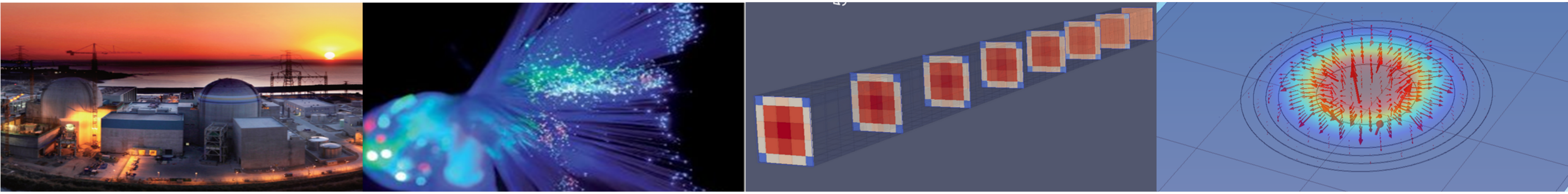

INTRODUCTION TO NUMERICAL ANALYSIS

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NuTHEL

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8. NUMERICAL DIFFERNTIATION

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Nuclear Thermal Hydraulic Engineering Lab.

Contents

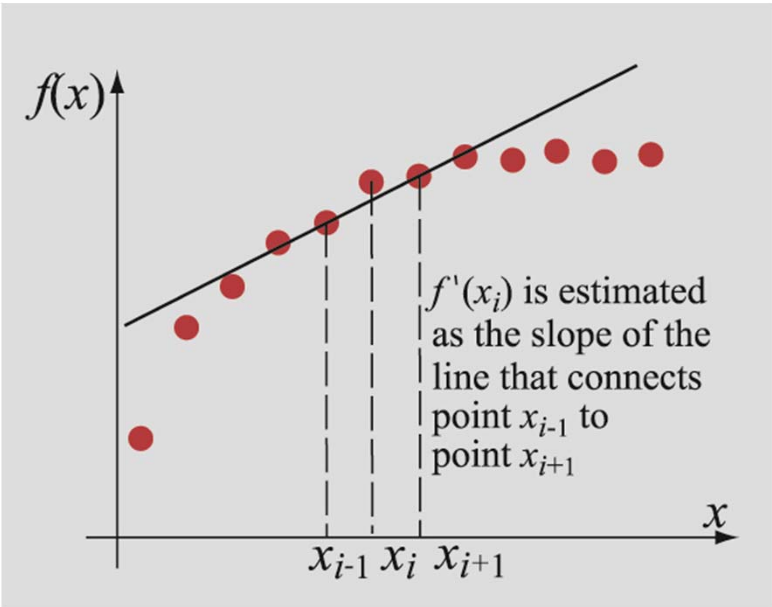
The need for numerical differentiation

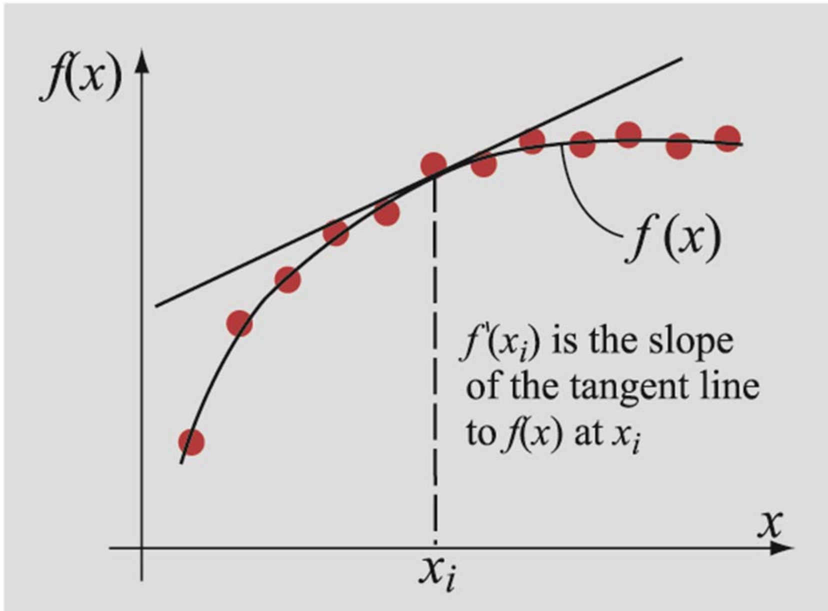
- The function to be differentiated can be given as an analytical expression or as a set of discrete points (tabulated data).
- When the function is given as a simple mathematical expression, the derivative can be determined analytically.
- When analytical differentiation of the expression is difficult or not possible, numerical differentiation has to be used.
- When the function is specified as a set of discrete points, differentiation is done by using a numerical method.
- Numerical differentiation also plays an important role in some of the numerical methods used for solving differential equations.

8.1 Background

Approaches to numerical differentiation

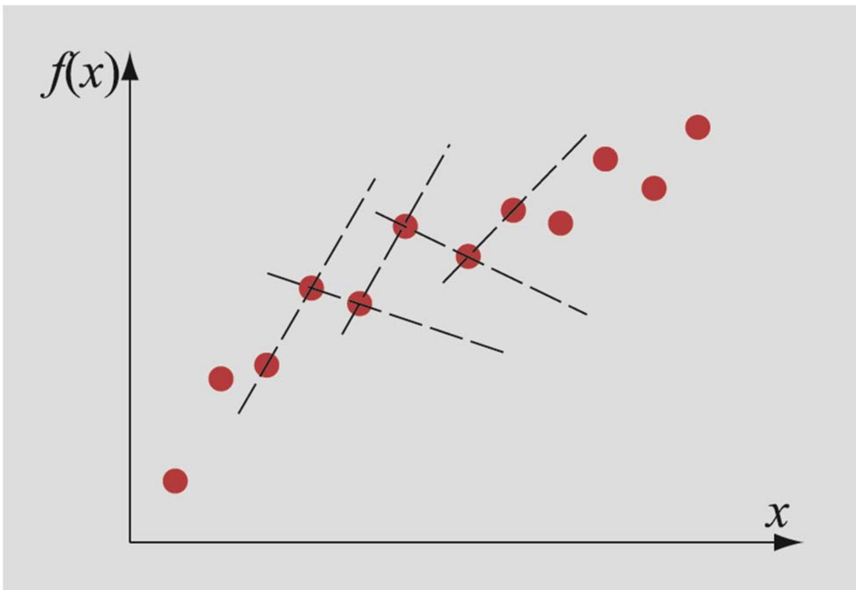
-
  - Derivative at a point x_i $\Longrightarrow$ based on the value of points in the neighborhood of x_i
- Approximate analytical expression
  - Analytical expression that can be easily differentiated
  - Derived by using curve fitting
  - Derivative at a point x_i $\Longrightarrow$ analytical differentiation





Noise and scatter in the data points

- Scatter in data
  - Experimental error, uncertainties in the measurement (electrical noise)
- Simplest form of finite difference approximation
  - Large variations !
  - Better results with ***higher-order formulas*** of finite difference approximation
    - Ex) four, five and seven-point finite difference formulas
  - Curve fitting can smooth out the data before the differentiation

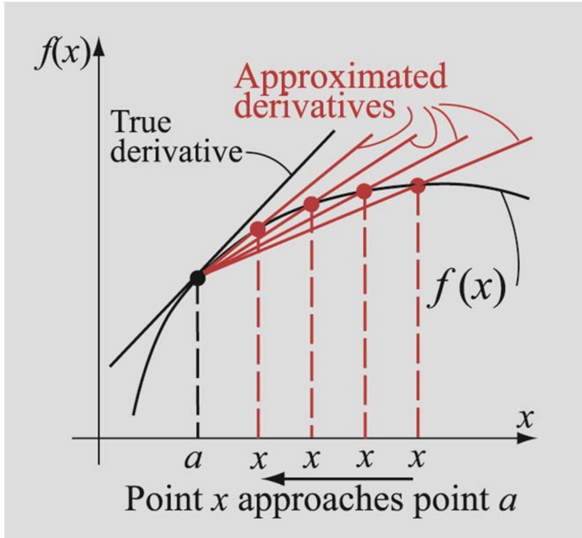


8.2 Finite Difference Approximation of the Derivative

The derivative $f'(x)$ of a function $f(x)$ at $x = a$

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

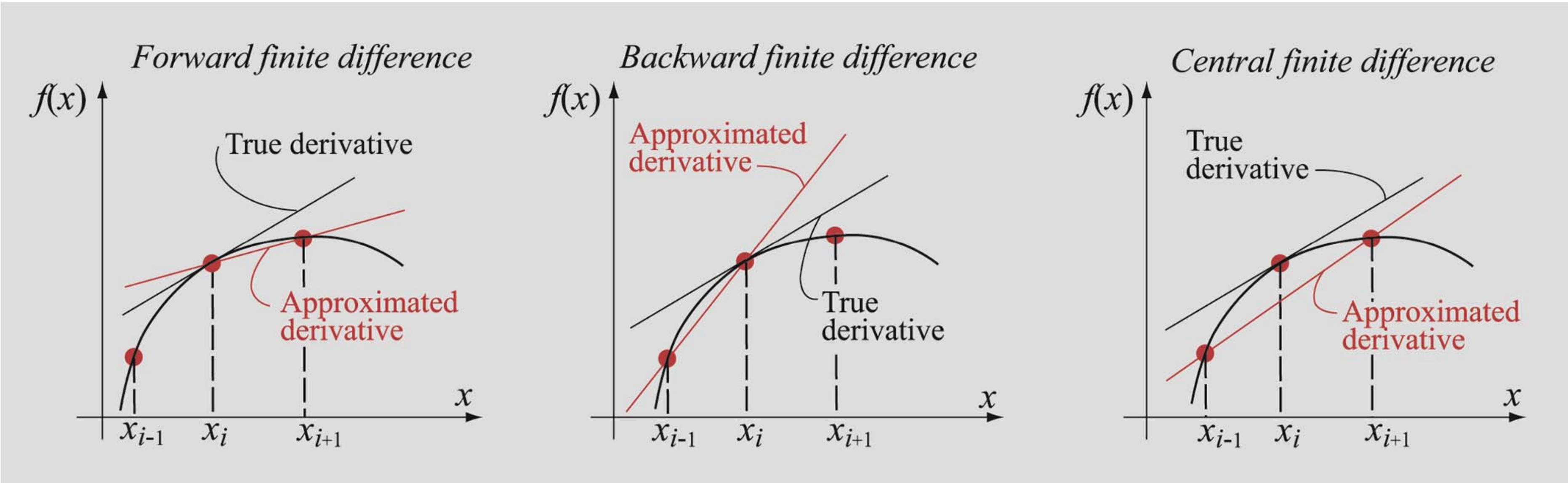
- Various finite difference formulas



Estimated derivative: value of the slope of the line that connects the two points

8.2 Finite Difference Approximation of the Derivative

❖ **Finite difference approximation of derivative**



8.2 Finite Difference Approximation of the Derivative

❖ Example 8-1: Comparing numerical and analytical differentiation

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

(*a*) Points $x = 2$, $x = 3$, and $x = 4$.

(*b*) Points $x = 2.75$, $x = 3$, and $x = 3.25$.

Compare the results with the exact (analytical) derivative.

x:	2	3	4
$f(x)$:	8	27	64

Forward finite difference:

$$\left.\frac{df}{dx}\right|_{x=3} = \frac{f(4)-f(3)}{4-3} = \frac{64-27}{1} = 37 \qquad error = \left|\frac{37-27}{27}\cdot 100\right| = 37.04\ \%$$

Backward finite difference:

$$\left.\frac{df}{dx}\right|_{x=3} = \frac{f(3)-f(2)}{3-2} = \frac{27-8}{1} = 19 \qquad error = \left|\frac{19-27}{27}\cdot 100\right| = 29.63\ \%$$

Central finite difference:

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

8.2 Finite Difference Approximation of the Derivative

❖ Example 8-1: Comparing numerical and analytical differentiation

Consider the function $f(x) = x^3$. Calculate its first derivative at point $x = 3$ numerically with the forward, backward, and central finite difference formulas and using:
(a) Points $x = 2$, $x = 3$, and $x = 4$.
(b) Points $x = 2.75$, $x = 3$, and $x = 3.25$.
Compare the results with the exact (analytical) derivative.

x:	2.75	3	3.25
$f(x)$:	2.75^3	3^3	3.25^3

Forward finite difference:

$$\left.\frac{df}{dx}\right|_{x=3} = \frac{f(3.25)-f(3)}{3.25-3} = \frac{3.25^3-27}{0.25} = 29.3125 \qquad error = \left|\frac{29.3125-27}{27}\right|\cdot 100 = 8.565 \quad \%$$

Backward finite difference:

$$\left.\frac{df}{dx}\right|_{x=3} = \frac{f(3)-f(2.75)}{3-2.75} = \frac{27-2.75^3}{0.25} = 24.8125 \qquad error = \left|\frac{24.8125-27}{27}\right|\cdot 100 = 8.102 \quad \%$$

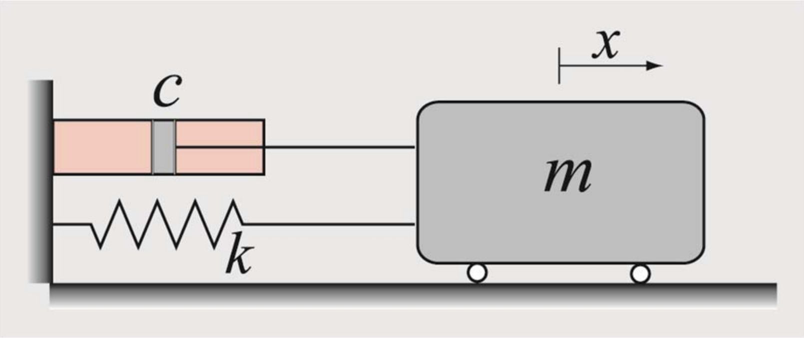
Central finite difference:

$$\left.\frac{df}{dx}\right|_{x=3} = \frac{f(3.25)-f(2.75)}{3.25-2.75} = \frac{3.25^3-2.75^3}{0.5} = 27.0625 \qquad error = \left|\frac{27.0625-27}{27}\right|\cdot 100 = 0.2315 \quad \%$$

8.2 Finite Difference Approximation of the Derivative

Example 8-2: Damped vibrations

- A block of mass m
  - Attached to a spring (k) and a dashpot (c)
- Data record for the block position: 5 Hz



(a) Calculate velocity at time $t = 5$ and $t = 6$

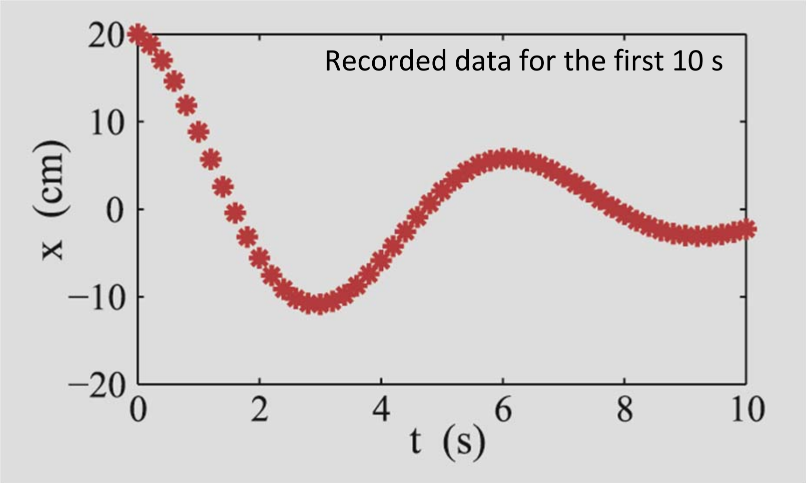
(b) Write a user-defined MATLAB function that

calculates the velocity: `dx=derivative(x,y)`

first point: forward difference , last point: backward difference

all the other: central difference

t (s)	4.0	4.2	4.4	4.6	4.8	5.0	5.2
x (cm)	–5.87	–4.23	–2.55	–0.89	0.67	2.09	3.31
t (s)	5.4	5.6	5.8	6.0	6.2	6.4	6.6
x (cm)	4.31	5.06	5.55	5.78	5.77	5.52	5.08
t (s)	6.8	7.0	7.2	7.4	7.6	7.8	8.0
x (cm)	4.46	3.72	2.88	2.00	1.10	0.23	–0.59



8.2 Finite Difference Approximation of the Derivative

Example 8-2: Damped vibrations

(a) Calculate velocity at time $t = 5$ and $t = 6$

The velocity is calculated by using Eq. (8.7):

for $t = 5$ s: $$\left.\frac{dx}{dt}\right|_{x=5} = \frac{f(5.2)-f(4.8)}{5.2-4.8} = \frac{3.31-0.67}{0.4} = 6.6 \quad \text{cm/s}$$

for $t = 6$ s: $$\left.\frac{dx}{dt}\right|_{x=5} = \frac{f(6.2)-f(5.8)}{6.2-5.8} = \frac{5.77-5.55}{0.4} = 0.55 \quad \text{cm/s}$$

(b) Write a user-defined MATLAB function that calculates the velocity

```
function dx = derivative(x,y)

n = length(x);
dx(1)=(y(2)-y(1))/(x(2)-x(1));
for i=2:n-1
    dx(i)=(y(i+1)-y(i-1))/(x(i+1)-x(i-1));
end
dx(n)=(y(n)-y(n-1))/(x(n)-x(n-1));
```

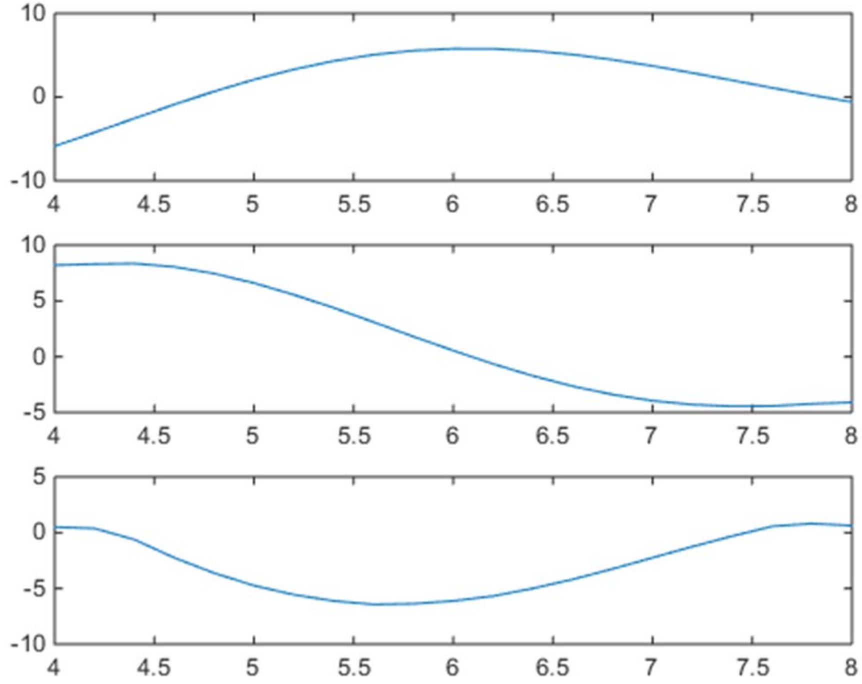
8.2 Finite Difference Approximation of the Derivative

❖ Example 8-2: Damped vibrations

(b) Write a user-defined MATLAB function that calculates the velocity.

(c) Make a plot of the displacement, velocity, and acceleration, versus time for $4 \le t \le 8\ s$

```
clear all
t = 4:0.2:8;
x = [-5.87 -4.23 -2.55 -0.89 0.67 2.09 3.31 4.31 5.06 ...
    5.55 5.78 5.77 5.52 5.08 4.46 3.72 2.88 2.00 1.10 0.23 -0.59];
vel = derivative(t,x)
acc = derivative(t,vel);
subplot (3,1,1)
plot(t,x)
subplot (3,1,2)
plot(t,vel)
subplot (3,1,3)
plot(t,acc)
```



8.3 Finite Difference Formulas Using Taylor Series Expansion

Using Taylor series expansion for approximating derivatives

- Many finite difference formulas can be derived by using Taylor series expansion.
- It also provides an estimate for the truncation error.
- First derivative
- Second derivative

Finite difference formulas of first derivative

- For the case where the points are equally spaced
- Two-point forward difference formula for first derivative
  - $f(x_{i+1})$: approximated by a Taylor series, $h = x_{i+1} - x_i$

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

$$f(x_{i+1}) = f(x_i) + f'(x_i)h +$$

$x_i \le \xi \le x_{i+1}$ Remainder theorem !

8.3 Finite Difference Formulas Using Taylor Series Expansion

Finite difference formulas of first derivative

- Two-point forward difference formula for first derivative

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

  -

  - The magnitude of the truncation error is not really known.

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

8.3 Finite Difference Formulas Using Taylor Series Expansion

❖ Finite difference formulas of first derivative

- Two-point backward difference formula for first derivative
  - $f(x_{i+1})$: approximated by a Taylor series, $h = x_i - x_{i-1}$

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

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

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

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

8.3 Finite Difference Formulas Using Taylor Series Expansion

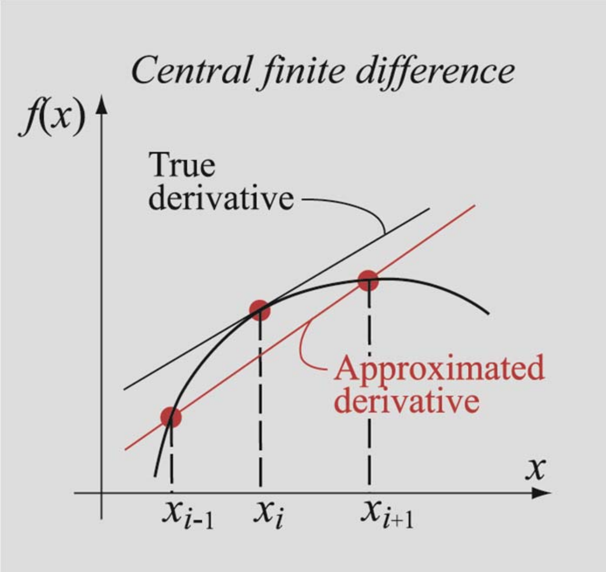
❖ Finite difference formulas of first derivative

- Two-point central difference formula for first derivative (for equal spacing)

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

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

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



  - Second order accuracy !
  - More accurate than the forward and backward differencing

8.3 Finite Difference Formulas Using Taylor Series Expansion

Finite difference formulas of first derivative

- Three-point forward/backward difference formula for first derivative (for equal spacing)
  - Central difference: second order accurate, but useful only for interior points
- Three-point forward difference
  - x_i , x_{i+1}, x_{i+2} with uniform space ($h = x_{i+2} - x_{i+1} = x_{i+1} - x_i$)

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

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

$$+\frac{4f'''(\xi_1)}{3!}h^3 - \frac{f'''(\xi_2)}{3!}(2h)^3$$

$$f'(x_i) = \qquad\qquad O(h^2)$$

Second order accuracy !

8.3 Finite Difference Formulas Using Taylor Series Expansion

❖ Finite difference formulas of first derivative

- Three-point backward difference
  - x_i , x_{i-1}, x_{i-2} with uniform space ($h = x_{i+2} - x_{i+1} = x_{i+1} - x_i$)

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

Second order accuracy !

8.3 Finite Difference Formulas Using Taylor Series Expansion

❖ Example 8-3: Comparing numerical and analytical differentiation

Consider the function $f(x) = x^3$. Calculate the first derivative at point $x = 3$ numerically with the three-point forward difference formula, using:
(*a*) Points $x = 3$, $x = 4$, and $x = 5$.
(*b*) Points $x = 3$, $x = 3.25$, and $x = 3.5$.
Compare the results with the exact value of the derivative, obtained analytically.

(*a*) The points used for numerical differentiation are:

x:	3	4	5
$f(x)$:	27	64	125

Using Eq. (8.24), the derivative using the three-point forward difference formula is:

$$f'(3) = \frac{-3f(3)+4f(4)-f(5)}{2\cdot 1} = \frac{-3\cdot 27+4\cdot 64-125}{2} = 25 \qquad error = \left|\frac{25-27}{27}\right|\cdot 100 = 7.41\ \%$$

(*b*) The points used for numerical differentiation are:

x:	3	3.25	3.5
$f(x)$:	27	3.25^3	3.5^3

Using Eq. (8.24), the derivative using the three points forward finite difference formula is:

$$f'(3) = \frac{-3f(3)+4f(3.25)-f(3.5)}{2\cdot 0.25} = \frac{-3\cdot 27+4\cdot 3.25^3-3.5^3}{0.5} = 26.875$$

$$error = \left|\frac{26.875-27}{27}\right|\cdot 100 = 0.46\ \%$$

Ex 8.1:

37.04%
8.56%

8.3 Finite Difference Formulas Using Taylor Series Expansion

Finite Difference Formulas for the Second Derivative

- Central difference
- One-sided forward difference
- One-sided backward difference
- Three-point central difference formula for the second derivative

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f'''(x_i)}{3!}h^3 + \frac{f^{(4)}(\xi_1)}{4!}h^4 \qquad x_i \le \xi_1 \le x_{i+1}$$

$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2!}h^2 - \frac{f'''(x_i)}{3!}h^3 + \frac{f^{(4)}(\xi_2)}{4!}h^4 \qquad x_{i-1} \le \xi_2 \le x_i$$

$$= \quad + \quad + \frac{f^{(4)}(\xi_1)}{4!}h^4 + \frac{f^{(4)}(\xi_2)}{4!}h^4$$

Second order truncation error

8.3 Finite Difference Formulas Using Taylor Series Expansion

Finite Difference Formulas for the Second Derivative

- Five-point central difference formula for the second derivative
  - 4^{th} order accurate

$$f''(x_i) = \frac{-f(x_{i-2}) + 16f(x_{i-1}) - 30f(x_i) + 16f(x_{i+1}) - f(x_{i+2})}{12h^2} + O(h^4)$$

- Three-point forward difference formula for the second derivative

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f'''(\xi_1)}{3!}h^3 \qquad \text{x2}$$

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

$$f''(x_i) = \qquad\qquad + O(h)$$

8.3 Finite Difference Formulas Using Taylor Series Expansion

❖ Finite Difference Formulas for the Second Derivative

- Three-point backward difference formula for the second derivative

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

x2

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

$f''(x_i) =$ $+O(h)$

8.3 Finite Difference Formulas Using Taylor Series Expansion

- Example 8-4: Comparing numerical and analytical differentiation

Consider the function $f(x) = \frac{2^x}{x}$. Calculate the second derivative at $x = 2$ numerically with the three-point central difference formula using:
(a) Points $x = 1.8$, $x = 2$, and $x = 2.2$.
(b) Points $x = 1.9$, $x = 2$, and $x = 2.1$.
Compare the results with the exact (analytical) derivative.

$$f''(x) = \frac{2^x[\ln(2)]^2}{x} - \frac{2 \cdot 2^x \ln(2)}{x^2} + \frac{2 \cdot 2^x}{x^3}$$

$$f''(2) = 0.574617$$

(a) `0.57748177389232`

(b) `0.57532441566441`

$$error = \frac{0.577482 - 0.574617}{0.574617} \cdot 100 = 0.4986\ \%$$

$$error = \frac{0.575324 - 0.574617}{0.574617} \cdot 100 = 0.1230\ \%$$

8.4 Summary of FD Formulas for Numerical Differentiation

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	$f'(x_i) = \dfrac{f(x_{i-2}) - 8f(x_{i-1}) + 8f(x_{i+1}) - f(x_{i+2})}{12h}$	$O(h^4)$

8.4 Summary of FD Formulas for Numerical Differentiation

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	$f''(x_i) = \dfrac{-f(x_{i-2}) + 16f(x_{i-1}) - 30f(x_i) + 16f(x_{i+1}) - f(x_{i+2})}{12h^2}$	$O(h^4)$

8.4 Summary of FD Formulas for Numerical Differentiation

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	$f'''(x_i) = \dfrac{f(x_{i-3})-8f(x_{i-2})+13f(x_{i-1})-13f(x_{i+1})+8f(x_{i+2})-f(x_{i+3})}{8h^3}$	$O(h^4)$

8.4 Summary of FD Formulas for Numerical Differentiation

Fourth Derivative		
Method	**Formula**	**Truncation Error**
Five-point forward difference	$f^{\text{iv}}(x_i) = \dfrac{f(x_i) - 4f(x_{i+1}) + 6f(x_{i+2}) - 4f(x_{i+3}) + f(x_{i+4})}{h^4}$	$O(h)$
Six-point forward difference	$f^{\text{iv}}(x_i) = \dfrac{3f(x_i) - 14f(x_{i+1}) + 26f(x_{i+2}) - 24f(x_{i+3}) + 11f(x_{i+4}) - 2f(x_{i+5})}{h^4}$	$O(h^2)$
Five-point backward difference	$f^{\text{iv}}(x_i) = \dfrac{f(x_{i-4}) - 4f(x_{i-3}) + 6f(x_{i-2}) - 4f(x_{i-1}) + f(x_i)}{h^4}$	$O(h)$
Six-point backward difference	$f^{\text{iv}}(x_i) = \dfrac{-2f(x_{i-5}) + 11f(x_{i-4}) - 24f(x_{i-3}) + 26f(x_{i-2}) - 14f(x_{i-1}) + 3f(x_i)}{h^4}$	$O(h^2)$
Five-point central difference	$f^{\text{iv}}(x_i) = \dfrac{f(x_{i-2}) - 4f(x_{i-1}) + 6f(x_i) - 4f(x_{i+1}) + f(x_{i+2})}{h^4}$	$O(h^2)$
Seven-point central difference	$f^{\text{iv}}(x_i) = \dfrac{-f(x_{i-3}) + 12f(x_{i-2}) - 39f(x_{i-1}) + 56f(x_i) - 39f(x_{i+1}) + 12f(x_{i+2}) - f(x_{i+3})}{6h^4}$	$O(h^4)$

8.5 Differentiation Formulas using Lagrange Polynomials

- Lagrange polynomials
  - First derivative
    - Two-point central, three-point forward, three-point backward difference formulas

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

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

    - $x_i \to x$

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

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

$$h = x_{i+1} - x_i = x_{i+2} - x_{i+1}$$

8.5 Differentiation Formulas using Lagrange Polynomials

- Lagrange polynomials
  - First derivative
    - Two-point central, three-point forward, three-point backward difference formulas

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

    - $x_{i+1} \to x$

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

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

8.5 Differentiation Formulas using Lagrange Polynomials

- Lagrange polynomials
  - First derivative
    - Two-point central, three-point forward, three-point backward difference formulas

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

    - $x_{i+2} \rightarrow x$

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

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

8.5 Differentiation Formulas using Lagrange Polynomials

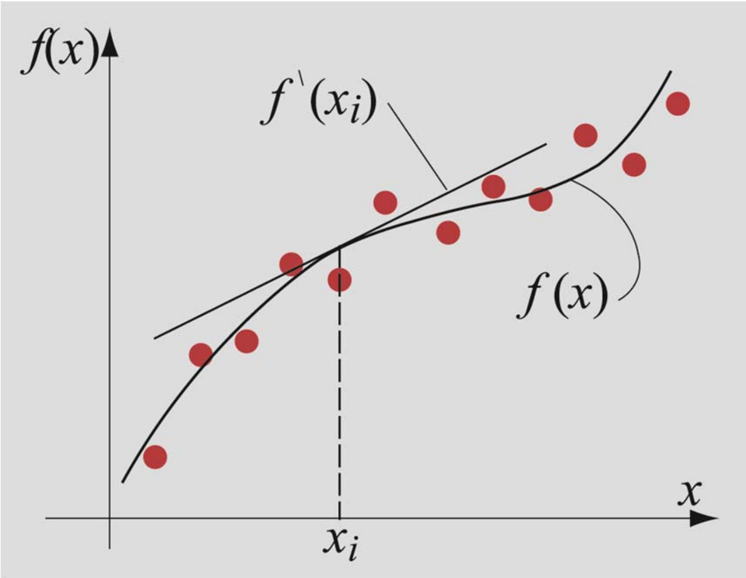
- Lagrange polynomials
  - Important features

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

    -
    - It can be used for calculating the value of the
    - With more points, higher order derivatives can be derived by Lagrange polynomials.
    - Use of Lagrange polynomials to
    - Taylor series provides

8.6 Differentiation using Curve Fitting

- Differentiation of data
  - A set of discrete points
  - Approximate with an analytical function
    - Easily differentiated
  - Differentiate the approximate function



  - Data of a non-linear relationship
    - Least square curve fitting
    - Ex) exponential function, power function, a combination of a non-linear functions

8.7 Use of MATLAB Built-in Functions for Numerical Differentiation

❖ `Diff` command

- Calculates the differences between adjacent elements of a vector

`d = diff(x)`

`d` is a vector with the differences between elements of x:

$$d=[(x_2-x_1),(x_3-x_2),\ldots,(x_n-x_{n-1})]$$

`x` is a vector: $[x_1, x_2, x_3, x_4, \ldots, x_{n-1}, x_n]$

One element shorter than **x**

- Derivative

```
diff(y)./diff(x)
```

$$\left[\frac{(y_2-y_1)}{(x_2-x_1)},\frac{(y_3-y_2)}{(x_3-x_2)},\frac{(y_4-y_3)}{(x_4-x_3)},\ldots,\frac{(y_n-y_{n-1})}{(x_n-x_{n-1})}\right]$$

  - Two-point forward difference formula

8.7 Use of MATLAB Built-in Functions for Numerical Differentiation

❖ `Diff` command

- High-order derivatives

```
d=diff(x,n)
```

  - n : number of times that `diff` is applied recursively
  - `diff(x,2) = diff((diff(x))`
  - With n-element vector $(x_1, \cdots, x_n)$
    - `diff(x)`: n-1 elements: $(x_2 - x_1, \cdots, x_n - x_{n-1})$
    - `diff(x,2)`: n-2 elements: $\left((x_3 - x_2) - (x_2 - x_1), \cdots, (x_n - x_{n-1}) - (x_{n-1} - x_{n-2})\right)$

$$\left((x_3 - 2x_2 + x_1), \cdots, (x_n - 2x_{n-1} + x_{n-2})\right)$$

  - Three-point forward difference
    - `diff(x,2)/h^2`

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

8.7 Use of MATLAB Built-in Functions for Numerical Differentiation

- `polyder` **command**

`dp = polyder(p)`

`dp` is a vector with the coefficients of the polynomial that is the derivative of the polynomial `p`.

`p` is a vector with the coefficients of the polynomial that is differentiated.

$$f(x) = 4x^3 + 5x + 7$$

```
p = [4 0 5 7]

df = polyder(p)

df = [12 0 5]
```

Richardson's extrapolation

- Method for calculating a more accurate approximation of a derivative from two less accurate approximations of that derivative

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

$D(h)$: approximated derivative

x4 $k_2 h^2$ and $k_4 h^4$: error terms

-

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

/3

Calculated with an error $O(h^2)$

Richardson's extrapolation

- Direct derivation from a FD formula

$$f(x_i+h)=f(x_i)+f'(x_i)h+\frac{f''(x_i)}{2!}h^2+\frac{f'''(x_i)}{3!}h^3+\frac{f^{\mathrm{iv}}(x_i)}{4!}h^4+\frac{f^{\mathrm{v}}(\xi_1)}{5!}h^5$$

$$f(x_i-h)=f(x_i)-f'(x_i)h+\frac{f''(x_i)}{2!}h^2-\frac{f'''(x_i)}{3!}h^3+\frac{f^{\mathrm{iv}}(x_i)}{4!}h^4-\frac{f^{\mathrm{v}}(\xi_2)}{5!}h^5 \qquad (-)$$

$$f(x_i+h)-f(x_i-h)=2f'(x_i)h+2\frac{f'''(x_i)}{3!}h^3+\frac{f^{\mathrm{v}}(\xi_1)}{5!}h^5+\frac{f^{\mathrm{v}}(\xi_2)}{5!}h^5$$

$$f'(x_i)=\frac{f(x_i+h)-f(x_i-h)}{2h}-$$

- Repeat with $h/2$

$$f'(x_i)=\frac{f(x_i+h/2)-f(x_i-h/2)}{2(h/2)}-\frac{f'''(x_i)}{3!}\left(\frac{h}{2}\right)^2+O(h^4)$$

$$f'(x_i)=\frac{f(x_i+h/2)-f(x_i-h/2)}{h}-$$

Richardson's extrapolation

- Direct derivation from a FD formula

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

$$f'(x_i) = \frac{f(x_i+h/2)-f(x_i-h/2)}{h} - \frac{f'''(x_i)}{4\cdot 3!}h^2 + O(h^4) \qquad (\times 4)$$

$$4f'(x_i) = 4\frac{f(x_i+h/2)-f(x_i-h/2)}{h} - \frac{f'''(x_i)}{3!}h^2 + O(h^4)$$

$$\boxed{f'(x_i) = \frac{1}{3}\left[4\underbrace{\frac{f(x_i+h/2)-f(x_i-h/2)}{h}} - \underbrace{\frac{f(x_i+h)-f(x_i-h)}{2h}}\right] + O(h^4)}$$

First derivative calculated with two-point central difference formula, Eq. (8.20), with error $O(h^2)$ for points with spacing of $h/2$.

First derivative calculated with two-point central difference formula, Eq. (8.20), with error $O(h^2)$ for points with spacing of h.

Richardson's extrapolation

- Higher-order extrapolation
  - Two approximated derivatives with different spacing (h and $h/2$)
  - 4th order accuracy
  - 6th order approximation

$$D = \frac{1}{15}\left(16D\left(\frac{h}{2}\right) - D(h)\right) + O(h^6)$$

$$D = D(h) + k_1 h^4 + k_2 h_6$$

$$D = D\left(\frac{h}{2}\right) + k_1\left(\frac{h}{2}\right)^4 + k_2\left(\frac{h}{2}\right)^6$$

❖ Using Richardson's extrapolation in differentiation

Use Richardson's extrapolation with the results in Example 8-4 to calculate a more accurate approximation for the derivative of the function $f(x) = \frac{2^x}{x}$ at the point $x = 2$. Compare the results with the exact (analytical) derivative.

$f''(2) = 0.574617$

for $h = 0.2$, $f''(2) = 0.577482$. The error in this approximation is 0.5016 %.
for $h = 0.1$, $f''(2) = 0.575324$. The error in this approximation is 0.126 %.

$$D = \frac{1}{3}\left(4D\left(\frac{h}{2}\right) - D(h)\right) + O(h^4) = \frac{1}{3}(4 \cdot 0.575324 - 0.577481) = 0.574605$$

$$error = \frac{0.574605 - 0.5746}{0.5746} \cdot 100 = 0.00087 \quad \%$$

Truncation error (or discretization error)

- Smaller error with smaller h
- For a set of discrete data points (the spacing is fixed)
  - The truncation error cannot be reduced.
  - A smaller truncation error can be obtained by using a FD formula with higher-order truncation error.

- h can be made arbitrarily small
  -
  - Round-off error can even grow as h is made smaller and smaller.

$$f(x) = e^x$$

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} - 2\frac{f'''(\xi)}{3!}h^2 \qquad f'(0) = \frac{e^h - e^{-h}}{2h} - 2\frac{f'''(\xi)}{3!}h^2$$

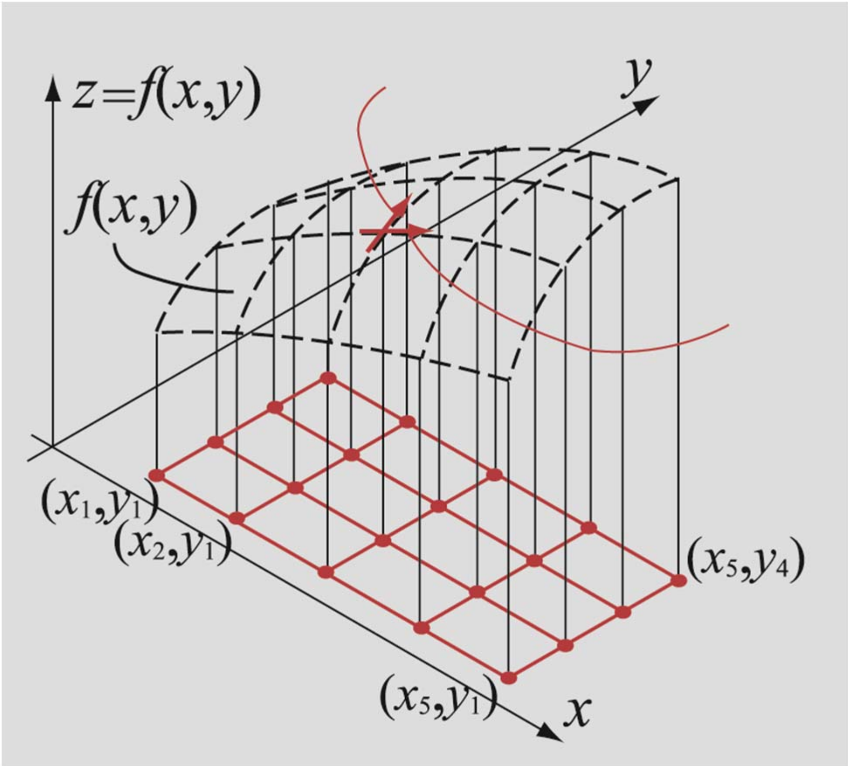
$$f'(0) = \frac{e^h + R_1 - e^{-h} - R_2}{2h} - 2\frac{f'''(\xi)}{3!}h^2 = \frac{e^h - e^{-h}}{2h} + \boxed{\frac{R_1 - R_2}{2h}} - 2\frac{f'''(\xi)}{3!}h^2$$

Partial differentiation

- 2-D and 3-D problem $T(x, y, z, t)$ $\dfrac{\partial T(x, y, z, t)}{\partial z}$
- Transient condition
- Rate of change of the value of the function with respect to this variable, while all the other variables are kept constant

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

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



- Two-point forward difference

$$\left.\frac{\partial f}{\partial x}\right|_{\substack{x=x_i\\y=y_i}} =$$

$$\left.\frac{\partial f}{\partial y}\right|_{\substack{x=x_i\\y=y_i}} =$$

$$h_x = x_{i+1} - x_i$$
$$h_y = y_{i+1} - y_i$$

8.10 Numerical Partial Differentiation

Partial differentiation

- Two-point backward and central difference

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

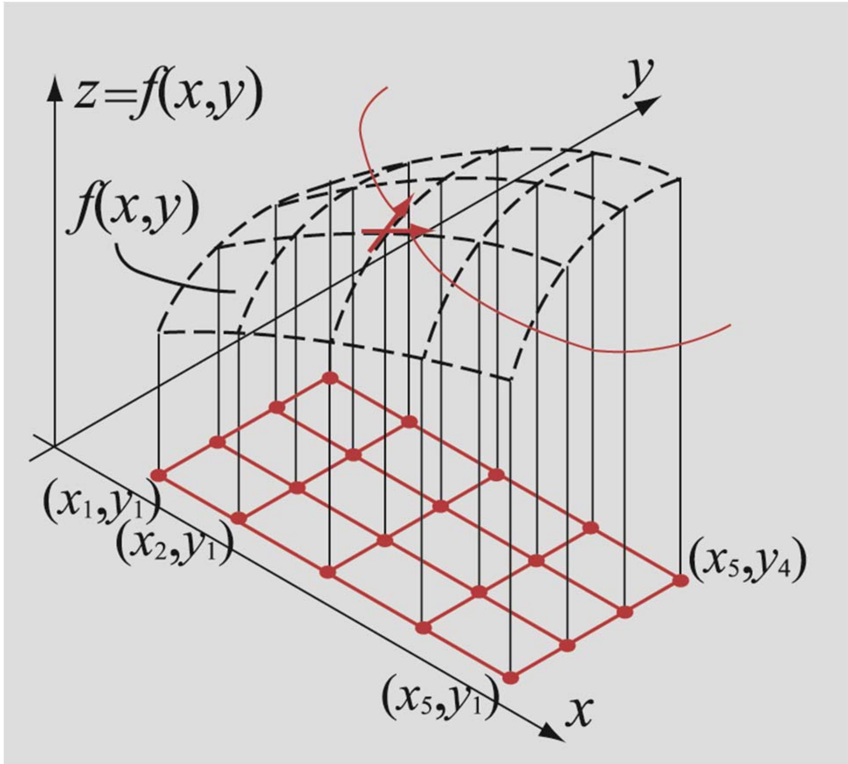
$$\left.\frac{\partial f}{\partial x}\right|_{\substack{x=x_i\\y=y_i}} = \qquad \left.\frac{\partial f}{\partial y}\right|_{\substack{x=x_i\\y=y_i}} =$$

Second derivatives

- Three-point central difference formula

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

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

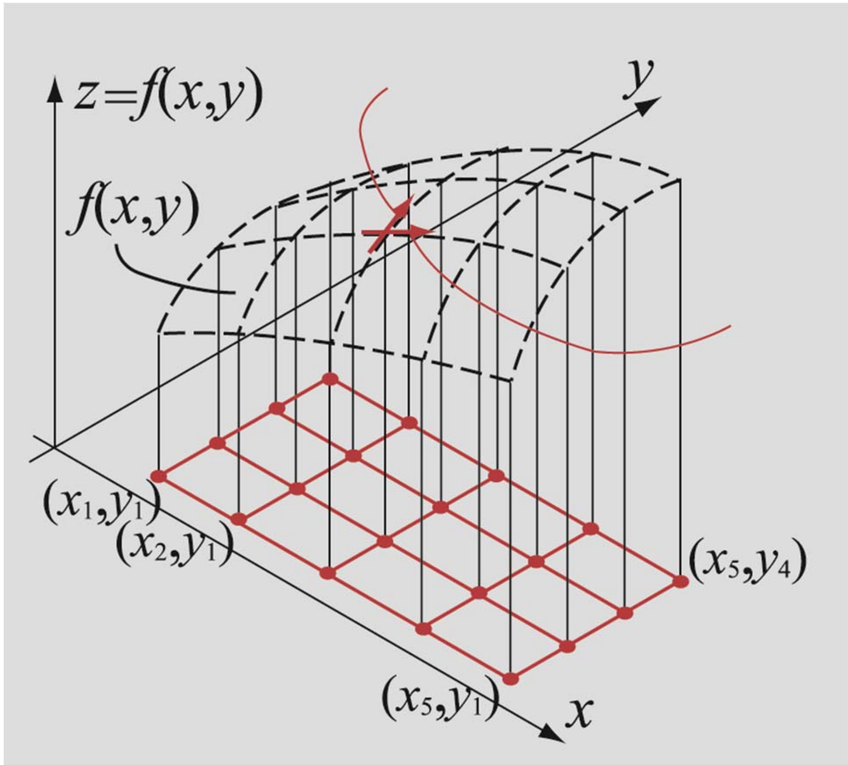


Second derivatives (mixed derivative)

$$\frac{\partial^2 f}{\partial x \partial y} = \frac{\partial}{\partial y}\left(\frac{\partial f}{\partial x}\right) = \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial y}\right)$$

- Obtained from the first-order finite difference formula for the first derivative

$$\left.\frac{\partial^2 f}{\partial x \partial y}\right|_{\substack{x = x_i \\ y = y_i}} =$$



❖ Example 8-7: Numerical partial differentiation

The following two-dimensional data for the x component of velocity u as a function of the two coordinates x and y is measured from an experiment:

	$x = 1.0$	$x = 1.5$	$x = 2.0$	$x = 2.5$	$x = 3.0$
$y = 1.0$	163	205	250	298	349
$y = 2.0$	228	291	361	437	517
$y = 3.0$	265	350	448	557	676

(a) Using central difference approximations, calculate $\partial u/\partial x$, $\partial u/(\partial y)$, $\partial^2 u/\partial y^2$, and $\partial^2 u/\partial x \partial y$ at the point $(2, 2)$.

$$\left.\frac{\partial u}{\partial x}\right|_{\substack{x = x_i \\ y = y_i}} = \frac{u(x_{i+1}, y_i) - u(x_{i-1}, y_i)}{2h_x} = \frac{u(2.5, 2) - u(1.5, 2)}{2 \cdot 0.5} = \frac{437 - 291}{1} = 146$$

$$\left.\frac{\partial u}{\partial y}\right|_{\substack{x = x_i \\ y = y_i}} = \frac{u(x_i, y_{i+1}) - u(x_i, y_{i-1})}{2h_y} = \frac{u(2, 3) - u(2, 1)}{2 \cdot 1} = \frac{448 - 250}{2} = 99$$

$$\left.\frac{\partial^2 u}{\partial y^2}\right|_{\substack{x = x_i \\ y = y_i}} = \frac{u(x_i, y_{i-1}) - 2u(x_i, y_i) + u(x_i, y_{i+1})}{h_y^2} = \frac{250 - (2 \cdot 361) + 448}{1^2} = -24$$

❖ Example 8-7: Numerical partial differentiation

The following two-dimensional data for the x component of velocity u as a function of the two coordinates x and y is measured from an experiment:

	$x = 1.0$	$x = 1.5$	$x = 2.0$	$x = 2.5$	$x = 3.0$
$y = 1.0$	163	205	250	298	349
$y = 2.0$	228	291	361	437	517
$y = 3.0$	265	350	448	557	676

(*a*) Using central difference approximations, calculate $\partial u/\partial x$, $\partial u/(\partial y)$, $\partial^2 u/\partial y^2$, and $\partial^2 u/\partial x \partial y$ at the point $(2, 2)$.

(*b*) Using a three-point forward difference approximation, calculate $\partial u/\partial x$ at the point (2,2).

(*c*) Using a three-point forward difference approximation, calculate $\partial u/\partial y$ at the point $(2, 1)$.

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

$$= \frac{[u(2.5, 3) - u(1.5, 3)] - [u(2.5, 1) - u(1.5, 1)]}{2 \cdot 0.5 \cdot 2 \cdot 1} = \frac{[557 - 350] - [298 - 205]}{2 \cdot 0.5 \cdot 2 \cdot 1} = 57$$

❖ Example 8-7: Numerical partial differentiation

The following two-dimensional data for the x component of velocity u as a function of the two coordinates x and y is measured from an experiment:

	$x = 1.0$	$x = 1.5$	$x = 2.0$	$x = 2.5$	$x = 3.0$
$y = 1.0$	163	205	250	298	349
$y = 2.0$	228	291	361	437	517
$y = 3.0$	265	350	448	557	676

(*b*) Using a three-point forward difference approximation, calculate $\partial u/\partial x$ at the point (2,2).

(*c*) Using a three-point forward difference approximation, calculate $\partial u/\partial y$ at the point $(2, 1)$.

$$\left.\frac{\partial u}{\partial x}\right|_{\substack{x = x_i \\ y = y_i}} = \frac{-3u(x_i, y_i) + 4u(x_{i+1}, y_i) - u(x_{i+2}, y_i)}{2h_x} =$$

$$= \frac{-3u(2,2) + 4u(2.5,2) - u(3.0,2)}{2\cdot 0.5} = \frac{-3\cdot 361 + 4\cdot 437 - 517}{2\cdot 0.5} = 148$$

$$\left.\frac{\partial u}{\partial y}\right|_{\substack{x = x_i \\ y = y_i}} = \frac{-3u(x_i, y_i) + 4u(x_i, y_{i+1}) - u(x_i, y_{i+2})}{2h_y} =$$

$$= \frac{-3u(2,1) + 4u(2,2) - u(2,3)}{2\cdot 1} = \frac{-3\cdot 250 + 4\cdot 361 - 448}{2\cdot 1} = 123$$