數值分析

Chapter 5
Numerical Differentiation

授課教師：劉耀先

國立陽明交通大學 機械工程學系 EE464

yhliu@nctu.edu.tw

110學年度第一學期

Outline

- Background (5.1)
- Finite difference approximation of the derivative (5.2)
- Finite difference using Taylor series expansion (5.3)
- Summary of finite difference formulas (5.4)
- Differentiation formulas using Lagrange polynomials (5.5)
- Differentiation using curve fitting (5.6)
- MATLAB built-in functions (5.7)
- Complementary topics (5.8 5.9 5.10)

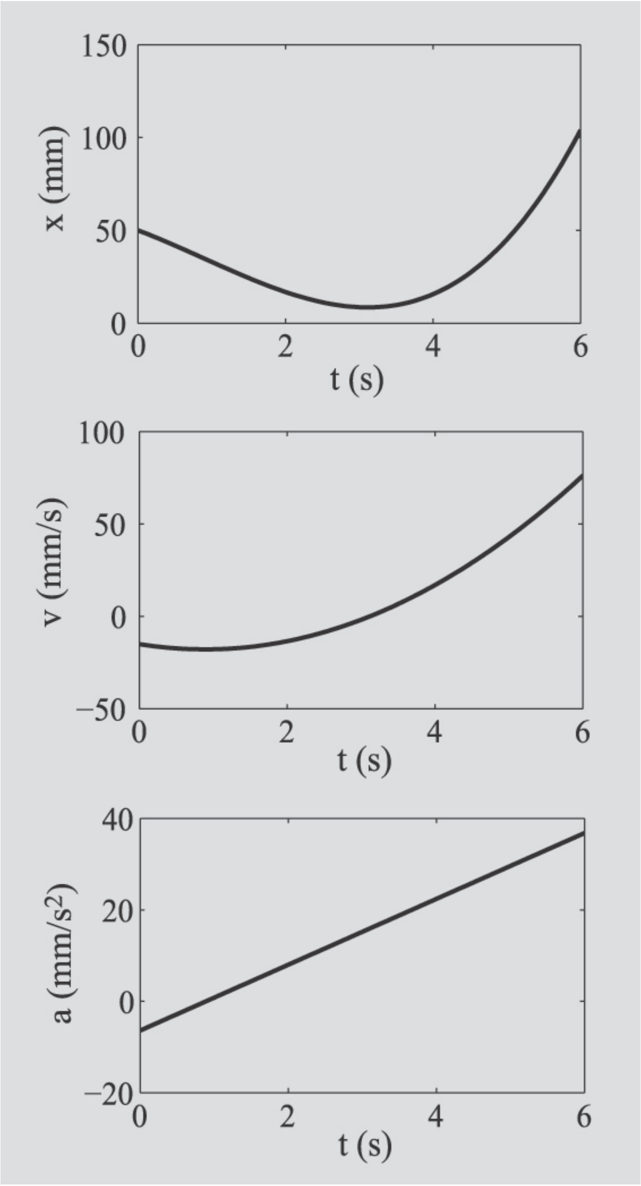
5.1 Background

- Differentiation gives a measure of the rate at which a quantity changes

- Position *x = f(t)*

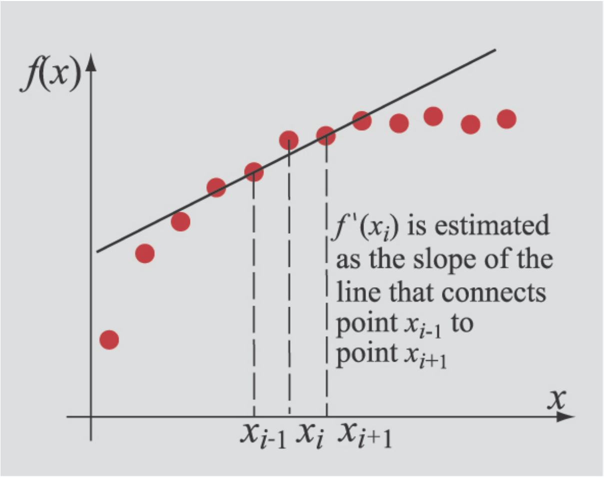
- Velocity $v = \dfrac{df(x)}{dt}$

- Acceleration $a = \dfrac{dv(x)}{dt}$



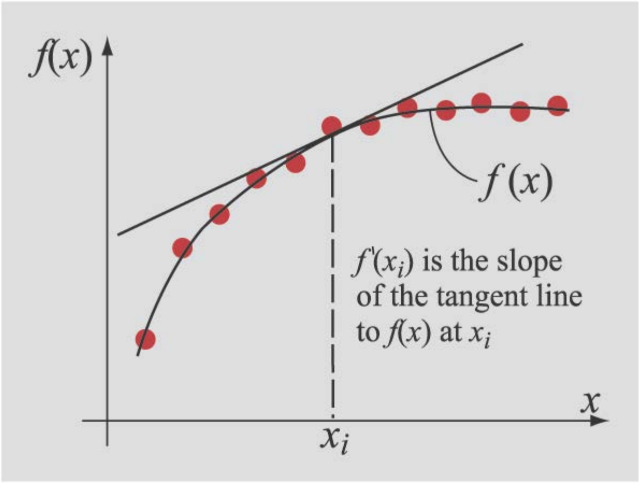
Numerical Differentiation

- The function to be differentiated can be:
  - Given as an analytical expression
  - Numerical differentiation if the analytical differentiation is impossible or difficult
- Numerical differentiation is carried out on data that are specified as a set of discrete points



(*a*)

Numerical differentiation using finite difference method



(*b*)

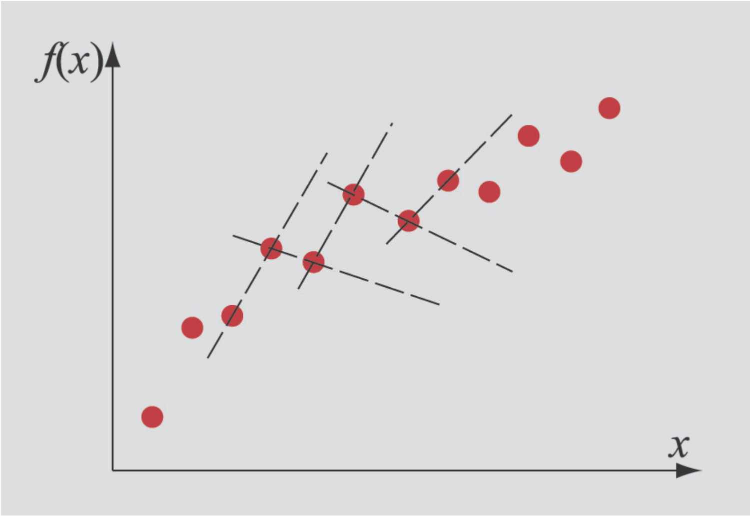
Analytical expression

Numerical Differentiation

- Numerical differentiation using finite difference method (5.2, 5.3)
  - Obtain the derivative of x_i based on the values of points in the neighborhood (x_{i-1} and x_{i+1})
  - The accuracy of the finite difference approximation depends on the
    - accuracy of the data points
    - the spacing between the points and
    - the specific formula used for approximation
- Function approximation using analytical expression (5.6)
  - Calculate the derivative by differentiating the analytical expression

Noise and scatter in the data points

- Because of experimental errors or uncertainties
- Two-point finite difference approximation will give large variations in the derivative from point to point
- Using higher-order formulas of finite difference approximation could give better results
- The differentiation could also be done by curve fitting the data to produce an analytical function and then differentiate



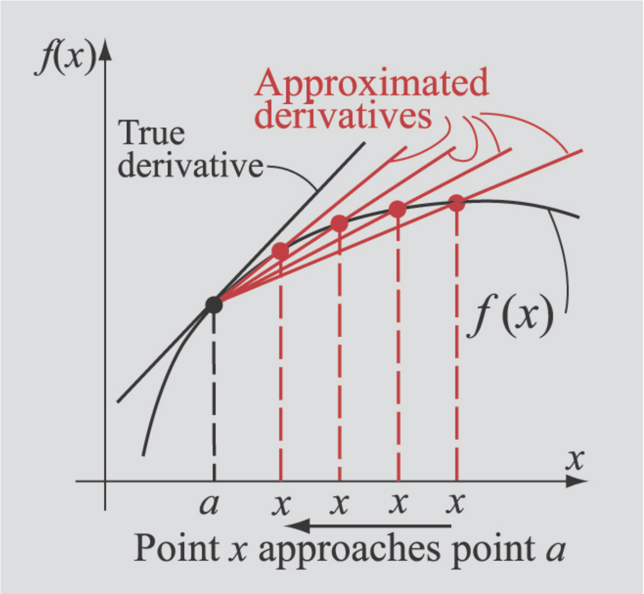
5.2 Finite Difference Approximation

- The derivative f'(x) of a function f(x) at the point x=a is defined by:

$$\left.\frac{df(x)}{dx}\right|_{x=a} = f'(a) = \lim_{x \to a} \frac{f(x) - f(a)}{x - a}$$

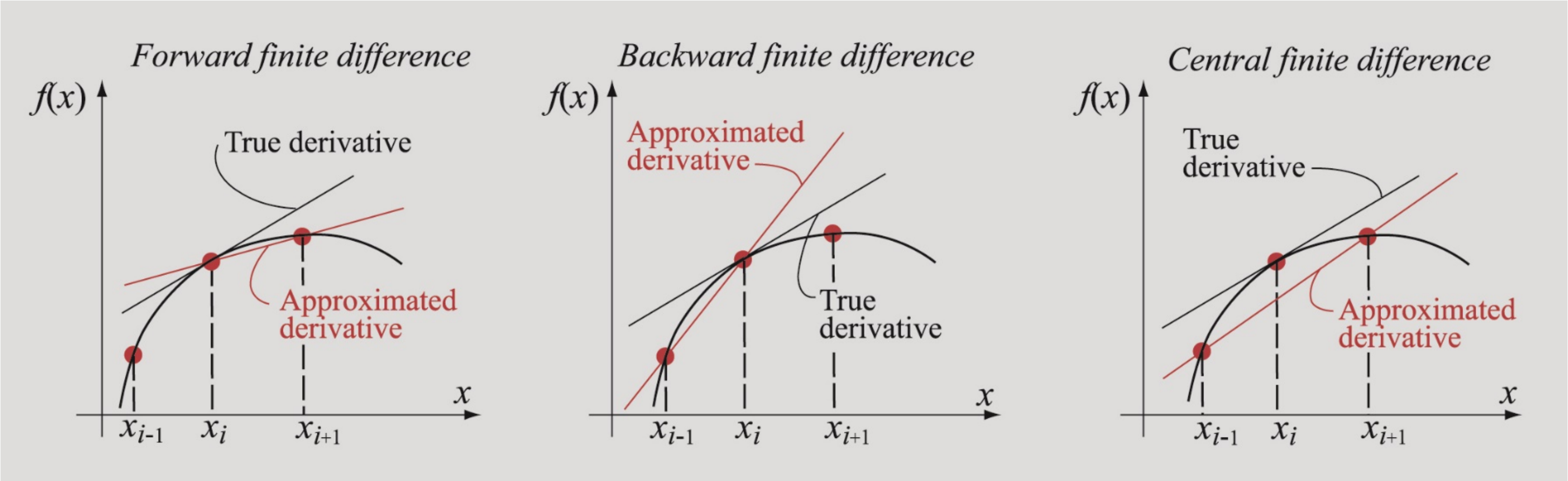
- The accuracy of calculating the derivative increases as point *x* is closer to point *a*

- Using the data points near point *a*



Finite Difference Methods

- Forward difference: $$\left.\frac{df}{dx}\right|_{x=x_i} = \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i}$$
- Backward difference: $$\left.\frac{df}{dx}\right|_{x=x_i} = \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}}$$
- Central difference: $$\left.\frac{df}{dx}\right|_{x=x_i} = \frac{f(x_{i+1}) - f(x_{i-1})}{x_{i+1} - x_{i-1}}$$



Example 5-1

- Consider function f(x) = x^3. Calculate its first derivative at point x = 3 numerically with the forward, backward, and central finite formulas using x = 2, 3, 4

- Analytical differentiation: f'(x) = $3x^2$ and f'(3) =27
- Numerical differentiation:
- Forward:

$$\left.\frac{df}{dx}\right|_{x=3} = \frac{f(4)-f(3)}{4-3} = \frac{64-27}{4-3} = 37 \qquad error = \left|\frac{37-27}{27}\cdot 100\right| = 37.04\%$$

- Backward:

$$\left.\frac{df}{dx}\right|_{x=3} = \frac{f(3)-f(2)}{3-2} = \frac{27-8}{3-2} = 19 \qquad error = \left|\frac{19-27}{27}\cdot 100\right| = 29.63\%$$

- Central

$$\left.\frac{df}{dx}\right|_{x=3} = \frac{f(4)-f(2)}{4-2} = \frac{64-8}{4-2} = 28 \qquad error = \left|\frac{28-27}{27}\cdot 100\right| = 3.704\%$$

Example 5-2: Damped vibrations

- Calculate the derivative of the following data by:
  - Calculating the **first** and **last** points using the **forward** and **backward** finite difference formulas
  - Using the **central** finite difference formula for all of the other points

t (s)	4.0	4.2	4.4	4.6	4.8	5.0	5.2	5.4	5.6	5.8	6.0
X (cm)	-5.87	-4.23	-2.55	-0.89	0.67	2.09	3.31	4.31	5.06	5.55	5.78

t (s)	6.2	6.4	6.6	6.8	7.0	7.2	7.4	7.6	7.8	8.0	
X (cm)	5.77	5.52	5.08	4.46	3.72	2.88	2.00	1.10	0.23	-0.59	

5.3 Finite Difference Formulas Using Taylor Series Expansion

- Taylor series expansion gives an estimate of the derivative at a point from the values of points in its neighborhood
- One advantage is that the formula provides an estimate for the **truncation error**
- Forward, backward, and central difference formulas
- Taylor series expansion:

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f'''(x_i)}{3!}h^3 + \frac{f^{(4)}(x_i)}{4!}h^4 + \ldots$$

- where h is the spacing between the points

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

First Derivative – Forward Difference

- By two-term Taylor series expansion:

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

- where ξ is a value between x_i and x_{i+1}
- Therefore

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

- The derivative can be calculated if last term is ignored
- Ignoring this term introduces a truncation error which is to be the order of h (written as **O(h)**):

$$truncation \quad error = -\frac{f''(\xi)}{2!}h = O(h)$$

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

First Derivative – Backward Difference

- Taylor series expansion:

$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2!}h^2 - \frac{f'''(x_i)}{3!}h^3 + \frac{f^{(4)}(x_i)}{4!}h^4 + \ldots$$

- where h is $h = x_i - x_{i-1}$
- Two-term Taylor series expansion

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

- where ξ is a value between x_{i-1} and x_i
- Therefore

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

First Derivative – Central Difference

- Three terms Taylor series expansion using x_i and x_{i+1} :

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f'''(\xi_1)}{3!}h^3$$

- where ξ_1 is a value between x_i and x_{i+1}
- Three terms Taylor series expansion using x_{i-1} and x_i :

$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2!}h^2 - \frac{f'''(\xi_2)}{3!}h^3$$

- where ξ_2 is a value between x_{i-1} and x_i
- where h is $h = x_{i+1} - x_i = x_i - x_{i-1}$

$$f(x_{i+1}) - f(x_{i-1}) = 2f'(x_i)h + \frac{f'''(\xi_1)}{3!}h^3 + \frac{f'''(\xi_2)}{3!}h^3$$

$$\Rightarrow \quad f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} + O(h^2)$$

Three-point finite difference formula

- Forward difference: calculate the derivative of x_i using x_{i+1} and x_{i+2} :

$$f'(x_i) = \frac{-3f(x_i) + 4f(x_{i+1}) - f(x_{i+2})}{2h} + O(h^2)$$

- Backward difference: calculate the derivative of x_i using x_{i-1} and x_{i-2} :

$$f'(x_i) = \frac{f(x_{i-2}) - 4f(x_{i-1}) + 3f(x_i)}{2h} + O(h^2)$$

Example 5-3

- Consider the function $f(x)=x^3$. Calculate the first derivative at point x=3 numerically with the three point forward difference formula using x=3 x=4 and x=5

- Analytical differentiation: $f'(x) = 3x^2$
  - $f'(3)=27$

- Numerical differentiation: (three point forward difference)

$$f'(3) = \frac{-3f(3) + 4f(4) - f(5)}{2 \cdot 1} = 25$$

$$error = \left| \frac{25-27}{27} \cdot 100 \right| = 7.41\%$$

Finite Difference Formulas for the Second Derivative

- Three-point central difference formula:

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

- Three-point forward difference formula:

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

- Three-point backward difference formula:

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

5.4 Summary of Finite difference Formulas

Table 5-1: Finite difference formulas.

First Derivative		
Method	**Formula**	**Truncation Error**
Two-point forward difference	$f'(x_i) = \dfrac{f(x_{i+1}) - f(x_i)}{h}$	$O(h)$
Three-point forward difference	$f'(x_i) = \dfrac{-3f(x_i) + 4f(x_{i+1}) - f(x_{i+2})}{2h}$	$O(h^2)$
Two-point backward difference	$f'(x_i) = \dfrac{f(x_i) - f(x_{i-1})}{h}$	$O(h)$
Three-point backward difference	$f'(x_i) = \dfrac{f(x_{i-2}) - 4f(x_{i-1}) + 3f(x_i)}{2h}$	$O(h^2)$
Two-point central difference	$f'(x_i) = \dfrac{f(x_{i+1}) - f(x_{i-1})}{2h}$	$O(h^2)$
Four-point central difference	$f'(x_i) = \dfrac{f(x_{i-2}) - 8f(x_{i-1}) + 8f(x_{i+1}) - f(x_{i+2})}{12h}$	$O(h^4)$

5.4 Summary of Finite difference Formulas

Second Derivative

Method	Formula	Truncation Error
Three-point forward difference	$f''(x_i) = \dfrac{f(x_i) - 2f(x_{i+1}) + f(x_{i+2})}{h^2}$	$O(h)$
Four-point forward difference	$f''(x_i) = \dfrac{2f(x_i) - 5f(x_{i+1}) + 4f(x_{i+2}) - f(x_{i+3})}{h^2}$	$O(h^2)$
Three-point backward difference	$f''(x_i) = \dfrac{f(x_{i-2}) - 2f(x_{i-1}) + f(x_i)}{h^2}$	$O(h)$
Four-point backward difference	$f''(x_i) = \dfrac{-f(x_{i-3}) + 4f(x_{i-2}) - 5f(x_{i-1}) + 2f(x_i)}{h^2}$	$O(h^2)$
Three-point central difference	$f''(x_i) = \dfrac{f(x_{i-1}) - 2f(x_i) + f(x_{i+1})}{h^2}$	$O(h^2)$
Five-point central difference	$f''(x_i) = \dfrac{-f(x_{i-2}) + 16f(x_{i-1}) - 30f(x_i) + 16f(x_{i+1}) - f(x_{i+2})}{12h^2}$	$O(h^4)$

Third Derivative

Method	Formula	Truncation Error
Four-point forward difference	$f'''(x_i) = \dfrac{-f(x_i) + 3f(x_{i+1}) - 3f(x_{i+2}) + f(x_{i+3})}{h^3}$	$O(h)$
Five-point forward difference	$f'''(x_i) = \dfrac{-5f(x_i) + 18f(x_{i+1}) - 24f(x_{i+2}) + 14f(x_{i+3}) - 3f(x_{i+4})}{2h^3}$	$O(h^2)$
Four-point backward difference	$f'''(x_i) = \dfrac{-f(x_{i-3}) + 3f(x_{i-2}) - 3f(x_{i-1}) + f(x_i)}{h^3}$	$O(h)$
Five-point backward difference	$f'''(x_i) = \dfrac{3f(x_{i-4}) - 14f(x_{i-3}) + 24f(x_{i-2}) - 18f(x_{i-1}) + 5f(x_i)}{2h^3}$	$O(h^2)$
Four-point central difference	$f'''(x_i) = \dfrac{-f(x_{i-2}) + 2f(x_{i-1}) - 2f(x_{i+1}) + f(x_{i+2})}{2h^3}$	$O(h^2)$
Six-point central difference	$f'''(x_i) = \dfrac{f(x_{i-3}) - 8f(x_{i-2}) + 13f(x_{i-1}) - 13f(x_{i+1}) + 8f(x_{i+2}) - f(x_{i+3})}{8h^3}$	$O(h^4)$

5.5 Differentiation Formulas using Lagrange Polynomials

- The Lagrange polynomial passes through (x_i, y_i), (x_{i+1}, y_{i+1}), (x_{i+2}, y_{i+2}) is:

$$f(x) = \frac{(x - x_{i+1})(x - x_{i+2})}{(x_i - x_{i+1})(x_i - x_{i+2})} y_i + \frac{(x - x_i)(x - x_{i+2})}{(x_{i+1} - x_i)(x_{i+1} - x_{i+2})} y_{i+1} + \frac{(x - x_i)(x - x_{i+1})}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})} y_{i+2}$$

- Take the derivative:

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

- Therefore

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

5.5 Differentiation Formulas using Lagrange Polynomials

- Similarly

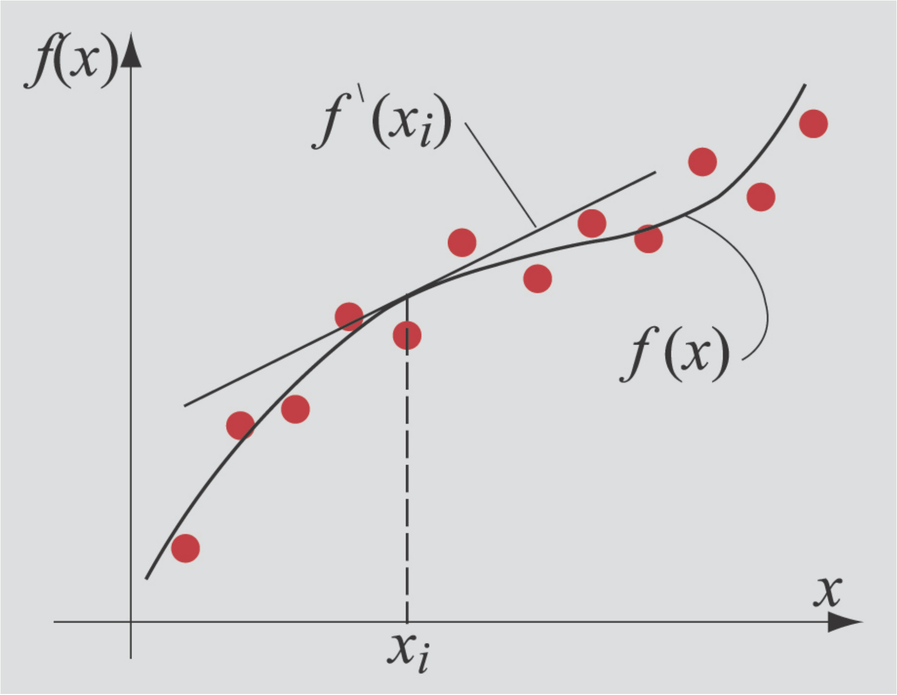
$$f'(x_{i+1}) = \frac{x_{i+1} - x_{i+2}}{(x_i - x_{i+1})(x_i - x_{i+2})} y_i + \frac{2x_{i+1} - x_i - x_{i+2}}{(x_{i+1} - x_i)(x_{i+1} - x_{i+2})} y_{i+1} + \frac{x_{i+1} - x_i}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})} y_{i+2}$$

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

- The formula can be used when the points **are not** spaced equally
- It can be used to calculate the value of first derivative at any point between x_i and x_{i+2}

5.6 Differentiation Using Curve Fitting

- First approximate the data points with an **analytical function** that can be easily differentiated
- The approximate function is then differentiated for calculating the derivative at any of the points
- Preferred when the data contains scatter or noise



5.7 MATLAB Built-in Functions

- **diff**: calculate the differences between adjacent elements of a vector
  - d = diff(x)
  - d is a vector with the differences between elements
  - d = [(x_2-x_1), (x_3-x_2),…,(x_n-x_{n-1})]
  - x is a vector: [x_1, x_2,…, x_n]
  - The first derivative can be calculated using **diff(y)./diff(x)**
  - d = diff(x,n)
  - N is a number that specifies the number of times that **diff** is applied recursively

5.7 MATLAB Built-in Functions

- **polyder**: calculate the derivative of a polynomial
  - dp = polyder (p)
  - dp is a vector with the coefficients of the polynomial that is the derivative of polynomial p
  - p is a vector with the coefficients of the polynomial

  - For $f(x) = 4x^3+5x+7$
  - P = [4 0 5 7]
  - dp = polyder(p)

  - This function can be used for calculating the derivative when a function is given

5.8 Richardson's Extrapolation

- Richardson's extrapolation is a method for calculating **a more accurate** approximation of a derivative from **two less accurate** approximations of that derivative
- Consider the value, D, of a derivative is calculated:

$$D = D(h) + k_2 h^2 + k_4 h^4$$

- Using a spacing of h/2:

$$D = D(h/2) + k_2 (h/2)^2 + k_4 (h/2)^4$$

- Combining the above two terms:

$$3D = 4D(h/2) - D(h) - k_4 \frac{3h^4}{4}$$

$$D = \frac{1}{3}\left(4D\left(\frac{h}{2}\right) - D(h) \right) - k_4 \frac{h^4}{4} = \frac{1}{3}\left(4D\left(\frac{h}{2}\right) - D(h) \right) + O(h^4)$$

Example 5-5

- Using Richardson's extrapolation to calculate the derivative of $f(x) = 2^x/x$ at the point $x=2$

- For $h = 0.2$ $f'(2)=0.577482$ error = 0.5016%
- For $h=0.1$, $f'(2)=0.575324$ error = 0.126%

- Use Richardson's extrapolation:

$$D = \frac{1}{3}\left(4D\left(\frac{h}{2}\right) - D(h)\right) + O(h^4) = \frac{1}{3}\left(4\cdot 0.575324 - 0.577482\right) = 0.574605$$

$$error = 0.00087\%$$

- Note: Richardson's extrapolation can be used with approximations that have errors of higher order

5.9 Error in Numerical Differentiation

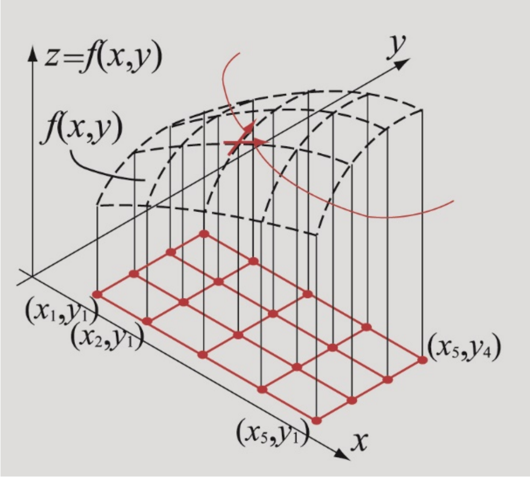
- The truncation error (discretization error) can be reduced by:
  - Reduce the spacing h between the points (not possible when a set of discrete data points are given)
  - Use the finite difference formula with higher-order truncation error
- When the function is given by a mathematical expression, choosing smaller spacing h can give smaller error
- However, round-off error still exists due to the finite precision of the particular computer used
- The total error can even **grow** as h is made smaller and smaller

5.10 Numerical Partial Differentiation

- Finite difference formulas can be used for approximating the derivatives of functions with **one independent variable** can be adopted for calculating the partial derivative

$$\left.\frac{\partial f(x,y)}{\partial x}\right|_{\substack{x=a\\y=b}} = \lim_{x\to a}\frac{f(x,b)-f(a,b)}{x-a}$$

$$\left.\frac{\partial f(x,y)}{\partial y}\right|_{\substack{x=a\\y=b}} = \lim_{y\to b}\frac{f(a,y)-f(a,b)}{y-b}$$



- Two-point forward difference formula is:

$$\left.\frac{\partial f}{\partial x}\right|_{\substack{x=x_i\\y=y_i}} = \frac{f(x_{i+1},y_i)-f(x_i,y_i)}{h_x} \qquad h_x = x_{i+1}-x_i$$

$$\left.\frac{\partial f}{\partial y}\right|_{\substack{x=x_i\\y=y_i}} = \frac{f(x_i,y_{i+1})-f(x_i,y_i)}{h_y} \qquad h_y = y_{i+1}-y_i$$

5.10 Numerical Partial Differentiation

- Two-point backward formula:

$$\left.\frac{\partial f}{\partial x}\right|_{\substack{x=x_i\\y=y_i}} = \frac{f(x_i, y_i) - f(x_{i-1}, y_i)}{h_x} \qquad \left.\frac{\partial f}{\partial y}\right|_{\substack{x=x_i\\y=y_i}} = \frac{f(x_i, y_i) - f(x_i, y_{i-1})}{h_y}$$

- Two-point central difference formula:

$$\left.\frac{\partial f}{\partial x}\right|_{\substack{x=x_i\\y=y_i}} = \frac{f(x_{i+1}, y_i) - f(x_{i-1}, y_i)}{2h_x} \qquad \left.\frac{\partial f}{\partial y}\right|_{\substack{x=x_i\\y=y_i}} = \frac{f(x_i, y_{i+1}) - f(x_i, y_{i-1})}{2h_y}$$

- The second partial derivative with the 3-point central difference:

$$\left.\frac{\partial^2 f}{\partial x^2}\right|_{\substack{x=x_i\\y=y_i}} = \frac{f(x_{i+1}, y_i) - 2f(x_i, y_i) + f(x_{i-1}, y_i)}{h_x^2}$$

Read Example 5-7

$$\left.\frac{\partial^2 f}{\partial y^2}\right|_{\substack{x=x_i\\y=y_i}} = \frac{f(x_i, y_{i+1}) - 2f(x_i, y_i) + f(x_i, y_{i-1})}{h_y^2}$$