Numerical Differentiation: Uneven spacing

- What if the given data is not equally spaced

$$\left(x_k, f\left(x_k\right)\right) \quad k = 0,1,2,\ldots,n$$

- Forward and backward difference formula for the first derivative will still be valid

$$f_i' \approx \frac{f_{i+1} - f_i}{x_{i+1} - x_i} \qquad\qquad f_i' \approx \frac{f_i - f_{i-1}}{x_i - x_{i-1}}$$

- Central difference? $$f_i' \approx \frac{f_{i+1} - f_{i-1}}{x_{i+1} - x_{i-1}}$$

- We may use it but error will NOT be O(h^2)

Uneven spacing: Taylor's series

$$f_{i-1} = f_i - h_i f'(x_i) + \frac{h_i^{\,2}}{2} f''(x_i) - \frac{h_i^{\,3}}{6} f'''(x_i) + \frac{h_i^{\,4}}{4!} f''''(\zeta_b)$$

$$f_{i+1} = f_i + h_{i+1} f'(x_i) + \frac{h_{i+1}^{\,2}}{2} f''(x_i) + \frac{h_{i+1}^{\,3}}{6} f'''(x_i) + \frac{h_{i+1}^{\,4}}{4!} f''''(\zeta_f)$$

$\zeta_b \in (x_{i\text{-}1}, x_i)$ and $\zeta_f \in (x_i, x_{i+1})$

$$f'(x_i) = \frac{f_i - f_{i-1}}{h_i} + \frac{h_i}{2} f''(x_i) - \frac{h_i^{\,2}}{6} f'''(x_i) + \frac{h_i^{\,3}}{4!} f''''(\zeta_b)$$

$$f'(x_i) = \frac{f_{i+1} - f_i}{h_{i+1}} - \frac{h_{i+1}}{2} f''(x_i) + \frac{h_{i+1}^{\,2}}{6} f'''(x_i) + \frac{h_{i+1}^{\,3}}{4!} f''''(\zeta_f)$$

Uneven spacing: Taylor's series

- Eliminate the 2nd derivative

$$f' = -\frac{h_{i+1}}{h_i\left(h_i + h_{i+1}\right)} f_{i-1} + \frac{h_{i+1} - h_i}{h_i h_{i+1}} f_i + \frac{h_i}{h_{i+1}\left(h_i + h_{i+1}\right)} f_{i+1}$$

$$\text{Error} = -\frac{h_i h_{i+1} f'''}{6}$$

Equally spaced points: Seond Derivative

– Forward difference, *O*(*h*):

$$f_i'' = \frac{\dfrac{f_{i+2} - f_{i+1}}{h} - \dfrac{f_{i+1} - f_i}{h}}{h} = \frac{f_i - 2f_{i+1} + f_{i+2}}{h^2}$$

– Backward difference, *O*(*h*):

$$f_i'' = \frac{f_i - 2f_{i-1} + f_{i-2}}{h^2}$$

– Central difference, *O*(h^2):

$$f_i'' = \frac{f_{i-1} - 2f_i + f_{i+1}}{h^2}$$

Central Difference: Richardson method

- Combine 2 estimates of $O(h^2)$ accuracy:

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

$$f''(x_i) = \frac{f_{i-2} - 2f_i + f_{i+2}}{4h^2} + 4E + O(h^4)$$

- And get $O(h^4)$ estimate:

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

$$\Rightarrow f_i'' = \frac{-f_{i-2} + 16f_{i-1} - 30f_i + 16f_{i+1} - f_{i+2}}{12h^2}$$

Central Difference: Taylor's series

- $O(h^4)$ accuracy:

$$\begin{aligned}
f_i'' &= \frac{1}{h^2}\left(c_{i-2}f_{i-2}+c_{i-1}f_{i-1}+c_i f_i+c_{i+1}f_{i+1}+c_{i+2}f_{i+2}\right) \\
&= \frac{c_{i-2}+c_{i-1}+c_i+c_{i+1}+c_{i+2}}{h^2}f_i+\frac{-2c_{i-2}-c_{i-1}+c_{i+1}+2c_{i+2}}{h}f'(x_i) \\
&+\frac{1}{2}\left(4c_{i-2}+c_{i-1}+c_{i+1}+4c_{i+2}\right)f''(x_i)+\frac{h}{6}\left(-8c_{i-2}-c_{i-1}+c_{i+1}+8c_{i+2}\right)f'''(x_i) \\
&+\frac{h^2}{24}\left(16c_{i-2}+c_{i-1}+c_{i+1}+16c_{i+2}\right)f''''(x_i)+\ldots
\end{aligned}$$

$$\begin{aligned}
&c_{i-2}+c_{i-1}+c_i+c_{i+1}+c_{i+2}=0 \\
&-2c_{i-2}-c_{i-1}+c_{i+1}+2c_{i+2}=0 \\
&\frac{1}{2}\left(4c_{i-2}+c_{i-1}+c_{i+1}+4c_{i+2}\right)=1 \\
&-8c_{i-2}-c_{i-1}+c_{i+1}+8c_{i+2}=0 \\
&16c_{i-2}+c_{i-1}+c_{i+1}+16c_{i+2}=0
\end{aligned}$$

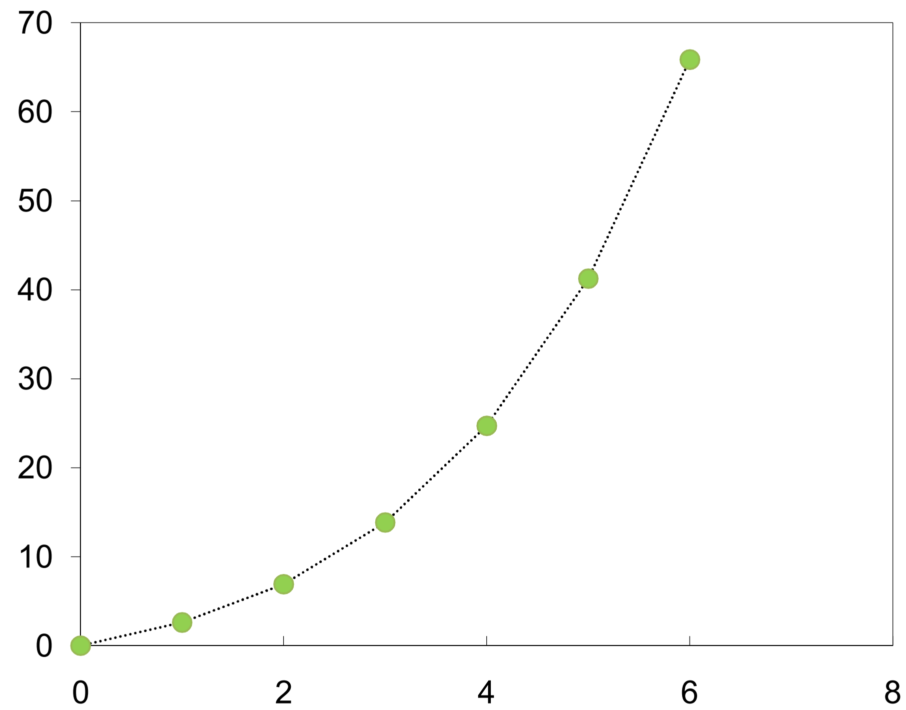
$$f_i''=\frac{-f_{i-2}+16f_{i-1}-30f_i+16f_{i+1}-f_{i+2}}{12h^2}$$

$$\text{Error}:\frac{h^4}{90}f^{[6]}(x_i)+O(h^8)$$

Numerical Differentiation: Example

- Given: Location of an object at different times

Time (s)	Location (cm)
0	0.00
1	2.61
2	6.91
3	13.85
4	24.70
5	41.25
6	65.86



- Estimate : Velocity and Acceleration at 3 sec

(The true values are 8.65 cm/s and 3.88 cm/s^2)

Numerical Differentiation: Velocity

Time (s)	Location (cm)
0	0.00
1	2.61
2	6.91
3	13.85
4	24.70
5	41.25
6	65.86

- Velocity, $O(h)$ estimates:
  - Forward: 24.70-13.85=10.85 cm/s
  - Backward: 13.85-6.91=6.94 cm/s
- Velocity, $O(h^2)$ estimates:
  - Forward: (-3x13.85+4x24.70-41.25)/2=8.00 cm/s (T.V. 8.65)
  - Backward: (3x13.85-4x6.91+2.61)/2=8.26 cm/s
  - Central: (24.70-6.91)/2=8.90 cm/s
- Velocity, $O(h^3/h^4)$ estimates:
  - Forward: -11/6x13.85+3x24.70-3/2x41.25+1/3x65.86=8.79 cm/s
  - Backward: 11/6x13.85-3x6.91+3/2x2.61-1/3x0=8.58 cm/s
  - Central (h^4): 1/12x2.61-2/3x6.91+2/3x27.70-1/12x41.25=8.64 cm/s

Numerical Differentiation: Velocity

Time (s)	Location (cm)
0	0.00
1	2.61
2	6.91
3	13.85
4	24.70
5	41.25
6	65.86

(T.V. 8.65)

- Velocity, Two O(h) estimates:
  - Forward, h: 24.70-13.85=10.85 cm/s
  - Forward, 2h: (41.25-13.85)/2=13.70 cm/s
- Velocity, O(h^2) estimates:
  - Forward: (2x10.85-13.70)=8.00 cm/s
- Velocity, Two O(h^2) estimates:
  - Central, h: (24.70-6.91)/2=8.90 cm/s
  - Central, 2h: (41.25-2.61)/4=9.66 cm/s
- Velocity, O(h^4) estimates:
  - Central: (4x8.90-9.66)/3=8.64 cm/s

Numerical Differentiation: Acceleration

Time (s)	Location (cm)
0	0.00
1	2.61
2	6.91
3	13.85
4	24.70
5	41.25
6	65.86

- Acceleration, O(h) estimates:
  - Forward: 41.25-2x24.70+13.85=5.70 cm/s^2
  - Backward: 13.85-2x6.91+2.61=2.64 cm/s^2
- Acceleration, O(h^2) estimates:
  - Forward: 2x13.85-5x24.70+4x41.25-65.86 = 3.34 cm/s^2 (T.V. 3.88)
  - Backward: 2x13.85-5x6.91+4x2.61-0 = 3.59 cm/s^2
  - Central: 6.91-2x13.85+24.70=3.91 cm/s^2
- Acceleration, O(h^4) estimate:
  - Central: -1/12x2.61+4/3x6.91-5/2x13.85+4/3x24.70-1/12x41.25=3.87 cm/s^2

Numerical Differentiation: Example

- Accl., Two $O(h^2)$ estimates:
  - Central, h: 6.91-2x13.85+24.70=3.91 cm/s^2
  - Central, 2h: 2.61-2x13.85+41.25=4.04 cm/s^2
- Accl., $O(h^4)$ estimates:
  - Forward: (4x3.91-4.04)/3=3.87 cm/s^2

Time (s)	Location (cm)
0	0.00
1	2.61
2	6.91
3	13.85
4	24.70
5	41.25
6	65.86

(T.V. 3.88)

Error Estimation : An alternative approach

- If we know that the forward difference estimate of the first derivative

$$f_i' = \frac{f_{i+1} - f_i}{h}$$

is $O(h)$ accurate, from dimensional analysis and the form of Taylor's series, it may be seen that the error must be of the form

$$f'(x_i) - f_i' = Chf''(\zeta_f)$$

- How do we obtain C?

Error Estimation

- Take any function which has a constant second derivative, simplest being $f(x)=x^2$
- Take any x and any h, find the true value of the derivative and the estimated value of the derivative, to obtain the error
- Divide the error by hf'' to obtain *C*
- E.g., $f(1)=1$; $f(2)=4$; $f'(1)=2$, $f_1' = \dfrac{4-1}{1} = 3$

$$\text{Error} = f'(x_i) - f_i' = 2 - 3 = -1 = Chf''(\zeta_f) \Rightarrow C = -\frac{1}{2}$$

as obtained earlier

Error Estimation

- Similarly, for central difference, the error in

$$f_i' = \frac{f_{i+1} - f_{i-1}}{2h}$$

should be of the form $f'(x_i) - f_i' = Ch^2 f'''(\zeta_c)$

- Take $f(x)=x^3$
- Take $x=1$ and $h=1$
- $f(1)=1; f(0)=0; f(2)=8; f'(1)=3,$ $f_1' = \frac{8-0}{2} = 4$

$$\text{Error } = f'(x_i) - f_i' = 3 - 4 = -1 = Ch^2 f'''(\zeta_c) \Rightarrow C = -\frac{1}{6}$$

as obtained earlier

Error Estimation

- If the order of error is not known, we could progressively increase the degree of the polynomial, and see up to what degree the finite difference approximations provide exact answer.
- E.g., forward difference approximation for the first derivative $$f_i' = \frac{f_{i+1} - f_i}{x_{i+1} - x_i}$$

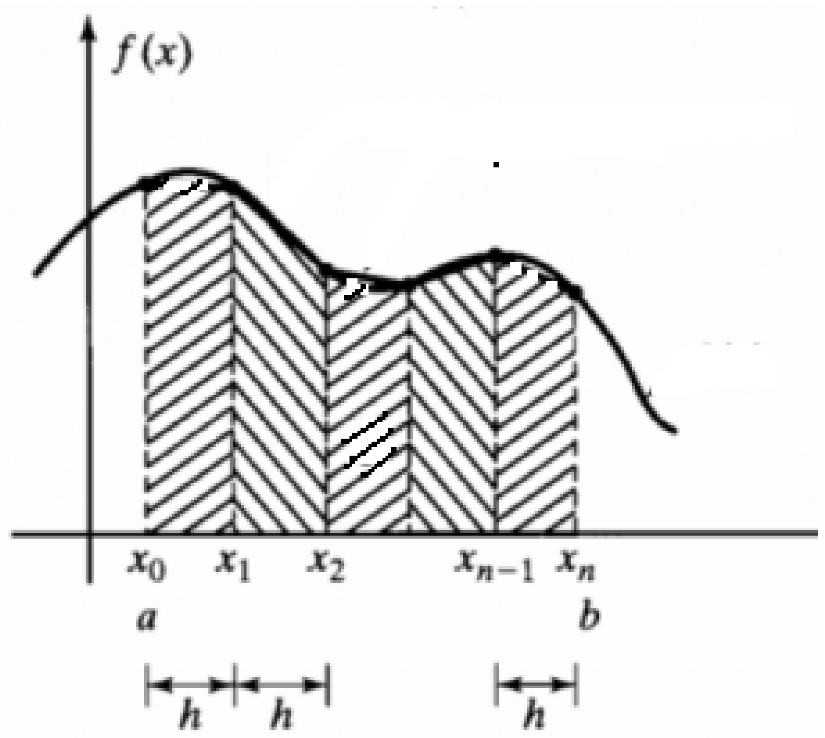
will be exact for $f(x)=x$ but not for $f(x)=x^2$

Numerical Integration

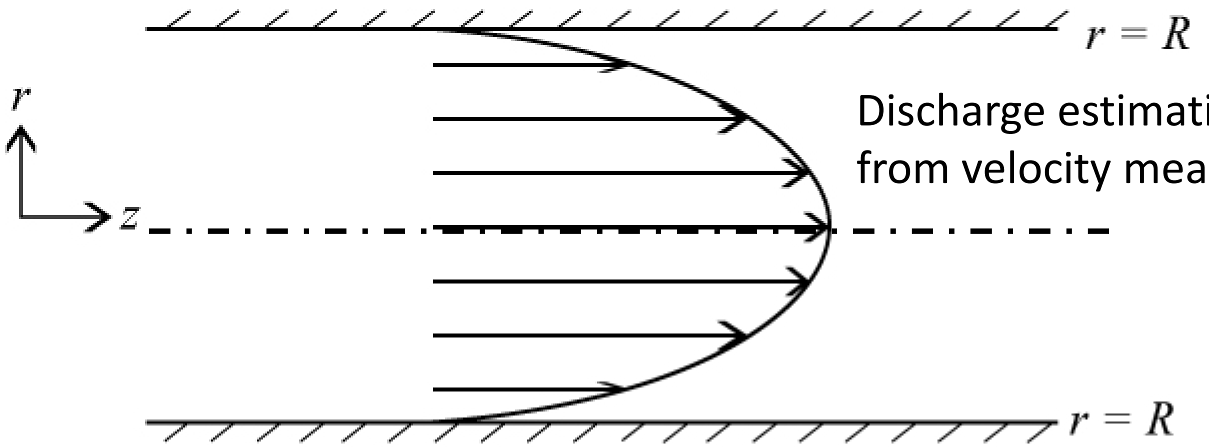
- Given data $\left(x_k, f\left(x_k\right)\right) \quad k = 0,1,2,\ldots,n$

- Estimate the integral:

$$I = \int_a^b f(x)dx$$

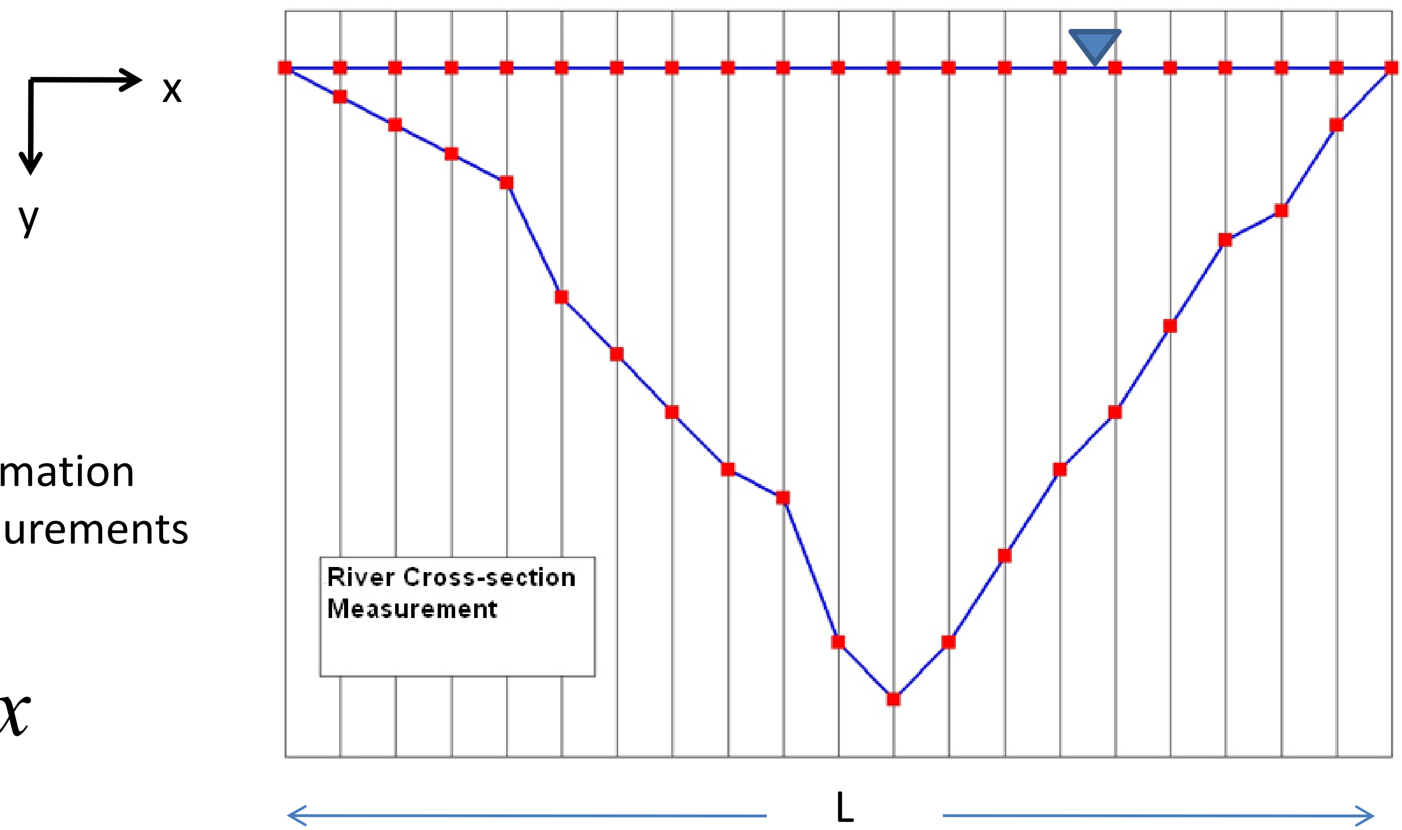


- Assume
  - increasing order
  - equidistant (with $\Delta x = h$)
  - $x_0 = a$ and $x_n = b$



Discharge estimation
from velocity measurements

$$Q = \int_0^R 2\pi r v\,dr$$

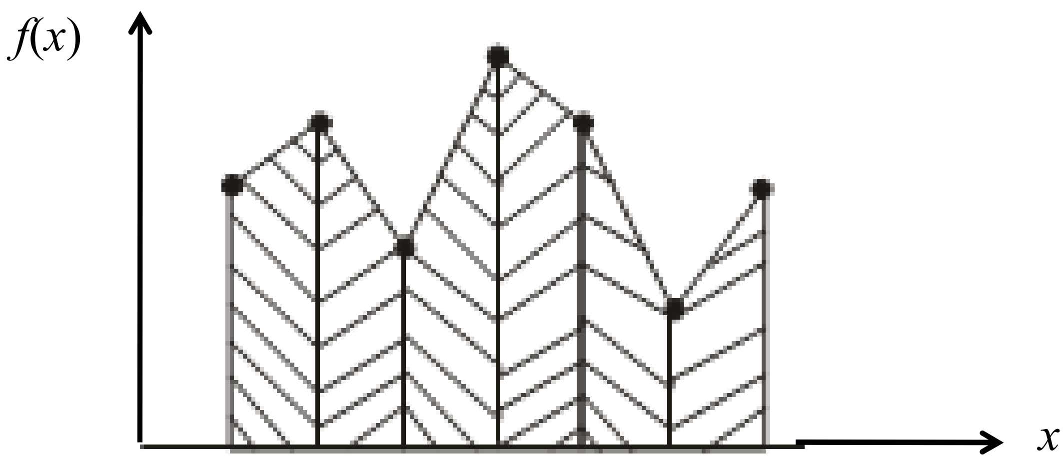


River section area estimation
from flow depth measurements

$$A = \int_0^L y\,dx$$

Numerical Integration

- Simplest: Join the function values by straight lines and find the area of the resulting shapes



- The shape is a trapezoid (sometimes triangle)
- Hence the method is called "Trapezoidal Rule"

(Even simpler - Rectangular rule, not common)

Trapezoidal Rule

- There are *n* segments. The integral over the *i*th segment is written as (using Newton D.D.):

$$\int_{x_{i-1}}^{x_i} f(x)dx \approx \widetilde{I}_i = \int_{x_{i-1}}^{x_i} \left[f_{i-1} + (x - x_{i-1}) \frac{f_i - f_{i-1}}{h} \right] dx$$

- Resulting in:

$$\widetilde{I}_i = \int_0^h \left[f_{i-1} + x \frac{f_i - f_{i-1}}{h} \right] dx = h \frac{f_{i-1} + f_i}{2}$$

which is the area of the trapezoid

Trapezoidal Rule

- The desired integral is written as

$$\widetilde{I} = \sum_{i=1}^{n} \widetilde{I}_i = h\left(\frac{f_0}{2} + \sum_{i=1}^{n-1} f_i + \frac{f_n}{2}\right)$$

- How to find the error?
- Take the ith segment:

$$E_i = I_i - \widetilde{I}_i = \int_{x_{i-1}}^{x_i} \left[f(x) - \left(f_{i-1} + (x - x_{i-1}) \frac{f_i - f_{i-1}}{h} \right) \right] dx$$

- From the divided difference method, we have an estimate of the error as

$$f(x) - \left(f_{i-1} + (x - x_{i-1}) \frac{f_i - f_{i-1}}{h} \right) = (x - x_{i-1})(x - x_i) f[x, x_{i-1}, x_i]$$