}) + \delta_y(b_{i,j}\delta_y u_{i,j})$$

$$\begin{aligned} &\approx \frac{b_{i+1,j}u_{i+2,j} + b_{i-1,j}u_{i-2,j} + b_{i,j+1}u_{i,j+2} + b_{i,j-1}u_{i,j-2}}{4h^2} \\ &\quad - \frac{(b_{i+1,j} + b_{i-1,j} + b_{i,j+1} + b_{i,j-1})u_{ij}}{4h^2} \end{aligned}$$



# Divergence Operator





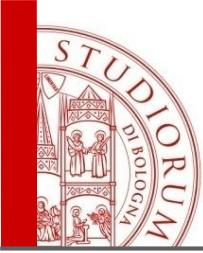
# Divergence Operator (2)

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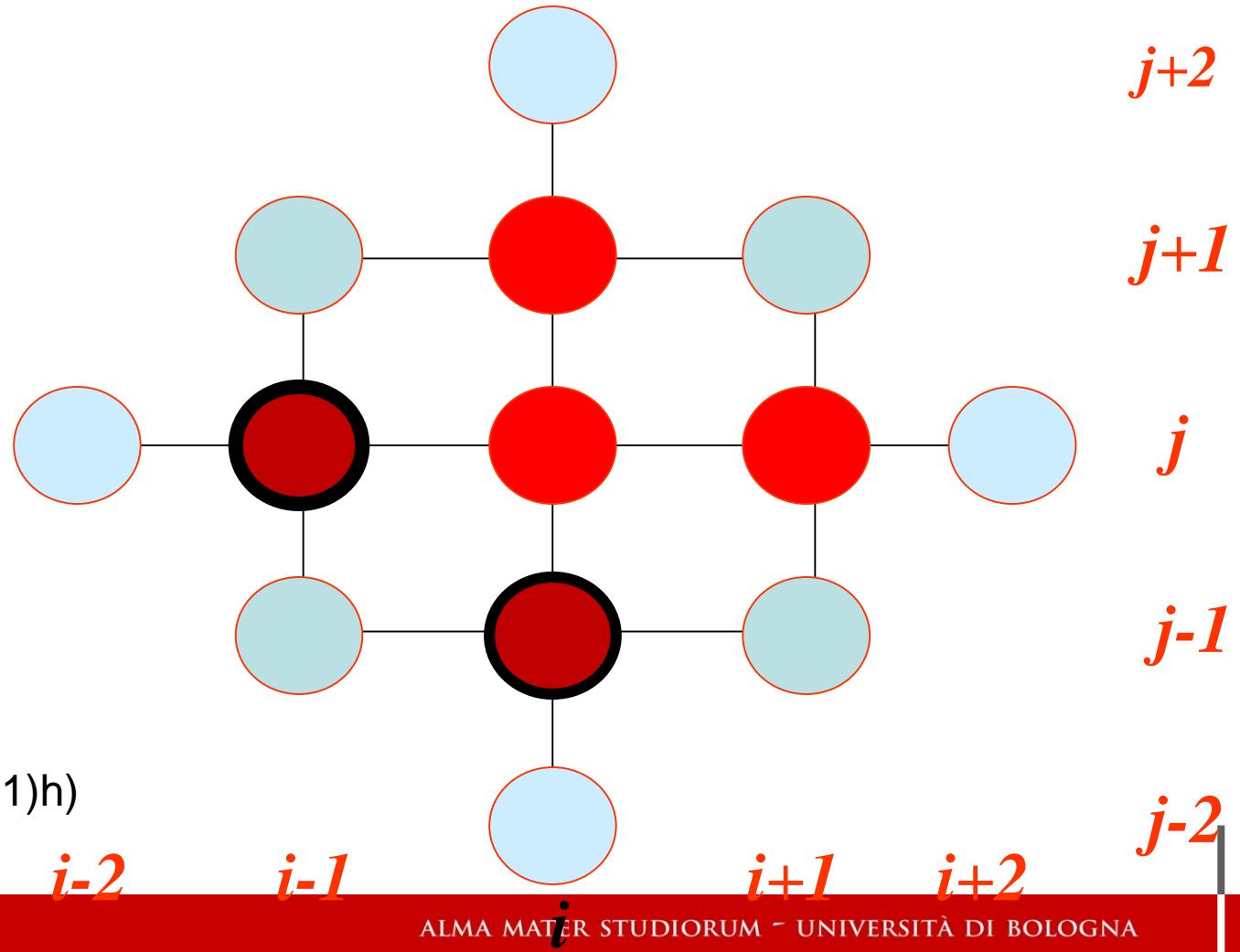
$$\operatorname{div}(b\nabla u) = \frac{\partial}{\partial x} \left( b \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left( b \frac{\partial u}{\partial y} \right)$$

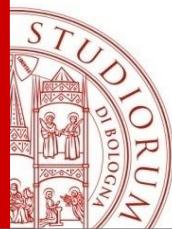
$$\operatorname{div}(b\nabla u) \approx D_x^+(b_{i,j}D_x^-u_{i,j}) + D_y^+(b_{i,j}D_y^-u_{i,j})$$

$$\begin{aligned} &\approx \frac{b_{i+1,j}u_{i+1,j} + b_{i,j}u_{i-1,j} + b_{i,j+1}u_{i,j+1} + b_{i,j}u_{i,j-1}}{h^2} \\ &- \frac{(b_{i+1,j} + b_{i,j+1} + 2b_{i,j})u_{ij}}{h^2} \end{aligned}$$



# Divergence Operator





# Divergence Operator (3)

$$\operatorname{div}(b\nabla u) = \frac{\partial}{\partial x} \left( b \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left( b \frac{\partial u}{\partial y} \right)$$

$$\delta_x^* = \frac{u_{i+\frac{1}{2},j} - u_{i-\frac{1}{2},j}}{h} \quad \delta_y^* = \frac{u_{i,j+\frac{1}{2}} - u_{i,j-\frac{1}{2}}}{h}$$

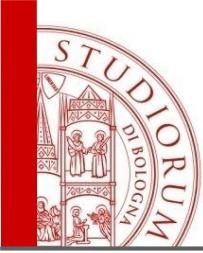
$$\operatorname{div}(b\nabla u) \approx \delta_x^*(b_{i,j}\delta_x^*u_{i,j}) + \delta_y^*(b_{i,j}\delta_y^*u_{i,j})$$

$$\approx \frac{b_{+0,j}u_{i+1,j} + b_{-0}u_{i-1,j} + b_{0+}u_{i,j+1} + b_{0-}u_{i,j-1}}{h^2} - \frac{(b_{+0} + b_{-0} + b_{0+} + b_{0-})u_{ij}}{h^2}$$

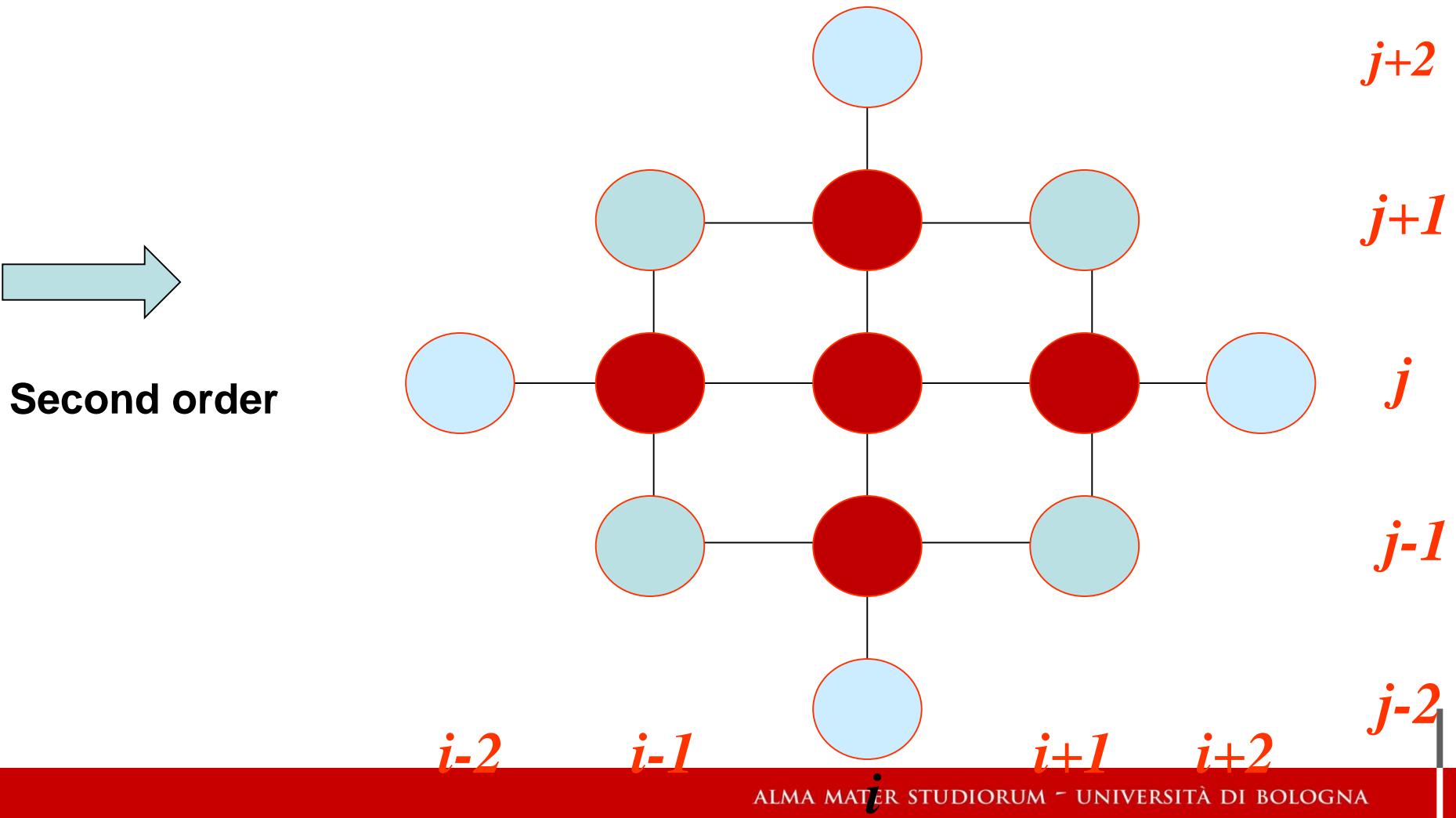
where

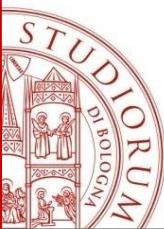
$$b_{\pm 0} = b_{i \pm \frac{1}{2}, j} \quad e \quad b_{0\pm} = b_{i, j \pm \frac{1}{2}}$$

Interpolated Values



# Divergence Operator

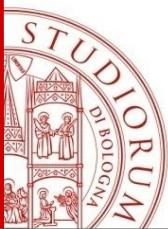




# Remarks

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- To increase the order of accuracy of the formulas is necessary to increase the number of points involved in the calculation.
- Higher precision is equivalent to a higher computational complexity.
- To achieve greater accuracy without increasing the order of the formulas we can use extrapolation techniques such as that of Richardson.

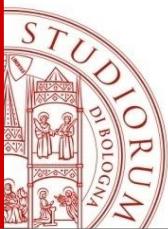


# Richardson's Extrapolation

This technique uses the concept of grids with variable amplitude step procedure for improving the accuracy of approximations.

Example in which we show how to turn a **second-order approximation of the second derivative** into a fourth order approximation of the same quantity

$$f''(x_i) = \left( \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{\Delta x^2} \right) + a_1 \Delta x^2 + a_2 \Delta x^4 + \dots$$



# Richardson's Extrapolation

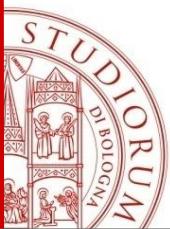
second-order approximation of the second-derivative:

$$f''(x_i) = \left( \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{\Delta x^2} \right) + a_1 \Delta x^2 + a_2 \Delta x^4 + \dots$$

We write the equation for grids of different sizes

$$f''(x_i) = F(\Delta x) + a_1 \Delta x^2 + a_2 \Delta x^4 + \dots$$

$$f''(x_i) = F\left(\frac{\Delta x}{2}\right) + a_1\left(\frac{\Delta x}{2}\right)^2 + a_2\left(\frac{\Delta x}{2}\right)^4 + \dots$$

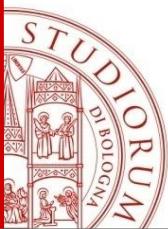


# Richardson's Extrapolation

This, of course, is still a second-order approximation of the derivative. However, the idea is to combine [1] with [2] such that the  $\Delta x^2$  term in the error vanishes.

$$f''(x_i) = F(\Delta x) + a_1 \Delta x^2 + a_2 \Delta x^4 + \dots \quad [1]$$

$$f''(x_i) = F\left(\frac{\Delta x}{2}\right) + a_1\left(\frac{\Delta x^2}{4}\right) + a_2\left(\frac{\Delta x^4}{16}\right) + \dots \quad [2]$$



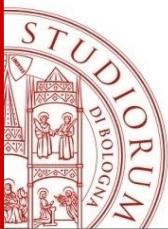
# Richardson's Extrapolation

Indeed, multiplying eq.[2] by 4 and subtracting [1] from [2]

$$4f''(x_i) = 4F\left(\frac{\Delta x}{2}\right) + 4a_1\left(\frac{\Delta x^2}{4}\right) + 4a_2\left(\frac{\Delta x^4}{16}\right) + \dots$$
$$-f''(x_i) = -F(\Delta x) - a_1\Delta x^2 - a_2\Delta x^4 + \dots$$

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$$3f''(x_i) = 4F\left(\frac{\Delta x}{2}\right) - F(\Delta x) - 12a_2\left(\frac{\Delta x^4}{16}\right) + \dots$$

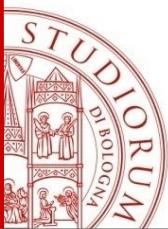


# Richardson's Extrapolation

The equation can be rewritten as:

$$f''(x_i) = \left( \frac{4F\left(\frac{\Delta x}{2}\right) - F(\Delta x)}{3} \right) - a_2 \left( \frac{\Delta x^4}{4} \right) + \dots$$

The accuracy of the new estimation of  $f''(x_i)$  is  $O(\Delta x^4)$  instead of  $O(\Delta x^2)$

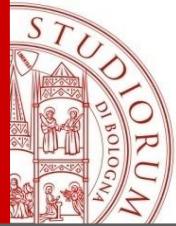


# Richardson's Extrapolation

We can continue to eliminate higher order terms of the error using a grid even finer:

$$f''(x_i) = B(\Delta x) + b_1 \Delta x^4 + b_2 \Delta x^6 + \dots$$

$$f''(x_i) = \left( \frac{16B\left(\frac{\Delta x}{2}\right) - B(\Delta x)}{15} \right) + O(\Delta x^6) + \dots$$



# Richardson's Extrapolation example

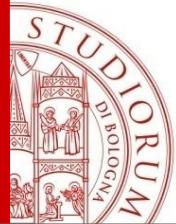
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Given the function

$$f(x) = x^3 - 2x^2 + 4x - 8$$

Find the first derivative at  $x=1.25$  using a centered difference formula and step  $\Delta h = 0.25$ .

$$f'(x) = 3x^2 - 4x + 4 = 3(1.25)^2 - 4(1.25) + 4 = 3.6875$$



# Richardson's Extrapolation example

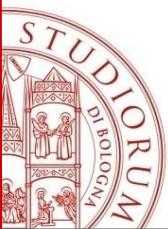
Given the discrete data set:

x	f(x)
1	-5
1.125	-4.607
1.25	-4.172
1.375	-3.682
1.5	-3.125

Compute first derivatives using centered differencing

$$F(\Delta x) \approx f'(1.25) = \frac{f(1.5) - f(1.0)}{2(0.25)} = \frac{-3.125 + 5}{0.5} = 3.75$$

$$F(\Delta x/2) \approx f'(1.25) = \frac{f(1.375) - f(1.125)}{2(0.125)} = \frac{-3.6816 + 4.6074}{0.25} = 3.7032$$



# Richardson's Extrapolation example

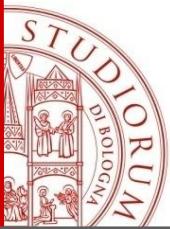
Compute the error with the exact first derivatives:

$$F(\Delta x) \approx f'(1.25) = 3.75 \quad \text{Error} = 1.69\%$$

$$F\left(\frac{\Delta x}{2}\right) \approx f'(1.25) = 3.7032 \quad \text{Error} = 0.425\%$$

Apply Richardson's extrapolation using these results to find a better solution

$$f'(1.25) = \frac{4F\left(\frac{\Delta x}{2}\right) - F(\Delta x)}{3} = \frac{4(3.7032) - 3.75}{3} = 3.6876 \quad \text{Error} = 0.003\%$$



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