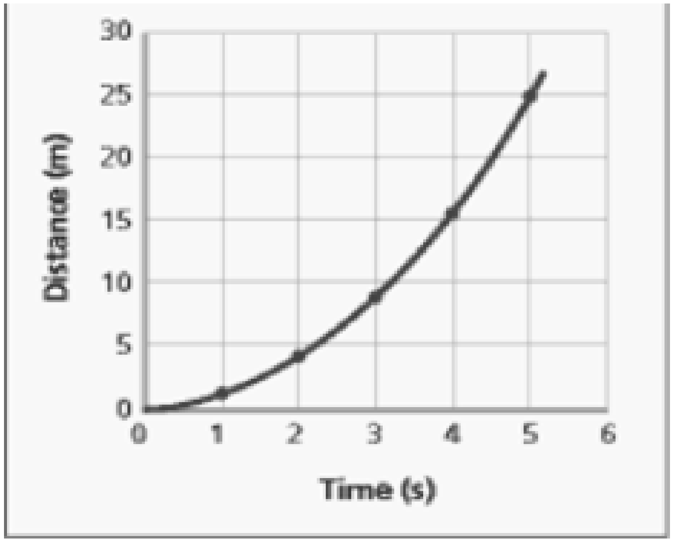
Numerical Differentiation and Integration

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

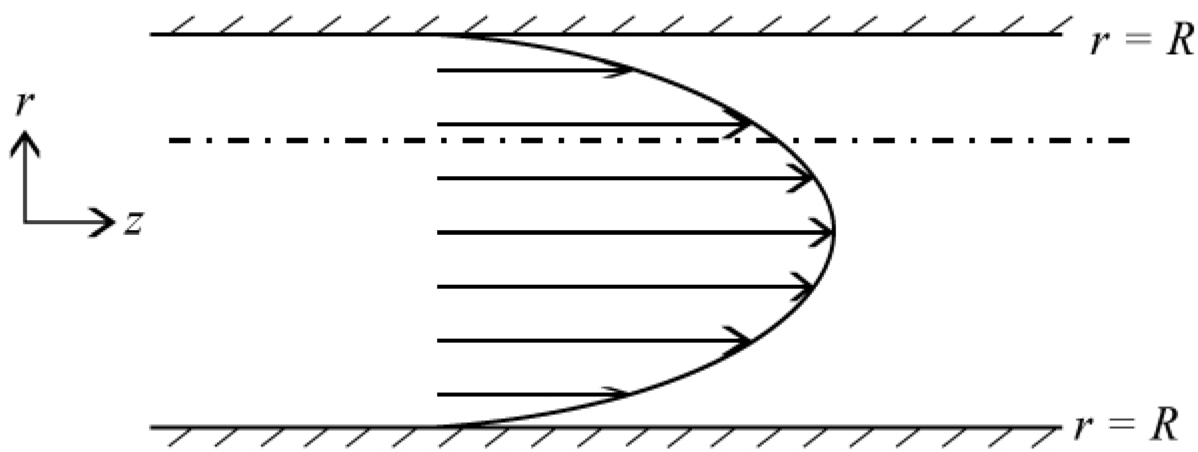
- Estimate the derivatives: e.g., from measured distances, estimate the velocity/acceleration, i.e., given a set of (t,x) values, find dx/dt, d^2x/dt^2

➢ Numerical Differentiation



- Estimate the integral: e.g., from measured flow velocities in a pipe, estimate discharge, i.e., given a set of (*r*,*v*) values, find $\int_0^R 2\pi r v \, dr$

  - Numerical Integration

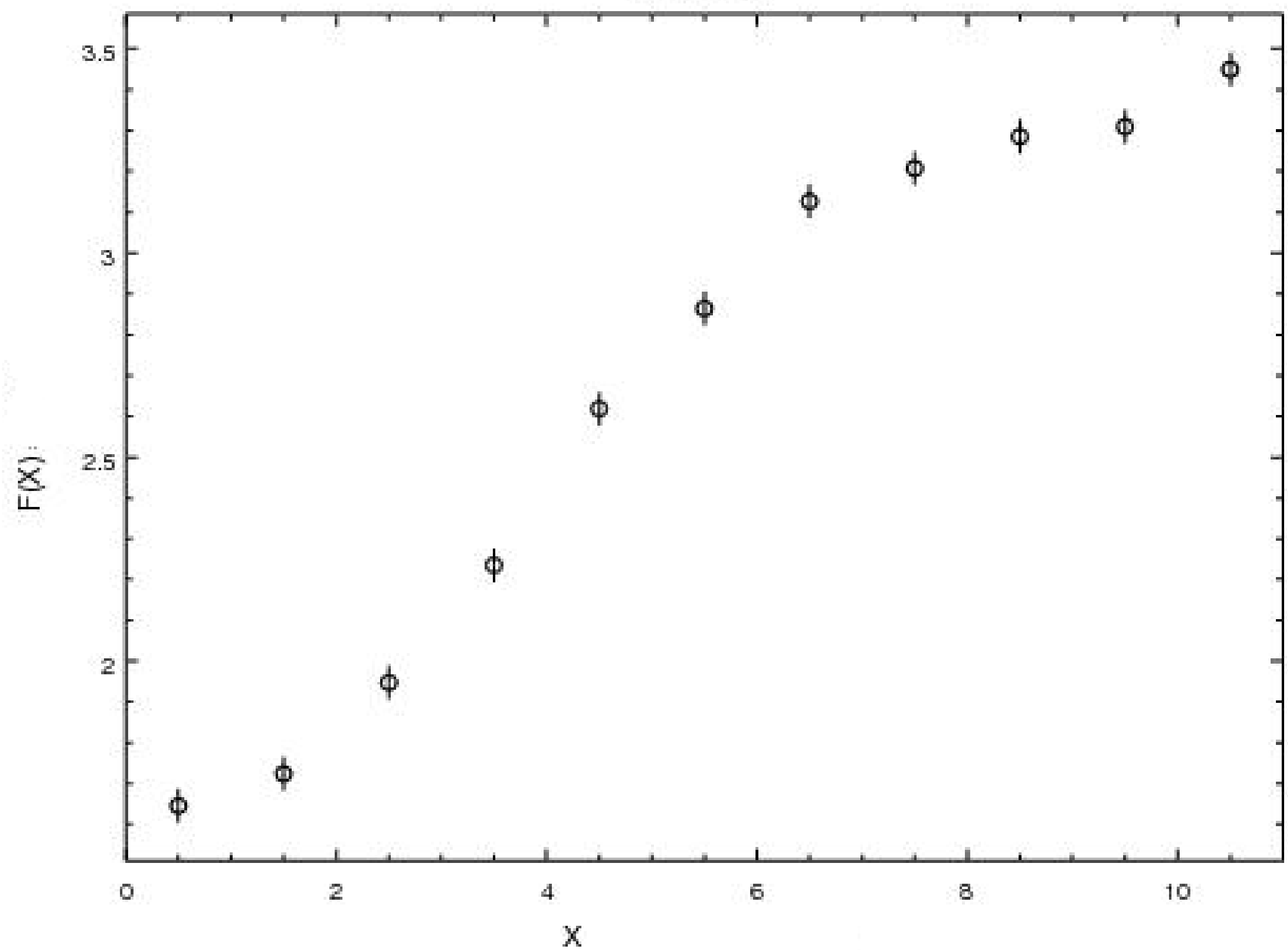


Numerical Differentiation

- Estimate the derivatives of a function from given data

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

- Start with the first derivative
- Simplest: The difference of the function values at two consecutive points divided by the difference in the x values
- Finite Difference: The analytical derivative has zero Δx, but we use a finite value
- What if we want more accurate estimates?


3.5
3
2.5
2
F(X)
0
2
4
6
8
10
X

First Derivative

- For simplicity, let us use f_i for $f(x_i)$
- Assume that the x's are arranged in increasing order ($x_n > x_{n-1} > \ldots > x_0$).
- For estimating the first derivative at x_i :
  - Forward difference: $$f_i' = \frac{f_{i+1} - f_i}{x_{i+1} - x_i}$$
  - Backward difference: $$f_i' = \frac{f_i - f_{i-1}}{x_i - x_{i-1}}$$
  - Central difference: $$f_i' = \frac{f_{i+1} - f_{i-1}}{x_{i+1} - x_{i-1}}$$

First Derivative

- Most of the times, the function is “measured” at equal intervals
- Assume that $x_n - x_{n\text{-}1} = x_{n\text{-}1} - x_{n\text{-}2} = \ldots = x_1 - x_0 = h$
- Then, the first derivative at x_i :
  - Forward difference: $$f_i' = \frac{f_{i+1} - f_i}{h}$$
  - Backward difference: $$f_i' = \frac{f_i - f_{i-1}}{h}$$
  - Central difference: $$f_i' = \frac{f_{i+1} - f_{i-1}}{2h}$$

First Derivative: Error Analysis

- What is the error in these approximations?
- As an example, if the exact function is a straight line, the estimate would have no error
- For forward difference, use Taylor's series:

$$f_{i+1} = f_i + hf'(x_i) + \frac{h^2}{2} f''(x_i) + \ldots + \frac{h^m}{m!} f^{[m]}(x_i) + \frac{h^{m+1}}{(m+1)!} f^{[m+1]}(\zeta_f)$$

$$\zeta_f \in \left(x_i, x_{i+1}\right)$$

ζ_f is a point in the forward interval (x_i, x_{i+1})

- We use $f'(x_i)$ to denote the exact value of the derivative at x_i (the estimation is f_i')

First Derivative: Error Analysis

- Truncating at the linear term

$$f_{i+1} = f_i + hf'(x_i) + \frac{h^2}{2} f''(\zeta_f)$$

- Which implies that

$$f'(x_i) = \frac{f_{i+1} - f_i}{h} - \frac{h}{2} f''(\zeta_f)$$

- The error in the forward difference approximation is, therefore,

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

First Derivative: Error Analysis

- Since the error is proportional to *h*, the method is called O(*h*) accurate.
- Similarly, the error in backward difference is obtained by expansion of f_{i-1}, as

$$f'(x_i) = \frac{f_i - f_{i-1}}{h} + \frac{h}{2} f''(\zeta_b)$$

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

ζ_b is a point in the backward interval, $(x_{i\text{-}1}, x_i)$

First Derivative: Error Analysis

- The error in central difference is obtained by expansion of both f_{i+1} and f_{i-1}, as

$$f_{i+1} = f_i + hf'(x_i) + \frac{h^2}{2} f''(x_i) + \frac{h^3}{6} f'''(\zeta_f)$$

$$f_{i-1} = f_i - hf'(x_i) + \frac{h^2}{2} f''(x_i) - \frac{h^3}{6} f'''(\zeta_b)$$

- Using intermediate value theorem

$$f'(x_i) = \frac{f_{i+1} - f_{i-1}}{2h} - \frac{h^2}{6} f'''(\zeta_c)$$

$$f'(x_i) - f_i' = -\frac{h^2}{6} f'''(\zeta_c)$$

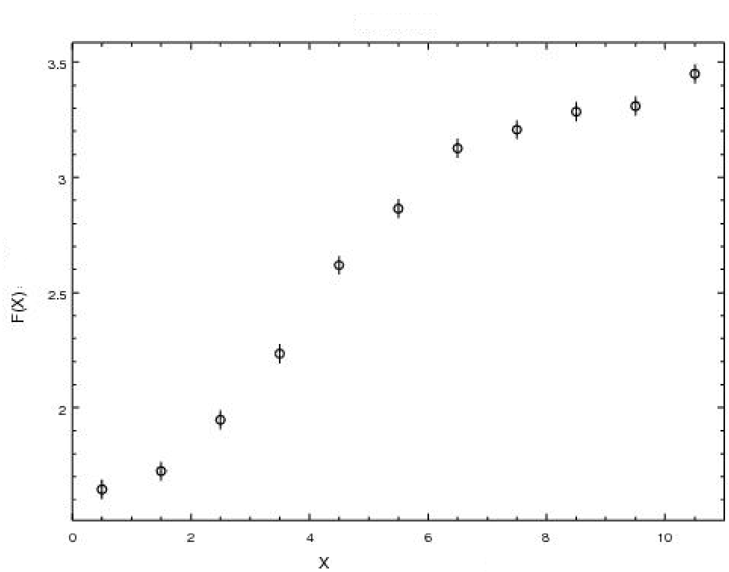
ζ_c is a point in the interval, $(x_{i\text{-}1}, x_{i+1})$

First Derivative: Error Analysis

- Clearly, the method is $O(h^2)$ accurate.
- If we reduce the step size by half, the error in the estimation by forward or backward difference should reduce by half, but that in central difference should reduce to one-fourth
- The presence of the derivatives in the error expression complicates this simple deduction!
- Note that the error in the forward/backward differences has the second derivative, while that in central difference has the third.

First Derivative: Error Analysis

- The forward/backward differences are exact for a linear function, central difference is exact for a quadratic function
- How to get more accurate forward difference?
- In addition to *i* and *i*+1, use *i*+2 also



First Derivative: Error Analysis

- Use a quadratic interpolating polynomial and find its slope at *i*
- Or, combine two lower order estimates
- Or, use Taylor's series expansion, which will provide an error estimate also

First Derivative: Quadratic interpolation

- Using Newton's divided difference

$$f_2(x) = f_i + (x - x_i)\frac{f_{i+1} - f_i}{h} + (x - x_i)(x - x_{i+1})\frac{\dfrac{f_{i+2} - f_{i+1}}{h} - \dfrac{f_{i+1} - f_i}{h}}{2h}$$

- Derivative at x_i

$$\frac{f_{i+1} - f_i}{h} + (-h)\frac{\dfrac{f_{i+2} - f_{i+1}}{h} - \dfrac{f_{i+1} - f_i}{h}}{2h} = \frac{-3f_i + 4f_{i+1} - f_{i+2}}{2h}$$

Combine two estimates: Richardson Extrapolation

- O(h) accurate: $$f'(x_i) = \frac{f_{i+1} - f_i}{h} + O(h)$$
- Write $$f'(x_i) = \frac{f_{i+1} - f_i}{h} + E + O(h^2)$$
- and $$f'(x_i) = \frac{f_{i+2} - f_i}{2h} + 2E + O(h^2)$$
- Eliminate E: $$2f'(x_i) - f'(x_i) = 2\frac{f_{i+1} - f_i}{h} - \frac{f_{i+2} - f_i}{2h}$$

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

First Derivative: Taylor's series

$$f_{i+1} = f_i + hf'(x_i) + \frac{h^2}{2} f''(x_i) + \frac{h^3}{6} f'''(x_i) + \frac{h^4}{4!} f''''(\zeta_{f1})$$

$$f_{i+2} = f_i + 2hf'(x_i) + \frac{4h^2}{2} f''(x_i) + \frac{8h^3}{6} f'''(x_i) + \frac{16h^4}{4!} f''''(\zeta_{f1})$$

$\zeta_{f1} \in (x_i, x_{i+1})$ and $\zeta_{f2} \in (x_i, x_{i+2})$

- Eliminate the 2nd derivative

$$4f_{i+1} - f_{i+2} = 3f_i + 2hf'(x_i) - \frac{4h^3}{6} f'''(x_i) + O(h^4)$$

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

Taylor's series

- $O(h^2)$ accurate

$$f_i' = \frac{-3f_i + 4f_{i+1} - f_{i+2}}{2h}$$

$$\text{Error}: -\frac{h^2}{3} f'''(x_i) + O(h^3)$$

- General Method:

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

- Equate coefficients:

$$\begin{aligned}
c_i + c_{i+1} + c_{i+2} &= 0 \\
c_{i+1} + 2c_{i+2} &= 1 \\
c_{i+1} + 4c_{i+2} &= 0
\end{aligned}$$

=> -3/2,2,-1/2

Backward difference

- Similarly, for backward difference, O(h^2) accurate:

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

$$
\begin{aligned}
c_i + c_{i-1} + c_{i-2} &= 0 \\
c_{i-1} + 2c_{i-2} &= -1 \\
c_{i-1} + 4c_{i-2} &= 0
\end{aligned}
$$

$$f_i' = \frac{3f_i - 4f_{i-1} + f_{i-2}}{2h}$$

$$\text{Error}: \frac{h^2}{3} f''(x_i) + O(h^3)$$

Central Difference

- And, for central difference, O(h^4) accurate:

$$
\begin{aligned}
f_i' &= \frac{1}{h}\left(c_{i-2}f_{i-2} + c_{i-1}f_{i-1} + c_i f_i + c_{i+1}f_{i+1} + c_{i+2}f_{i+2}\right) \\
&= \frac{c_{i-2} + c_{i-1} + c_i + c_{i+1} + c_{i+2}}{h} f_i + \left(-2c_{i-2} - c_{i-1} + c_{i+1} + 2c_{i+2}\right) f'(x_i) \\
&+ \frac{h}{2}\left(4c_{i-2} + c_{i-1} + c_{i+1} + 4c_{i+2}\right) f''(x_i) + \frac{h^2}{6}\left(-8c_{i-2} - c_{i-1} + c_{i+1} + 8c_{i+2}\right) f'''(x_i) \\
&+ \frac{h^3}{24}\left(16c_{i-2} + c_{i-1} + c_{i+1} + 16c_{i+2}\right) f''''(x_i) + \ldots
\end{aligned}
$$

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

$$f_i' = \frac{f_{i-2} - 8f_{i-1} + 0f_i + 8f_{i+1} - f_{i+2}}{12h}$$

$$\text{Error}: \frac{h^4}{30} f^{[5]}(x_i) + O(h^6)$$

General formulation

- In general, for the n^{th} derivative

$$f_i^{[n]} = \frac{1}{h^n} \sum_{j=-n_b}^{n_f} c_{i+j} f_{i+j}$$

where, n_b is the number of backward grid points, and n_f, forward grid points.

Forward difference formulae $f_i^n = \frac{1}{h^n}\sum_{j=0}^{n_f} c_{i+j} f(x_{i+j})$

Accuracy	Derivative	c_i	c_{i+1}	c_{i+2}	c_{i+3}	c_{i+4}	Error
$O(h)$	f_i'	–1	1				$-hf''/2$
	f_i''	1	–2	1			$-hf'''$
	f_i'''	–1	3	–3	1		$-3hf^{iv}/2$
	f_i^{iv}	1	– 4	6	– 4	1	$-2hf^{v}$
$O(h^2)$	f_i'	–3/2	2	– 1/2			$h^2 f'''/3$
	f_i''	2	–5	4	– 1		$11h^2 f^{iv}/12$
	f_i'''	–5/2	9	– 12	7	– 3/2	$7h^2 f^{v}/4$
$O(h^3)$	f_i'	–11/6	3	– 3/2	1/3		$-h^3 f^{iv}/4$
	f_i''	35/12	– 26/3	19/2	– 14/3	11/12	$-5h^3 f^{v}/6$

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

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

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

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