Numerical Differentiation

ME 2004

Outline

- 1.1: Numerical Differentiation via Taylor Series
- 1.2: Example

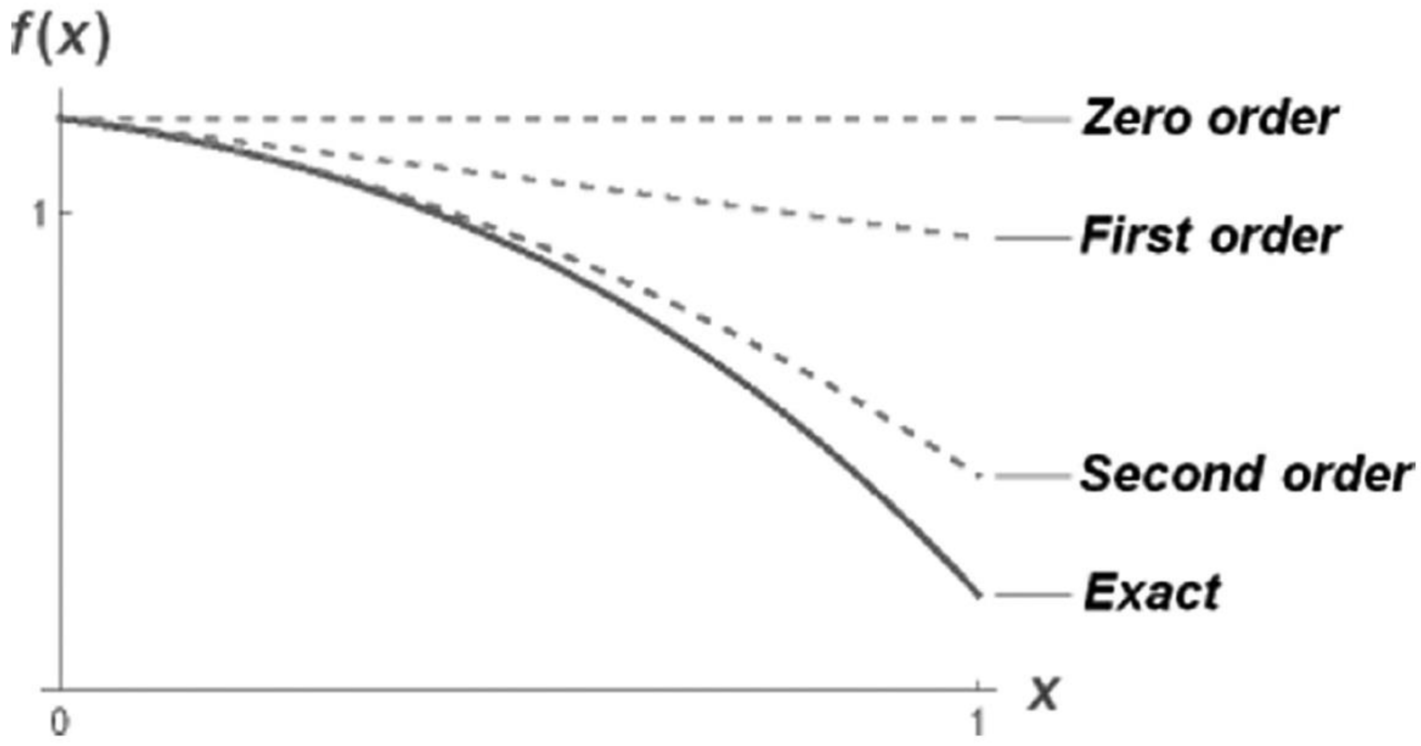
1.1: Numerical Differentiation via Taylor Series

Numerical Differentiation

- Given $f(x)$, compute $\frac{d^n x}{dy^n}$ at the point x_i
  - Can be difficult, especially if $f(x)$ is discrete data instead of a mathematical function
- Numerical differentiation suffers from a conflict between truncation errors and computation time/data availability

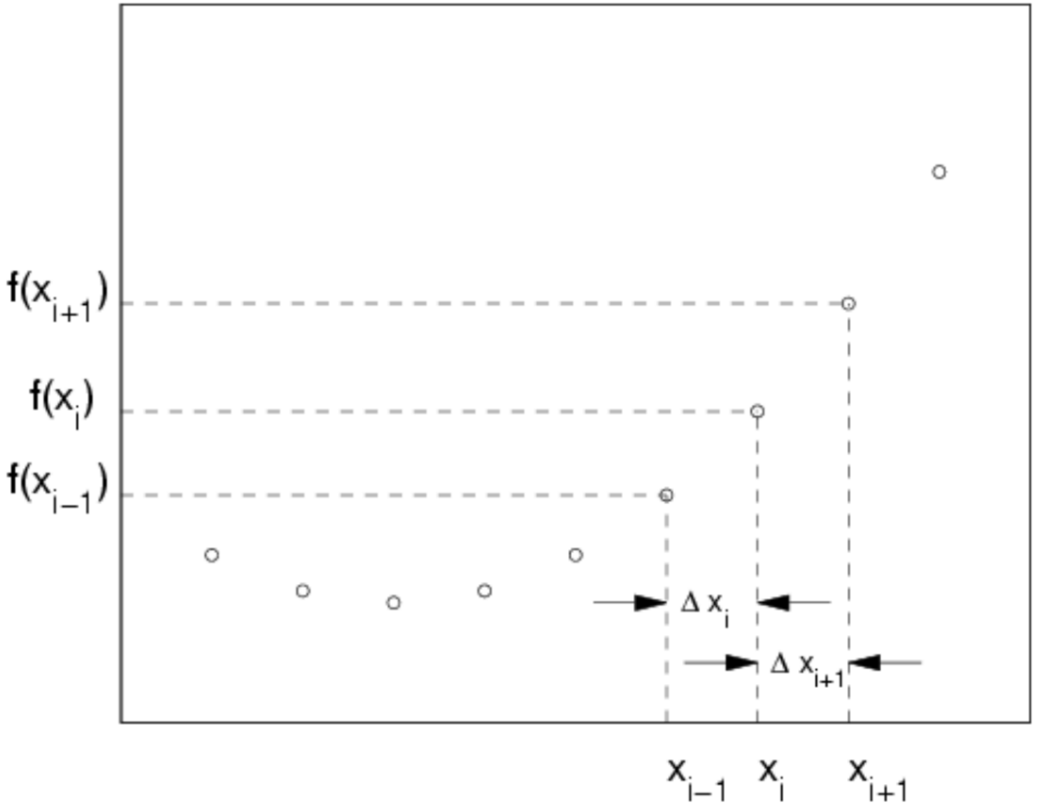
Taylor Series Revisited

- The Taylor Series can be used to predict $f(x_{i+1})$ given x_i and $\frac{d^n x}{dy^n}$
- → If we have $f(x_{i+1})$ and x_i, we can estimate $\frac{d^n x}{dy^n}$



Taylor Series Revisited

- Suppose we have N potentially unevenly spaced data points
  - $\Delta x_i \neq \Delta x_{i+1}$ (potentially)



- Taylor Series expansion about $x = x_i$:

$$f(x_{i+1}) = f(x_i) + (\Delta x_{i+1})\left(\left.\frac{dy}{dx}\right|_{x=x_i}\right) + \left(\frac{(\Delta x_{i+1})^2}{2}\right)\left(\left.\frac{d^2y}{dx^2}\right|_{x=x_i}\right) + \cdots + \left(\frac{(\Delta x_{i+1})^n}{n!}\right)\left(\left.\frac{d^ny}{dx^n}\right|_{x=x_i}\right)$$

Taylor Series Revisited

$$f(x_{i+1}) = f(x_i) + (\Delta x_{i+1})\left(\left.\frac{dy}{dx}\right|_{x=x_i}\right) + \cancel{\left(\frac{(\Delta x_{i+1})^2}{2}\right)\left(\left.\frac{d^2 y}{dx^2}\right|_{x=x_i}\right)} + \cdots + \cancel{\left(\frac{(\Delta x_{i+1})^n}{n!}\right)\left(\left.\frac{d^n y}{dx^n}\right|_{x=x_i}\right)}$$

$$\rightarrow f(x_{i+1}) \cong f(x_i) + (\Delta x_{i+1})\left(\left.\frac{dy}{dx}\right|_{x=x_i}\right) + O\left((\Delta x_{i+1})^2\right)$$

$$\rightarrow \boxed{\left.\frac{dy}{dx}\right|_{x=x_i} \cong \frac{f(x_{i+1}) - f(x_i)}{\Delta x_{i+1}} + O(\Delta x_{i+1})}$$

Forward Difference

Taylor Series Revisited

- Taylor Series expansion about $x = x_i$ (backwards):

$$f(x_{i-1}) = f(x_i) - (\Delta x_i)\left(\left.\frac{dy}{dx}\right|_{x=x_i}\right) + \left(\frac{(\Delta x_i)^2}{2}\right)\left(\left.\frac{d^2y}{dx^2}\right|_{x=x_i}\right) + \cdots + \left(\frac{(\Delta x_i)^n}{n!}\right)\left(\left.\frac{d^ny}{dx^n}\right|_{x=x_i}\right)$$

$$\rightarrow f(x_{i-1}) \cong f(x_i) - (\Delta x_i)\left(\left.\frac{dy}{dx}\right|_{x=x_i}\right) + O\big((\Delta x_i)^2\big)$$

$$\rightarrow \boxed{\left.\frac{dy}{dx}\right|_{x=x_i} \cong \frac{f(x_i) - f(x_{i-1})}{\Delta x_i} + O(\Delta x_i)}$$

Backward Difference

Taylor Series Revisited

- We have the forward and the backward differences, but surely there's a middle ground?

$$f(x_{i+1}) \cong f(x_i) + (\Delta x_{i+1})\left(\left.\frac{dy}{dx}\right|_{x=x_i}\right) + O\left((\Delta x_{i+1})^2\right)$$

$$f(x_{i-1}) = f(x_i) - (\Delta x_i)\left(\left.\frac{dy}{dx}\right|_{x=x_i}\right) + O\left((\Delta x_i)^2\right)$$

$$\rightarrow f(x_{i+1}) - f(x_{i-1}) \cong (\Delta x_{i+1})\left(\left.\frac{dy}{dx}\right|_{x=x_i}\right) - (\Delta x_i)\left(\left.\frac{dy}{dx}\right|_{x=x_i}\right) + O\left((\Delta x_{i+1})^2\right) + O\left((\Delta x_i)^2\right)$$

Taylor Series Revisited

$$f(x_{i+1}) - f(x_{i-1}) \cong (\Delta x_{i+1})\left(\left.\frac{dy}{dx}\right|_{x=x_i}\right) - (\Delta x_i)\left(\left.\frac{dy}{dx}\right|_{x=x_i}\right) + O\left((\Delta x_{i+1})^2\right) + O\left((\Delta x_i)^2\right)$$

$$\rightarrow f(x_{i+1}) - f(x_{i-1}) \cong (\Delta x_{i+1} - \Delta x_i)\left(\left.\frac{dy}{dx}\right|_{x=x_i}\right) + O\left((\Delta x_{i+1})^2\right) + O\left((\Delta x_i)^2\right)$$

$$\rightarrow \boxed{\left.\frac{dy}{dx}\right|_{x=x_i} \cong \frac{f(x_{i+1}) - f(x_{i-1})}{\Delta x_{i+1} - \Delta x_i} + O\left((\Delta x_i)^2\right) \cong \frac{f(x_{i+1}) - f(x_{i-1})}{2\Delta x_i} + O\left((\Delta x_i)^2\right)}$$

Central Difference

Taylor Series Revisited

- Forward difference: $\left.\frac{dy}{dx}\right|_{x=x_i} \cong \frac{f(x_{i+1})-f(x_i)}{\Delta x_{i+1}} + O(\Delta x_{i+1})$
- Backward difference: $\left.\frac{dy}{dx}\right|_{x=x_i} \cong \frac{f(x_i)-f(x_{i-1})}{\Delta x_i} + O(\Delta x_i)$
- Central difference: $\left.\frac{dy}{dx}\right|_{x=x_i} \cong \frac{f(x_{i+1})-f(x_{i-1})}{\Delta x_{i+1}-\Delta x_i} + O\left((\Delta x_i)^2\right)$

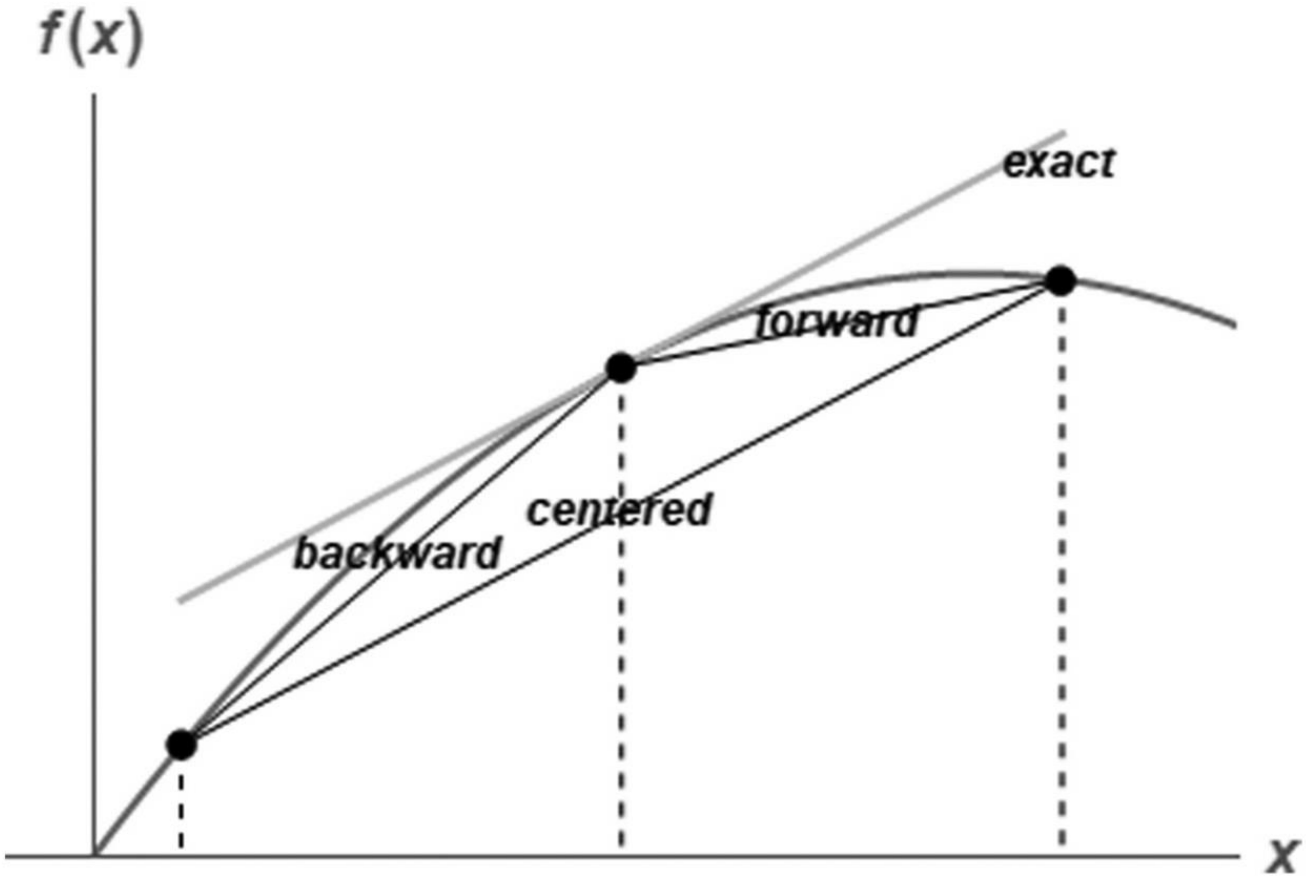
- These formulas apply for (un)equally spaced data, although more accurate methods exist for unequally spaced data

Taylor Series Revisited

- Assuming a constant step size, h:

- Forward difference: $\left.\frac{dy}{dx}\right|_{x=x_i} \cong \frac{f(x_{i+1})-f(x_i)}{h} + O(h)$
- Backward difference: $\left.\frac{dy}{dx}\right|_{x=x_i} \cong \frac{f(x_i)-f(x_{i-1})}{h} + O(h)$
- Central difference: $\left.\frac{dy}{dx}\right|_{x=x_i} \cong \frac{f(x_{i+1})-f(x_{i-1})}{2h} + O(h^2)$

Taylor Series Revisited



Taylor Series Revisited

- Big O notation: allows us to compare the truncation errors of numerical methods
- $O(h^n)$: truncation error is proportional to the step size raised to the nth power
- Forward and Backward differences have error $O(\Delta x_{i+1})$ and $O(\Delta x_i)$, so truncation errors are linearly proportional to the step size
    - Halving the step size halves the truncation error
- Central difference has error $O\left((\Delta x_i)^2\right)$, so truncation error is quadratically proportional to the step size
    - Halving the step size quarters the truncation error

Taylor Series Revisited

- To increase the accuracy (decrease truncation error), we could also algebraically combine multiple Taylor Series expansions about other points

$$\left.\frac{dy}{dx}\right|_{x=x_i} \cong \frac{\left(-\frac{11}{6}\right)f(x_i) + 3f(x_{i+1}) - \left(\frac{3}{2}\right)f(x_{i+2}) + \left(\frac{1}{3}\right)f(x_{i+3})}{h} + O\left((\Delta x_{i+1})^3\right)$$

Forward difference, 3rd order accuracy (assumes equal step size)

- …but computation time becomes a concern.

Taylor Series Revisited

- An even bigger concern is the lack of available data:

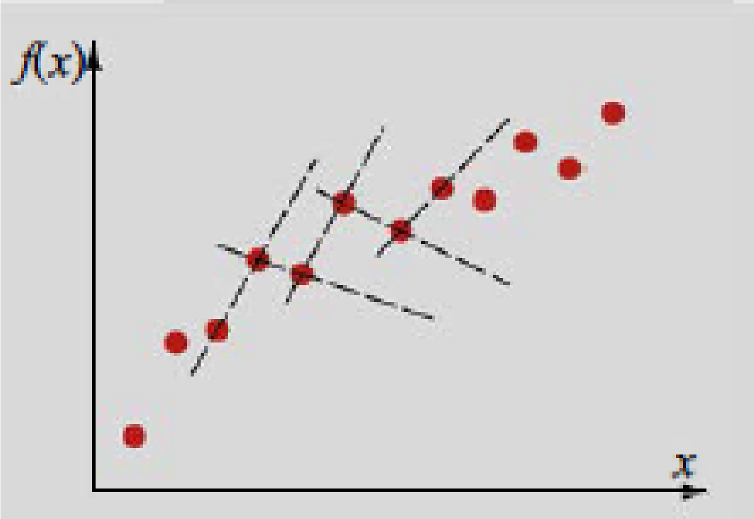
t (s)	0	1	2	3	4
x (m)	0	2	3	3.1	3.7

- Central difference: $\left.\frac{dy}{dx}\right|_{x=x_i} \cong \frac{f(x_{i+1})-f(x_{i-1})}{\Delta x_{i+1} - \Delta x_i} + O\left((\Delta x_i)^2\right)$

- …so we can't compute $\left.\frac{dx}{dt}\right|_{t=4}$ using the central (or forward) difference because the next point does not exist.

Taylor Series Revisited

- Minimizing error in the dataset is imperative!



- Large variations of $\frac{dy}{dx}$ will be seen from point to point

1.2: Example

Example

- Compute $\left.\frac{dx}{dt}\right|_{t=1}$ using the forward difference.

t (s)	0	1	2	3	4
x (m)	0	2	3	3.1	3.7

$$\left.\frac{dx}{dt}\right|_{t=1} \cong \frac{x(t_{i+1}) - x(t_i)}{\Delta t_{i+1}} = \frac{x(3) - x(2)}{t(3) - t(2)} = \frac{3-2}{2-1}$$

MATLAB Notation!!!!!!

$$\rightarrow \boxed{\left.\frac{dx}{dt}\right|_{t=1} \cong 1\frac{m}{s}}$$

Example

- Compute $\left.\frac{dx}{dt}\right|_{t=1}$ using the backward difference.

t (s)	0	1	2	3	4
x (m)	0	2	3	3.1	3.7

$$\left.\frac{dx}{dt}\right|_{t=1} \cong \frac{x(t_i) - x(t_{i-1})}{\Delta t_i} = \frac{x(2) - x(1)}{t(2) - t(1)} = \frac{2-0}{1-0}$$

MATLAB Notation!!!!!!

$$\rightarrow \boxed{\left.\frac{dx}{dt}\right|_{t=1} \cong 2\frac{m}{s}}$$

Example

- Compute $\left.\frac{dx}{dt}\right|_{t=1}$ using the central difference.

t (s)	0	1	2	3	4
x (m)	0	2	3	3.1	3.7

$$\left.\frac{dx}{dt}\right|_{t=1} \cong \frac{x(t_{i+1}) - x(t_{i-1})}{\Delta t_{i+1} - \Delta t_i} = \frac{x(3) - x(1)}{t(3) - t(1)} = \frac{3-0}{2-0}$$

MATLAB Notation!!!!!!

$$\rightarrow \boxed{\left.\frac{dx}{dt}\right|_{t=1} \cong 1.5\,\frac{m}{s}}$$

Higher-Order Derivatives

- To obtain higher-order derivatives $\left(\frac{d^2y}{dx^2}, etc.\right)$, incorporate more terms of the Taylor Series expansion

$$f(x_{i-1}) = f(x_i) - (\Delta x_i)\left(\left.\frac{dy}{dx}\right|_{x=x_i}\right) + \left(\frac{(\Delta x_i)^2}{2}\right)\left(\left.\frac{d^2y}{dx^2}\right|_{x=x_i}\right) + \cdots + \left(\frac{(\Delta x_i)^n}{n!}\right)\left(\left.\frac{d^ny}{dx^n}\right|_{x=x_i}\right)$$

- Common assumption is the data are equally spaced (constant step size)

Higher-Order Derivatives

- Finite difference tables: gives coefficients (weights) to various data points to compute high-order and/or high-accuracy derivatives

Central finite difference [edit]

This table contains the coefficients of the **central** differences, for several orders of accuracy and with uniform grid spacing:[1]

Derivative	Accuracy	−5	−4	−3	−2	−1	0	1	2	3	4	5
1	2					−1/2	0	1/2				
	4				1/12	−2/3	0	2/3	−1/12			
	6			−1/60	3/20	−3/4	0	3/4	−3/20	1/60		
	8		1/280	−4/105	1/5	−4/5	0	4/5	−1/5	4/105	−1/280	
2	2					1	−2	1				
	4				−1/12	4/3	−5/2	4/3	−1/12			
	6			1/90	−3/20	3/2	−49/18	3/2	−3/20	1/90		
	8		−1/560	8/315	−1/5	8/5	−205/72	8/5	−1/5	8/315	−1/560	

Higher-Order Derivatives

- High-order/high-accuracy schemes are best implemented in MATLAB, especially if the data is unequally spaced (many custom programs treat unequally spaced data with an advanced algorithm)

- `diffxy()` function: NOT built-in; download from MATLAB's File Exchange
  - Not used in this class, but may want to keep it for later

Summary

- Forward difference: $\left.\frac{dy}{dx}\right|_{x=x_i} \cong \frac{f(x_{i+1})-f(x_i)}{\Delta x_{i+1}} + O(\Delta x_{i+1})$
- Backward difference: $\left.\frac{dy}{dx}\right|_{x=x_i} \cong \frac{f(x_i)-f(x_{i-1})}{\Delta x_i} + O(\Delta x_i)$
- Central difference: $\left.\frac{dy}{dx}\right|_{x=x_i} \cong \frac{f(x_{i+1})-f(x_{i-1})}{\Delta x_{i+1} - \Delta x_i} + O\left((\Delta x_i)^2\right)$

- Accuracy can be increased by reducing step size and/or combining multiple Taylor Series expansions about other points
- Some schemes cannot be applied at the boundaries of a dataset (forward difference cannot be applied at the last point, etc.)
- Implement high-order/high-accuracy schemes in MATLAB if you ever need them in a future class/research