Numerical Differentiation

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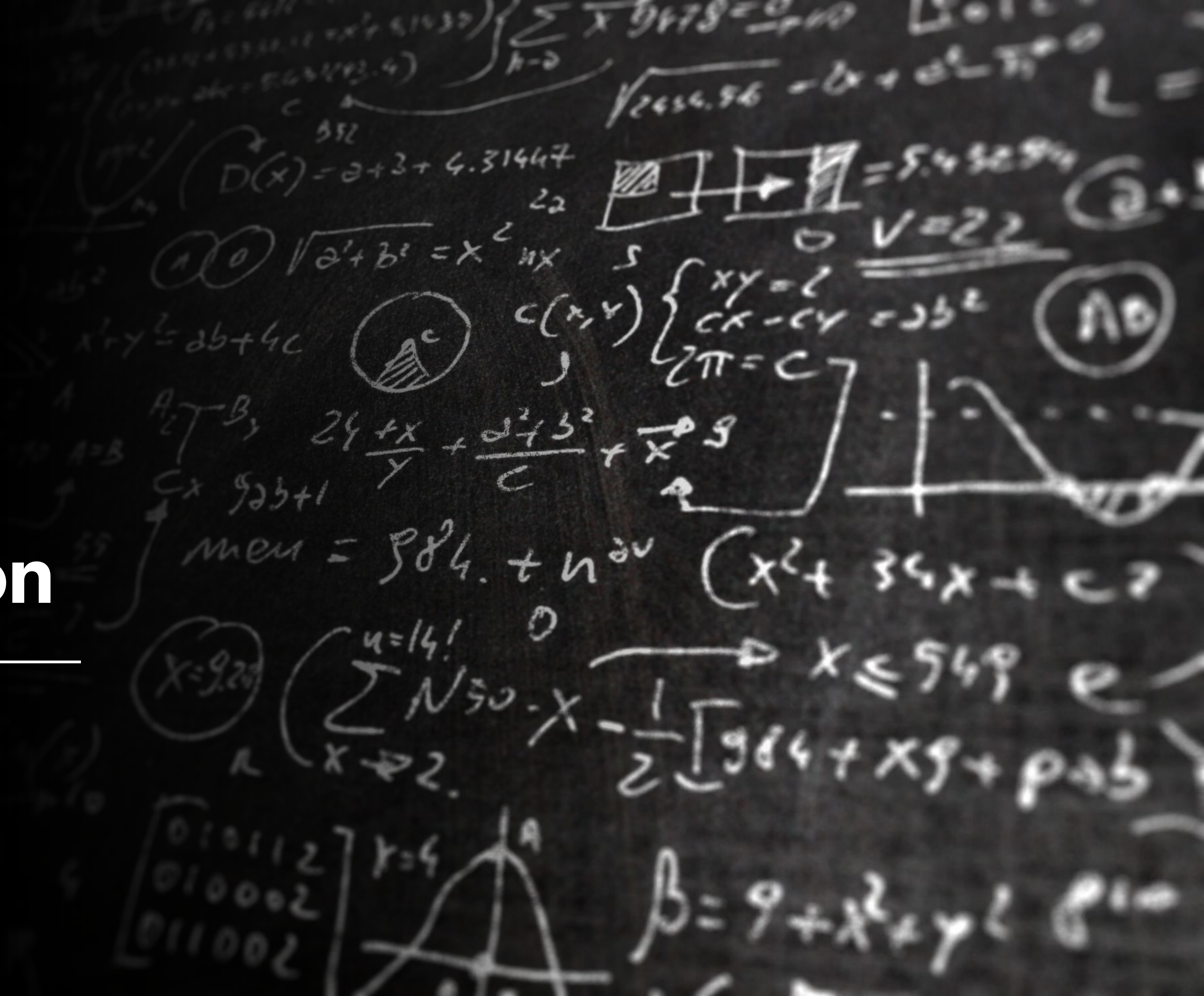

Capaian Pembelajaran

- Mahasiswa mampu menerapkan **metode numerik** (Euler, Taylor dan Rung-kutta) untuk penyelesaian persamaan **diferensial dan integral tertentu**

Numerical Differentiation

- Estimate the derivatives (slope, curvature, etc.) of a function by using the function values at only a set of discrete points
- Ordinary differential equation (ODE)
- Partial differential equation (PDE)

Euler’s Method

$$\frac{dy}{dx} = f(x, y), y(0) = y_0$$

$$\text{Slope} = \frac{Rise}{Run}$$

$$= \frac{y_1 - y_0}{x_1 - x_0}$$

$$= f(x_0, y_0)$$

$$y_1 = y_0 + f(x_0, y_0)(x_1 - x_0)$$

$$= y_0 + f(x_0, y_0)h$$

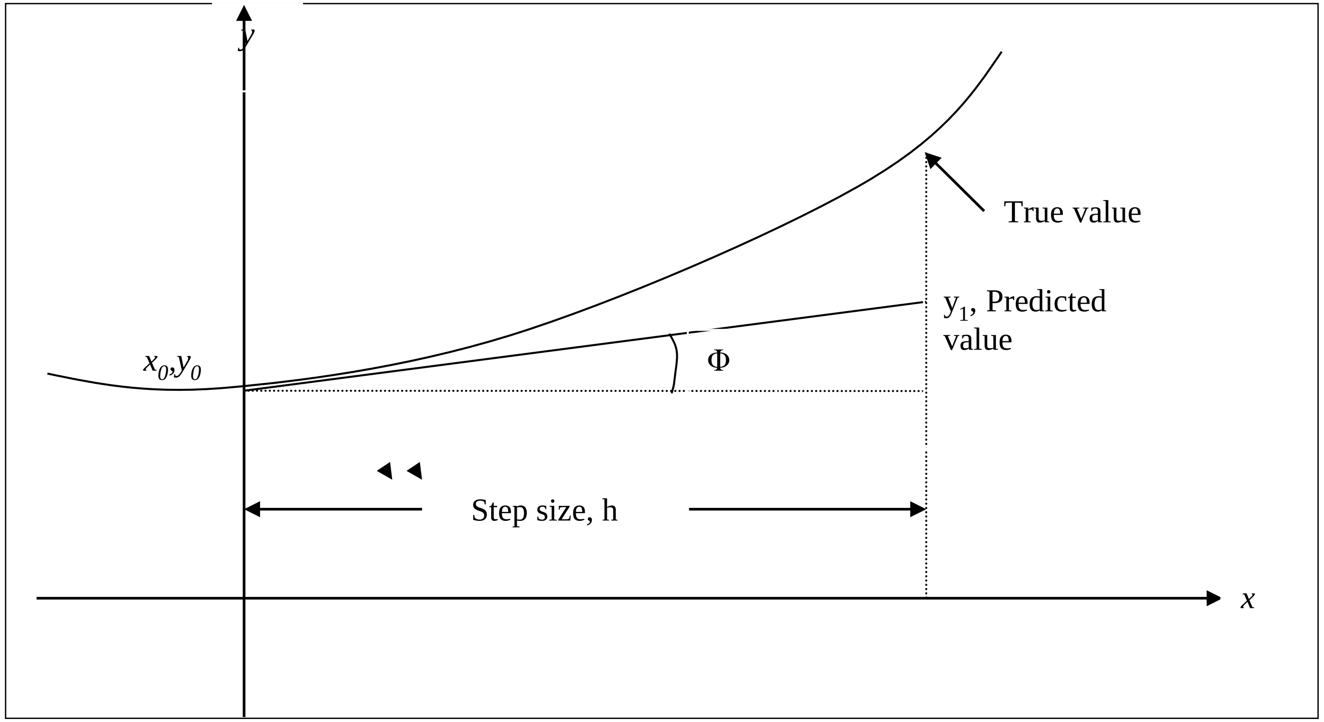

Figure 1 Graphical interpretation of the first step of Euler’s method

Euler's Method

$$y_{i+1} = y_i + f(x_i, y_i)h$$

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

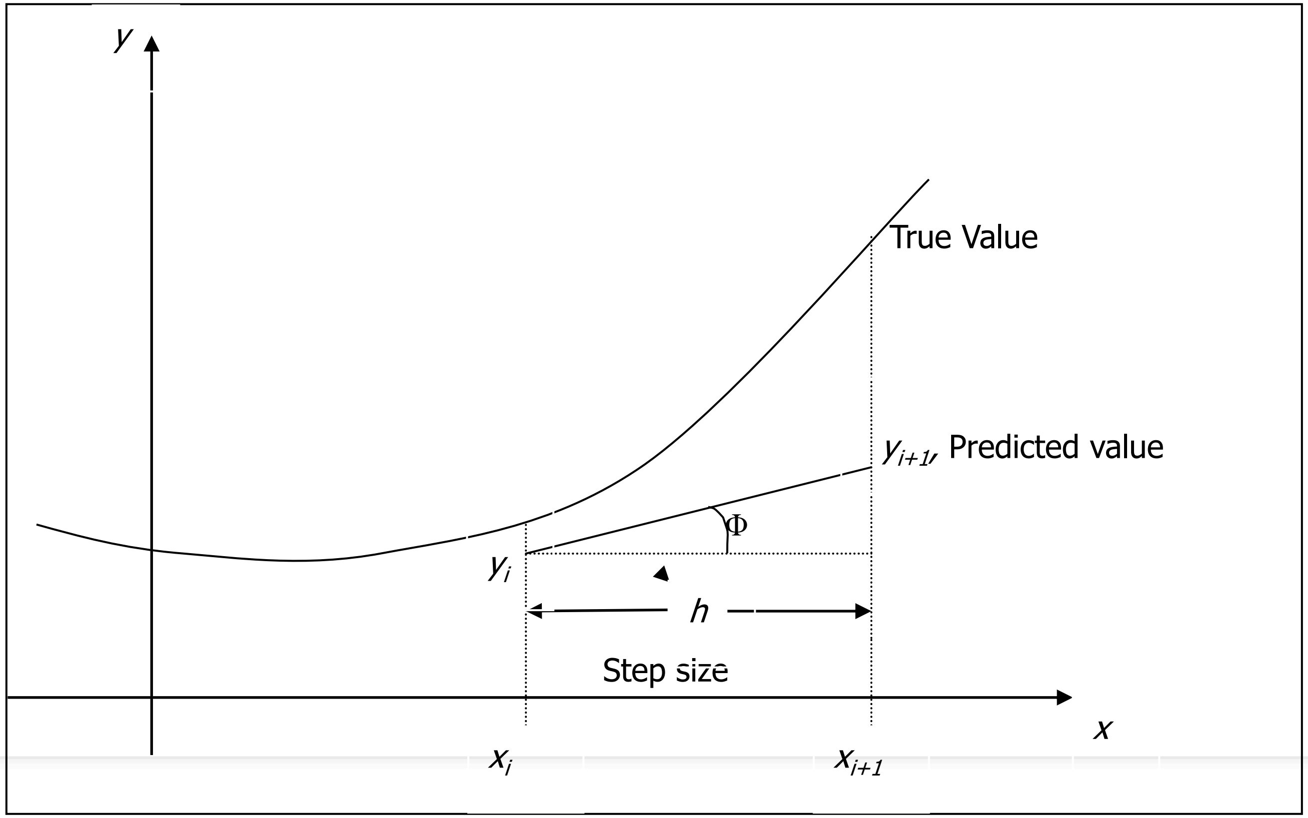

Figure 2. General graphical interpretation of Euler's method

How to write Ordinary Differential Equation

How does one write a first order differential equation in the form of

$$\frac{dy}{dx} = f(x, y)$$

Example

$$\frac{dy}{dx} + 2y = 1.3e^{-x}, y(0) = 5$$

is rewritten as

$$\frac{dy}{dx} = 1.3e^{-x} - 2y, y(0) = 5$$

In this case

$$f(x, y) = 1.3e^{-x} - 2y$$

Example

A ball at 1200K is allowed to cool down in air at an ambient temperature of 300K. Assuming heat is lost only due to radiation, the differential equation for the temperature of the ball is given by

$$\frac{d\theta}{dt} = -2.2067 \times 10^{-12}\left(\theta^4 - 81 \times 10^8\right), \theta(0) = 1200K$$

Find the temperature at $t = 480$ seconds using Euler's method. Assume a step size of $h = 240$ seconds.

Step 1:

$$\frac{d\theta}{dt} = -2.2067\times10^{-12}\left(\theta^4 - 81\times10^8\right)$$

$$f(t,\theta) = -2.2067\times10^{-12}\left(\theta^4 - 81\times10^8\right)$$

$$\theta_{i+1} = \theta_i + f(t_i,\theta_i)h$$

$$\begin{aligned}\theta_1 &= \theta_0 + f(t_0,\theta_0)h \\ &= 1200 + f(0,1200)240 \\ &= 1200 + \left(-2.2067\times10^{-12}\left(1200^4 - 81\times10^8\right)\right)240 \\ &= 1200 + (-4.5579)240 \\ &= 106.09K\end{aligned}$$

θ_1 is the approximate temperature at $t = t_1 = t_0 + h = 0 + 240 = 240$

$$\theta(240) \approx \theta_1 = 106.09K$$

Step 2: For $i = 1, \quad t_1 = 240, \quad \theta_1 = 106.09$

$$\begin{aligned}
\theta_2 &= \theta_1 + f(t_1, \theta_1)h \\
&= 106.09 + f(240, 106.09)240 \\
&= 106.09 + \left(-2.2067 \times 10^{-12}\left(106.09^4 - 81 \times 10^8\right)\right)240 \\
&= 106.09 + (0.017595)240 \\
&= 110.32K
\end{aligned}$$

θ_2 is the approximate temperature at $t = t_2 = t_1 + h = 240 + 240 = 480$

$$\theta(480) \approx \theta_2 = 110.32K$$

The exact solution of the ordinary differential equation is given by the solution of a non-linear equation as

$$0.92593\ln\frac{\theta-300}{\theta+300}-1.8519\tan^{-1}\left(0.00333\theta\right)=-0.22067\times10^{-3}t-2.9282$$

The solution to this nonlinear equation at t=480 seconds is

$$\theta(480)=647.57K$$

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Comparison of Exact and Numerical Solutions

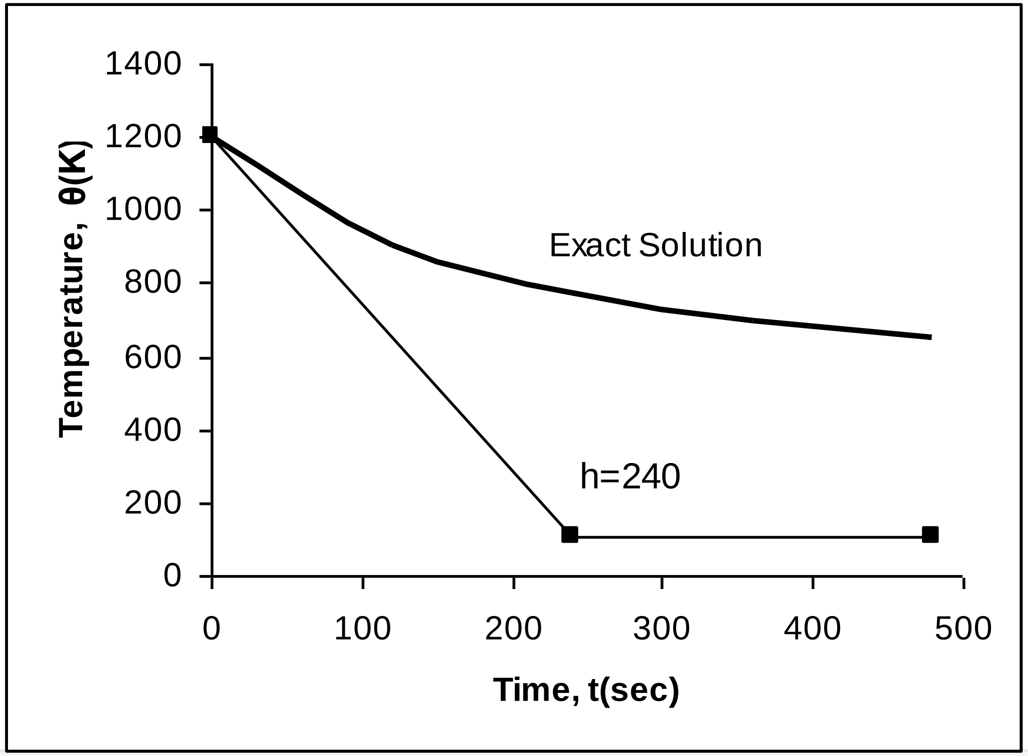


Figure 3. Comparing exact and Euler's method

Table 1. Temperature at 480 seconds as a function of step size, h

Step, h	$\theta(480)$	E_t	$\lvert\epsilon_t\rvert\%$
480	−987.81	1635.4	252.54
240	110.32	537.26	82.964
120	546.77	100.80	15.566
60	614.97	32.607	5.0352
30	632.77	14.806	2.2864

$\theta(480) = 647.57K$ (exact)

Comparison with exact results

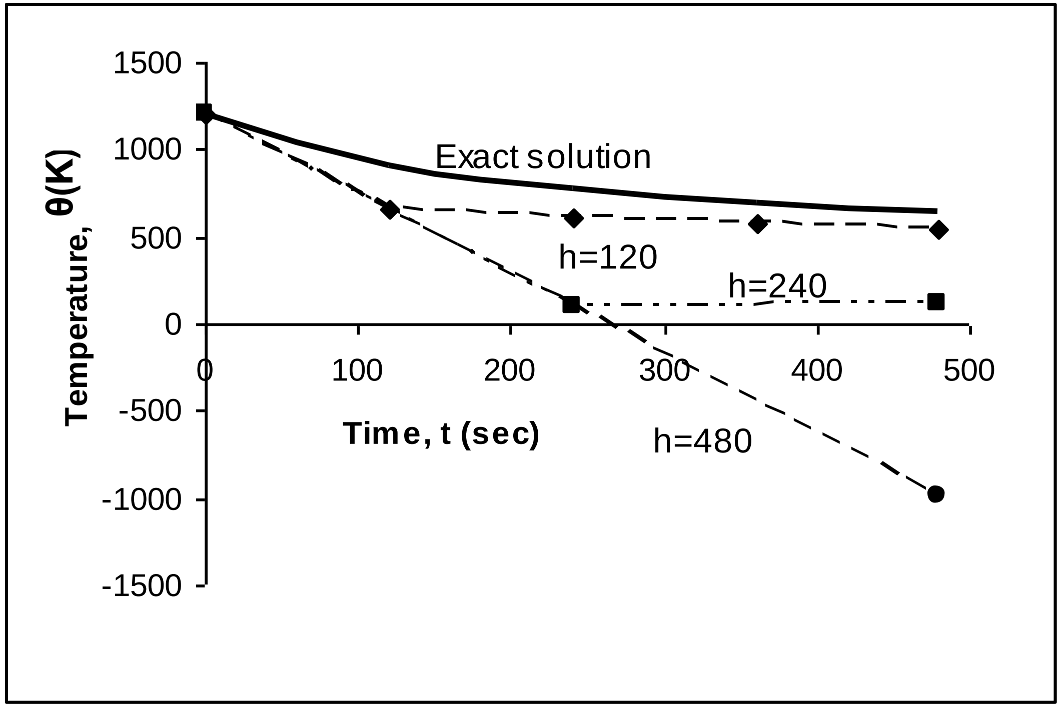


Figure 4. Comparison of Euler's method with exact solution for different step sizes

Errors in Euler's Method

It can be seen that Euler's method has large errors. This can be illustrated using Taylor series.

$$y_{i+1} = y_i + \left.\frac{dy}{dx}\right|_{x_i, y_i} (x_{i+1} - x_i) + \frac{1}{2!}\left.\frac{d^2y}{dx^2}\right|_{x_i, y_i} (x_{i+1} - x_i)^2 + \frac{1}{3!}\left.\frac{d^3y}{dx^3}\right|_{x_i, y_i} (x_{i+1} - x_i)^3 + \ldots$$

As you can see the first two terms of the Taylor series

$y_{i+1} = y_i + f(x_i, y_i)h$ are the Euler's method.

The true error in the approximation is given by

$$E_t = \frac{f'(x_i, y_i)}{2!}h^2 + \frac{f''(x_i, y_i)}{3!}h^3 + \ldots \qquad E_t \propto h^2$$

Numerical Differentiation

- Represent the function by Taylor polynomials or Lagrange interpolation
- Evaluate the derivatives of the interpolation polynomial at selected nodal points

Numerical Differentiation

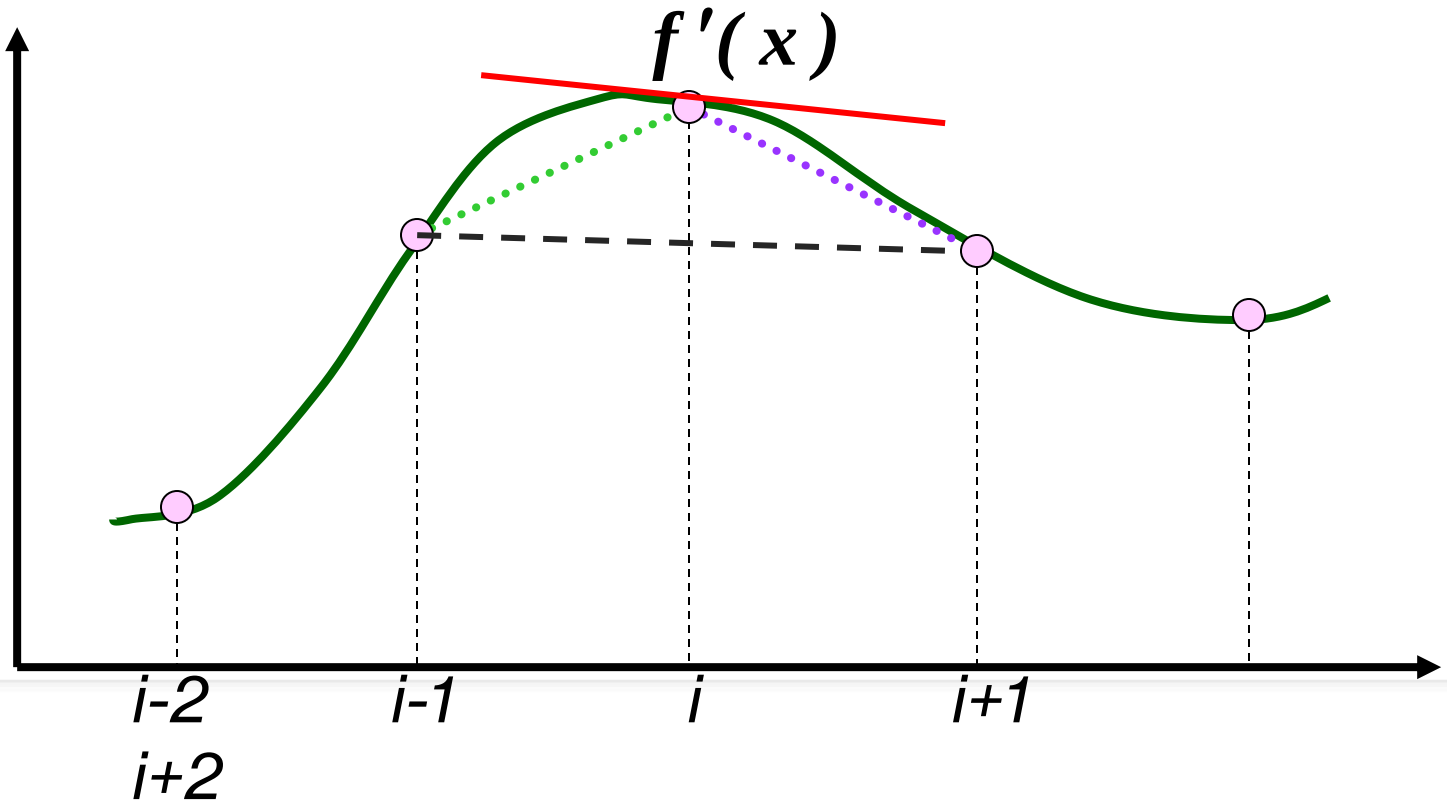
A Taylor series or Lagrange interpolation of points can be used to find the derivatives. The Taylor series expansion is defined as:

$$f(x_i) = f(x_0) + \Delta x \left.\frac{df}{dx}\right|_{x=x_0} + \frac{(\Delta x)^2}{2!} \left.\frac{d^2 f}{dx^2}\right|_{x=x_0} + \frac{(\Delta x)^3}{3!} \left.\frac{d^3 f}{dx^3}\right|_{x=x_0} + \ldots$$

$$\Delta x = x_i - x_0$$

$$f(x_i) = f(x_0) + (x_i - x_0) f'(x_0) + \frac{(x_i - x_0)^2}{2!} f''(x_0) + \frac{(x_i - x_0)^3}{3!} f'''(x_0) + \ldots$$

First Derivative at a Point



Numerical Differentiation

Use the Taylor series expansion to represent three points about single location:

$$f(x_{i+1}) = f(x_i) + (x_{i+1} - x_i) f'(x_i) + \frac{(x_{i+1} - x_i)^2}{2!} f''(x_i) + \ldots \quad [1]$$

$$f(x_i) = f(x_i) \quad [2]$$

$$f(x_{i-1}) = f(x_i) + (x_{i-1} - x_i) f'(x_i) + \frac{(x_{i-1} - x_i)^2}{2!} f''(x_i) + \ldots \quad [3]$$

Numerical Differentiation

Assume that the data points are "equally spaced" and the equations can be written as:

$$f(x_{i+1}) = f(x_i) + (\Delta x) f'(x_i) + \frac{(\Delta x)^2}{2!} f''(x_i) + \frac{(\Delta x)^3}{3!} f'''(x_i) + \ \ldots \quad [1]$$

$$f(x_i) = f(x_i) \quad [2]$$

$$f(x_{i-1}) = f(x_i) - (\Delta x) f'(x_i) + \frac{(\Delta x)^2}{2!} f''(x_i) - \frac{(\Delta x)^3}{3!} f'''(x_i) \ \ldots \quad [3]$$

Forward Differentiation

For a forward first derivative, subtract eqn[2] from eqn[1]:

$$f(x_{i+1}) - f(x_i) = (\Delta x) f'(x_i) + \frac{(\Delta x)^2}{2!} f''(x_i) + \frac{(\Delta x)^3}{3!} f'''(x_i) + \ldots$$

Rearrange the equation:

$$(\Delta x) f'(x_i) = f(x_{i+1}) - f(x_i) - \frac{(\Delta x)^2}{2!} f''(x_i) - \frac{(\Delta x)^3}{3!} f'''(x_i) + \ldots$$

$$f'(x_i) = \left(\frac{f(x_{i+1}) - f(x_i)}{\Delta x} \right) - \frac{(\Delta x)}{2!} f''(x_i) - \frac{(\Delta x)^2}{3!} f'''(x_i) + \ldots$$

Forward Differentiation

As the Δx gets smaller the error will get smaller

$$f'(x_i) = \left(\frac{f(x_{i+1}) - f(x_i)}{\Delta x} \right) - \text{Error}$$

The error is defined as:

$$\text{Error} = \frac{(\Delta x)}{2!} f''(x_i) + \frac{(\Delta x)^2}{3!} f'''(x_i) + \ldots$$

Backward Differentiation

Subtract eqn[3] from eqn[2]:

$$f'(x_i) = \left(\frac{f(x_i) - f(x_{i-1})}{\Delta x} \right) - \text{Error}$$

The error is defined as:

$$\text{Error} = \frac{(\Delta x)}{2!} f''(x_i) + \frac{(\Delta x)^2}{3!} f'''(x_i) + \ldots$$

Central Differentiation

Subtract eqn[3] from eqn[1]:

$$f'(x_i) = \left(\frac{f(x_{i+1}) - f(x_{i-1})}{2\Delta x} \right) - \text{Error}$$

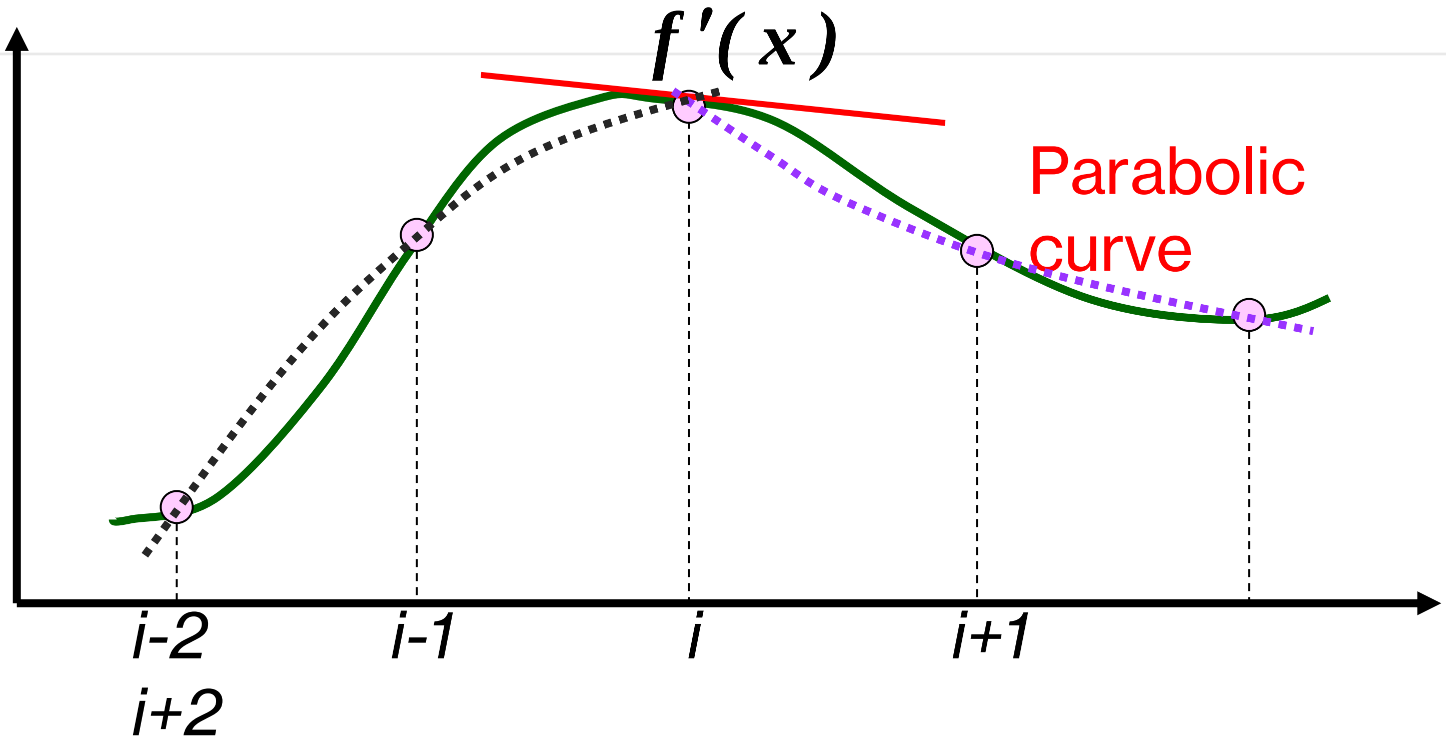
The error is defined as:

$$\text{Error} = \frac{(\Delta x)^2}{3!} f'''(x_i) + \ldots$$

Differential Error

Notice that the errors of the forward and backward 1st derivative of the equations have an error of the order of $O(\Delta x)$ and the central differentiation has an error of order $O(\Delta x^2)$.   The central difference has an better accuracy and lower error that the others. This can be improved by using more terms to model the first derivative.

Higher Order 1st Derivative



Forward difference

$$f'(x_i) = \left(\frac{3f(x_{i+2}) - 4f(x_{i+1}) + f(x_i)}{2\Delta x} \right) + \; E[O(\Delta x^2)]$$

Backward difference

$$f'(x_i) = \left(\frac{-3f(x_i) + 4f(x_{i-1}) - f(x_{i-2})}{2\Delta x} \right) + \; E[O(\Delta x^2)]$$

Higher Order Derivatives

To find higher derivatives, use the Taylor series expansions of term and eliminate the terms from the sum of equations. To improve the error in the problem add additional terms.

2^{nd} Derivative of the Function

It will require three terms to get a central 2^{nd} derivative of discrete set of data.

$$A * f(x_{i+1}) = f(x_i) + (\Delta x) f'(x_i) + \frac{(\Delta x)^2}{2!} f''(x_i) + \frac{(\Delta x)^3}{3!} f'''(x_i) + \ldots$$

$$B * f(x_i) = f(x_i)$$

$$C * f(x_{i-1}) = f(x_i) - (\Delta x) f'(x_i) + \frac{(\Delta x)^2}{2!} f''(x_i) - \frac{(\Delta x)^3}{3!} f'''(x_i) + \ldots$$

$f(x_i)$ column	$(\Delta x) f'(x_i)$ column	$\frac{(\Delta x)^2}{2!} f''(x_i)$ column
=	=	=
0	0	#

2nd Order Central Difference

The terms become：

$$A+B+C=0$$

$$A-C= 0$$

$$A+C= \#(2)$$

The terms become A=1,B=-2 and C=1. Therefore

$$f''(x_i)=\left(\frac{f(x_{i+1})-2f(x_i)+f(x_{i-1})}{\Delta x^2}\right)+ \mathrm{E}\left[\mathrm{O}\left(\Delta \mathrm{x}^2\right)\right]$$

Lagrange Differentiation

Another form of differentiation is to use the Lagrange interpolation between three points. The values can be determine for unevenly spaced points. Given:

$$L(x) = L_1(x)y_1 + L_2(x)y_2 + L_3(x)y_3$$

$$= \frac{(x-x_2)(x-x_3)}{(x_1-x_2)(x_1-x_3)}y_1 + \frac{(x-x_1)(x-x_3)}{(x_2-x_1)(x_2-x_3)}y_2 + \frac{(x-x_1)(x-x_2)}{(x_3-x_2)(x_3-x_1)}y_3$$

Lagrange Differentiation

Differentiate the Lagrange interpolation

$$f'(x) \cong L(x) = \frac{2x - x_2 - x_3}{(x_1 - x_2)(x_1 - x_3)} y_1 + \frac{2x - x_1 - x_3}{(x_2 - x_1)(x_2 - x_3)} y_2 + \frac{2x - x_1 - x_2}{(x_3 - x_2)(x_3 - x_1)} y_3$$

Assume a constant spacing

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

Lagrange Differentiation

Differentiate the Lagrange interpolation

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

Various locations

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

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

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

Lagrange Differentiation

To find a higher order derivative from the Lagrange interpolation for a three point Lagrange

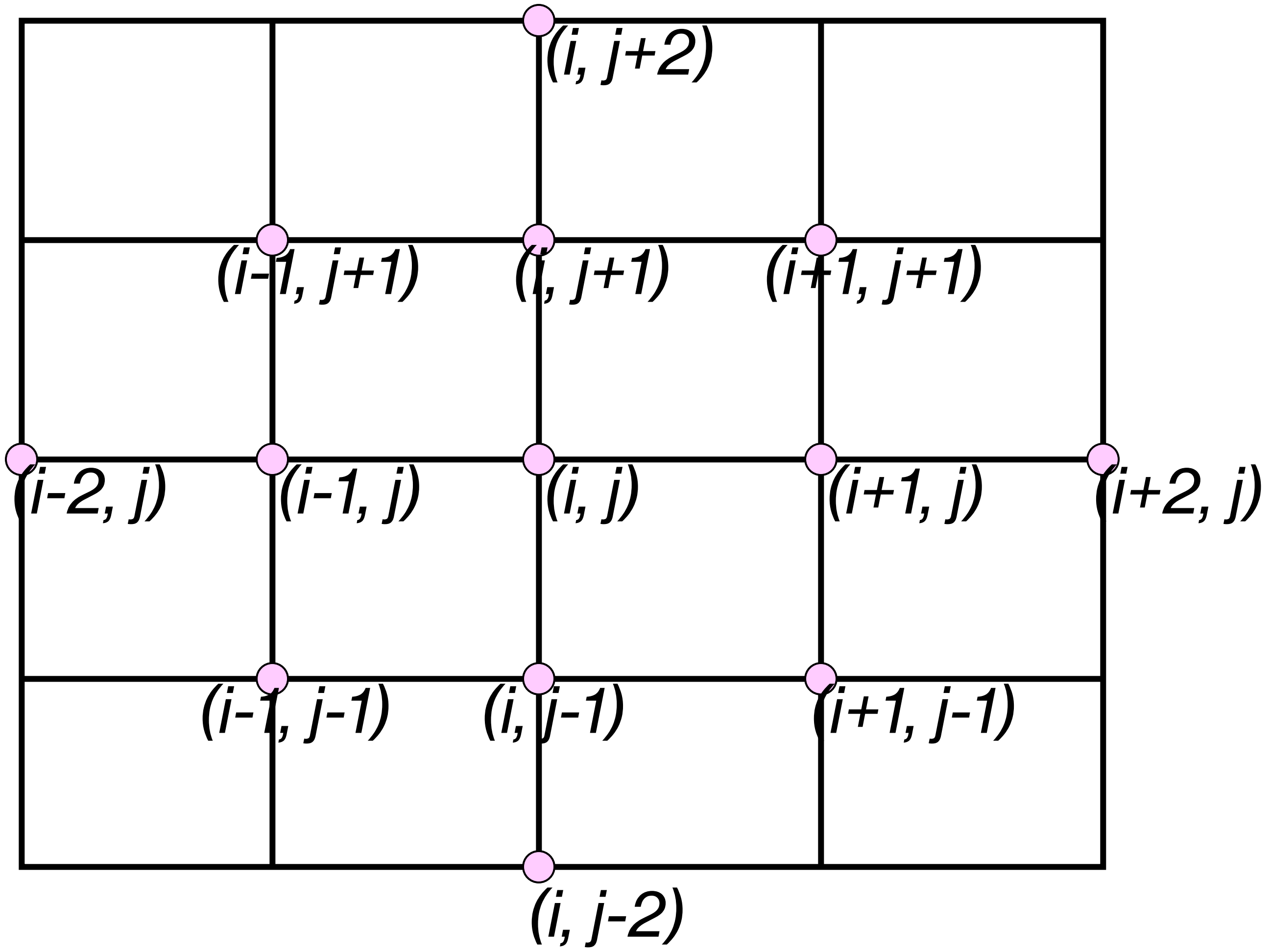
$$f'(x) = \frac{2x - x_2 - x_3}{2\Delta x^2} y_1 + \frac{2x - x_1 - x_3}{-\Delta x^2} y_2 + \frac{2x - x_1 - x_2}{2\Delta x^2} y_3$$

Take the derivative

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

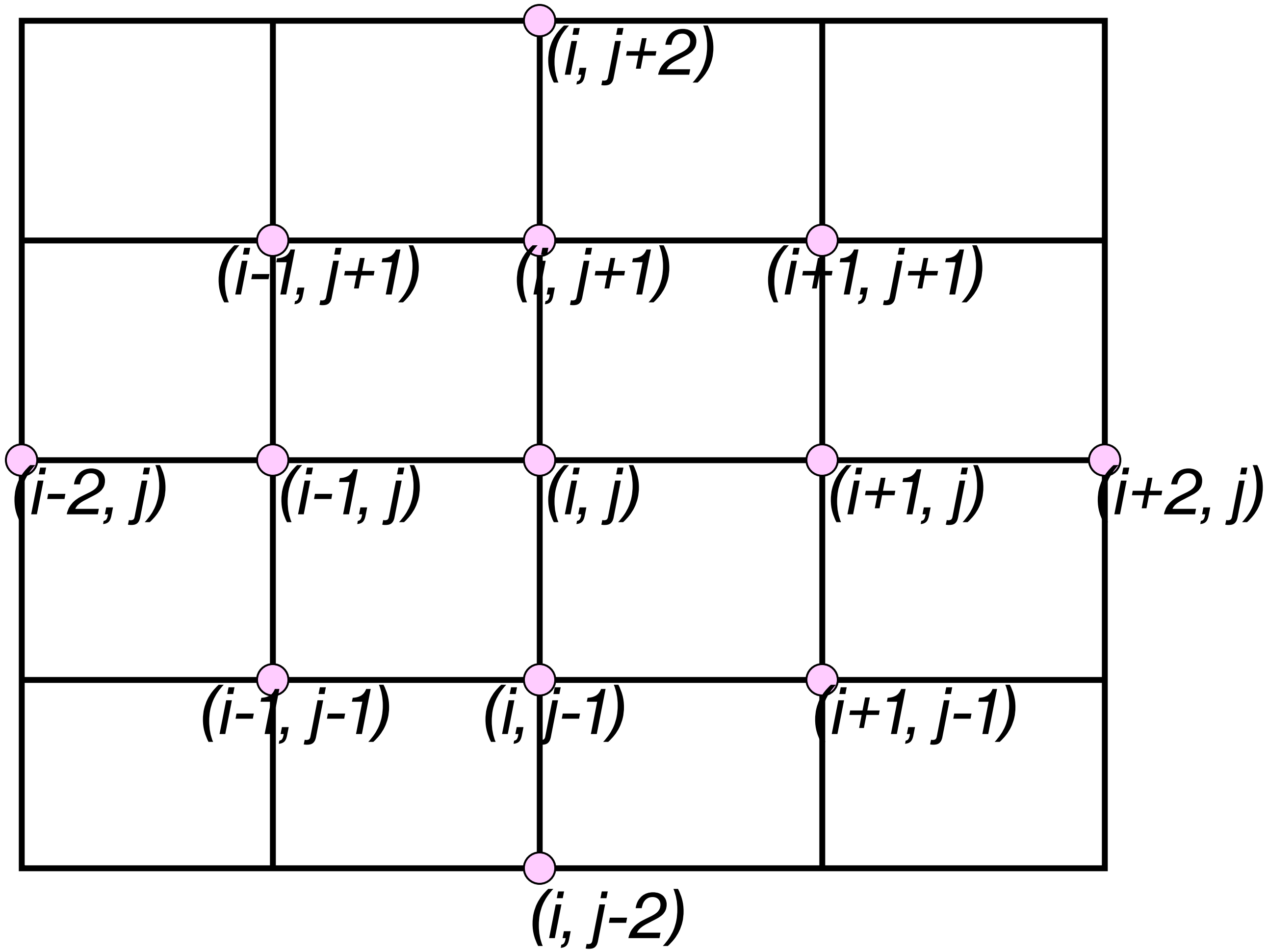
Partial Derivatives

- Straightforward extension of one-dimensional formula



$$u_x = \frac{\partial u}{\partial x} = \frac{1}{2h}\{ -1 \quad - \quad 0 \quad - \quad 1 \}$$

$$u_{xx} = \frac{\partial^2 u}{\partial x^2} = \frac{1}{h^2}\{ 1 \quad - \quad -2 \quad - \quad 1 \}$$



Partial Derivatives

Laplacian Operator

$$\nabla^2 u = u_{xx} + u_{yy} =$$

$$\frac{1}{h^2}\left\{\begin{array}{ccccc} & & 1 & & \\ & & | & & \\ 1 & - & -4 & - & 1 \\ & & | & & \\ & & 1 & & \end{array}\right\}\begin{array}{c} j+1 \\ \\ j \\ \\ j-1 \end{array}$$

$$\begin{array}{ccc} i-1 & i & i+1 \end{array}$$

Partial Derivatives

Mixed Derivative

$$u_{xy} = \frac{1}{4h^2} \left\{ \begin{matrix} -1 & - & 0 & - & 1 \\ | & & | & & | \\ 0 & - & 0 & - & 0 \\ | & & | & & | \\ 1 & - & 0 & - & -1 \end{matrix} \right\} \begin{matrix} j+1 \\ \\ j \\ \\ j-1 \end{matrix}$$

$$\begin{matrix} i-1 & \quad & i & \quad & i+1 \end{matrix}$$