MATH2089
Numerical Methods
Lecture 7

Numerical Differentiation

Numerical Differentiation

- The function to be differentiated can be in one of the following forms
  - A simple continuous function being linear, quadratic, higher order polynomial, exponential, etc. *They can be evaluated analytically using calculus.*
  - For example
    - $f(x) = y = a_0x + a_1$
    - $f(x) = y = a_0x^2 + a_1x + a_2$
    - $f(x) = y = a_0x^n + a_1x^{n-1} + a_2x^{n-2} + a_3x^{n-3} + \ldots..$
  - Differentiation with respect to x
    - $f'(x) = dydx = a_0$
    - $f'(x) = dydx = 2a_0x + a_1$
    - $f'(x) = dydx = na_0x^{n-1} + (n-1)a_1x^{n-2} + \ldots..$

Numerical Differentiation (continue)

- A complicated continuous function that is difficult or impossible to differentiate or integrate directly. Analytical solutions are often impractical, and sometimes impossible.

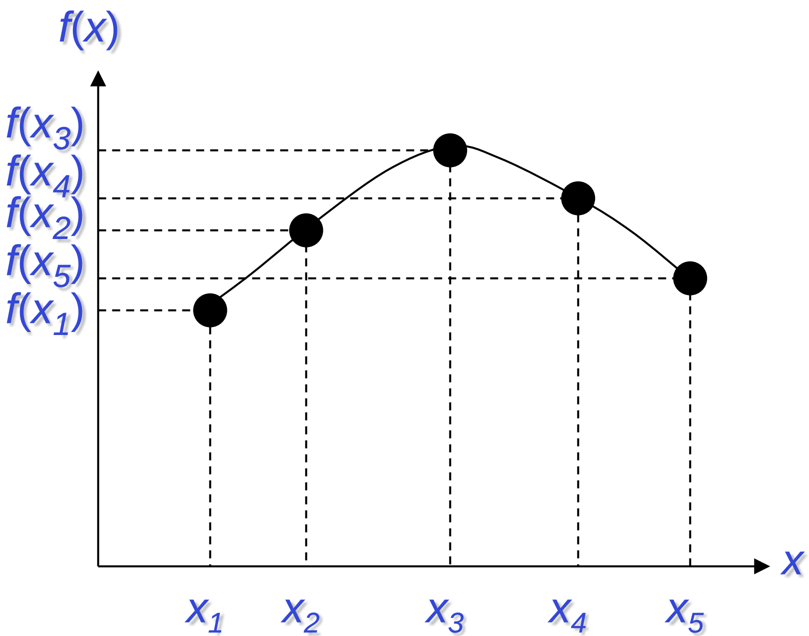
Approximate method must be employed.

- A tabulated function where values of x and $f(x)$ are given at a number of discrete points, as if often the case with experimental or field data.

Approximate method must be employed.

Numerical Differentiation (continue)

- Based on a set of discrete data, how we can best approximate
  - Slope (first order derivative) $f'(x) = dy/dx$
  - Curvature (second order derivative) $f''(x) = d^2y/dx^2$



Engineering Applications - Example

A plane is being tracked by radar, and data is taken every second in polar coordinates θ and *r*.

t (s)	100	101	102	103	104	105
θ (rad)	0.75	0.72	0.70	0.68	0.67	0.66
r (ft)	5120	5370	5560	5800	6030	6240

At t=103 seconds find the vector expression for velocity and acceleration. The velocity and acceleration given in polar coordinates are:

$$\vec{v} = \dot{r}\,\vec{e}_r + r\dot{\theta}\,\vec{e}_\theta$$

$$\vec{a} = \left(\ddot{r} - r\dot{\theta}^2\right)\vec{e}_r + \left(r\ddot{\theta} + 2\dot{r}\dot{\theta}\right)\vec{e}_\theta$$

Engineering Applications - Example

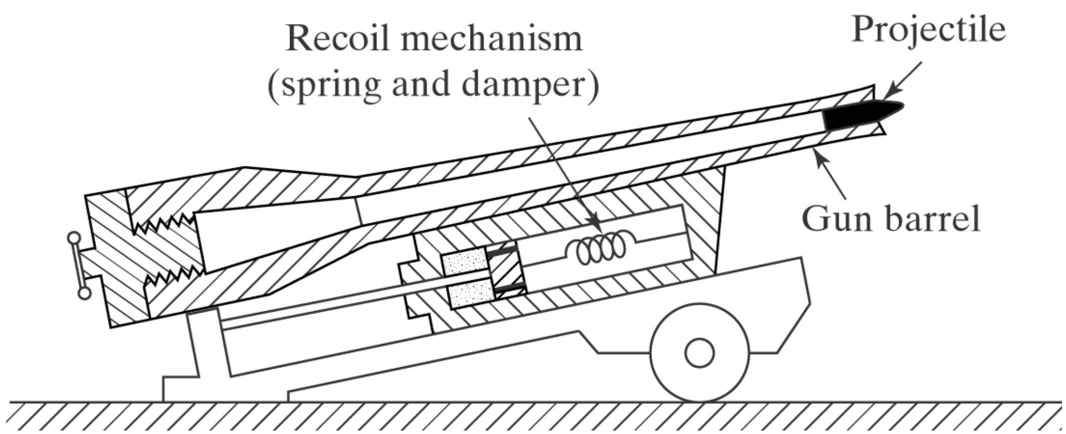


Figure 7.1
Recoil mechanism of a cannon.

$$x(t) = (c_1 + c_2 t) e^{-\omega_n t}$$

$$c_1 = x_0, \; c_2 = \dot{x}_0 + \omega_n x_0, \;\; \omega_n = \sqrt{k/m}$$

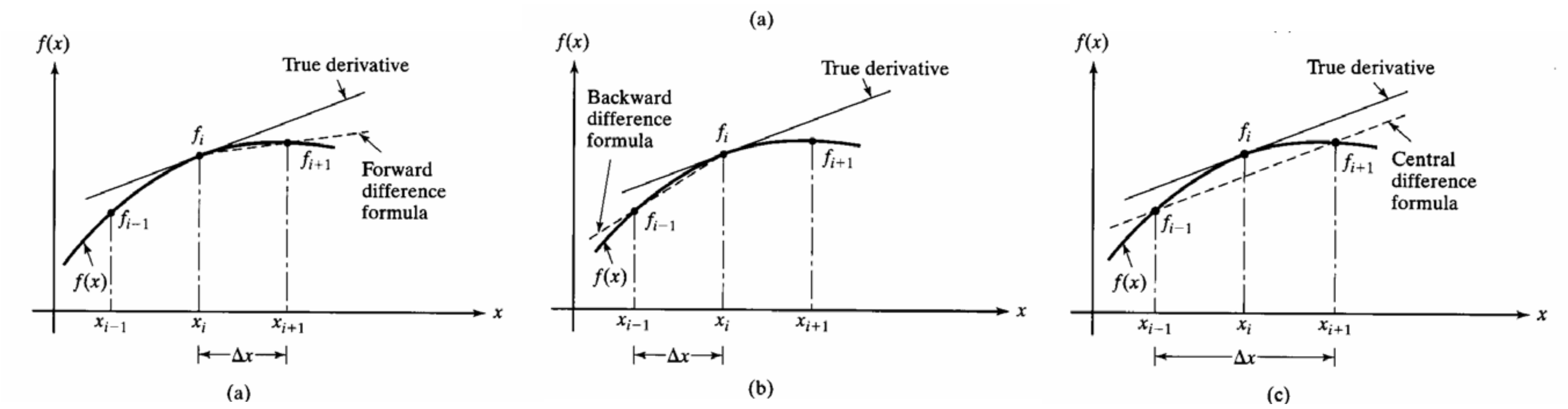
Find the maximum recoil velocity of the cannon using numerical differentiation with x_0=0 and $\dot{x}_0$ =5m/s.

Engineering Applications

The one-dimensional forms of some constitutive laws commonly used in engineering and science

Law	Equation	Physical Area	Gradient	Flux	Proportionality
Fourier's law	$q = -k\frac{dT}{dx}$	Heat conduction	Temperature	Heat flux	Thermal Conductivity
Fick's law	$J = -D\frac{dc}{dx}$	Mass diffusion	Concentration	Mass flux	Diffusivity
Darcy's law	$q = -k\frac{dh}{dx}$	Flow through porous media	Head	Flow flux	Hydraulic Conductivity
Ohm's law	$J = -\sigma\frac{dV}{dx}$	Current flow	Voltage	Current flux	Electrical Conductivity
Newton's viscosity law	$\tau = \mu\frac{du}{dx}$	Fluids	Velocity	Shear Stress	Dynamic Viscosity
Hooke's law	$\sigma = E\frac{\Delta L}{L}$	Elasticity	Deformation	Stress	Young's Modulus

Basic Finite-Difference Approximations (Graphic Interpretation)



(a) forward: $$\left.\frac{df}{dx}\right|_i \approx \frac{\Delta f}{\Delta x} = \frac{f_{i+1} - f_i}{x_{i+1} - x_i}$$

(b) backward: $$\left.\frac{df}{dx}\right|_i \approx \frac{\Delta f}{\Delta x} = \frac{f_i - f_{i-1}}{x_i - x_{i-1}}$$

(c) central: $$\left.\frac{df}{dx}\right|_i \approx \frac{\Delta f}{\Delta x} = \frac{f_{i+1} - f_{i-1}}{x_{i+1} - x_{i-1}}$$

Taylor Series Expansion

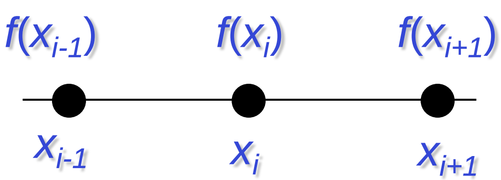
- Derivatives are replaced by discrete approximations – finite difference forms

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

$$+ \frac{(x_{i+1} - x_i)^n}{n!} f^{(n)}(x_i) + \dots$$

First order derivative

Second order derivative



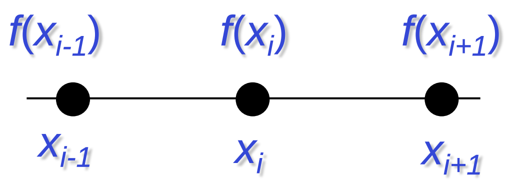
Taylor Series Expansion (continue)

- Let $\Delta x = x_{i+1} - x_i$

$$f_{i+1} = f_i + \Delta x\, f_i' + \frac{(\Delta x)^2}{2!} f_i'' + \frac{(\Delta x)^3}{3!} f_i''' + \frac{(\Delta x)^4}{4!} f_i^{(4)} + \ldots$$

- Rearranging the above equation,

$$f_i' = \frac{f_{i+1} - f_i}{\Delta x} - \frac{\Delta x}{2!} f_i'' - \frac{(\Delta x)^2}{3!} f_i''' - \ldots$$



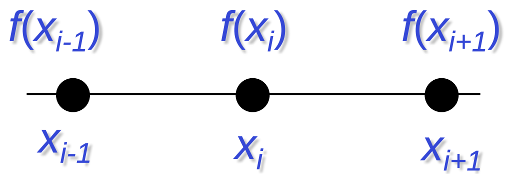
Taylor Series Expansion (continue)

- By applying the mean value theorem,

$$f_i' = \frac{f_{i+1} - f_i}{\Delta x} - \frac{\Delta x}{2!} f''(\xi); \quad x_i < \xi < x_{i+1}$$

- Truncation error term is $O(\Delta x) = -\frac{\Delta x}{2!} f''(\xi)$

- 1st forward difference $\boxed{f_i' = \frac{f_{i+1} - f_i}{\Delta x} + O(\Delta x)}$



Taylor Series Expansion (continue)

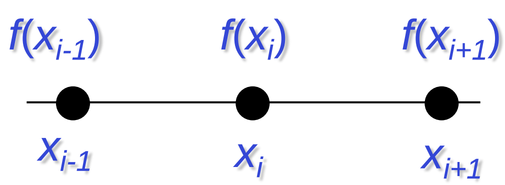
- Let $-\Delta x = x_{i-1} - x_i$

$$f_{i-1} = f_i - \Delta x\, f_i' + \frac{(\Delta x)^2}{2!} f_i'' - \frac{(\Delta x)^3}{3!} f_i''' + \frac{(\Delta x)^4}{4!} f_i^{(4)} - \dots$$

- Rearranging the above equation,

$$f_i' = \frac{f_i - f_{i-1}}{\Delta x} + \underbrace{\frac{\Delta x}{2!} f_i'' - \frac{(\Delta x)^2}{3!} f_i''' + \dots}_{\frac{\Delta x}{2!} f''(\xi) = O(\Delta x)}$$

- 1st backward difference $\boxed{f_i' = \dfrac{f_i - f_{i-1}}{\Delta x} + O(\Delta x)}$



Taylor Series Expansion (continue)

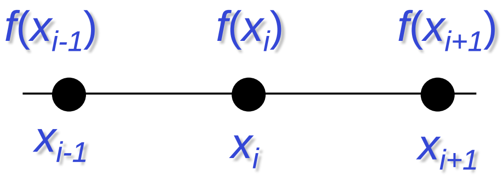
- Recapping that

$$f_{i+1} = f_i + \Delta x\, f_i' + \frac{(\Delta x)^2}{2!} f_i'' + \frac{(\Delta x)^3}{3!} f_i''' + \frac{(\Delta x)^4}{4!} f_i^{(4)} + \ldots$$

$$f_{i-1} = f_i - \Delta x\, f_i' + \frac{(\Delta x)^2}{2!} f_i'' - \frac{(\Delta x)^3}{3!} f_i''' + \frac{(\Delta x)^4}{4!} f_i^{(4)} - \ldots$$

- Removing f'(x_i) yields

$$f_{i+1} - f_{i-1} = 2\Delta x\, f_i' + \frac{(\Delta x)^3}{3} f_i''' + \frac{(\Delta x)^5}{60} f_i^{(5)} + \ldots$$



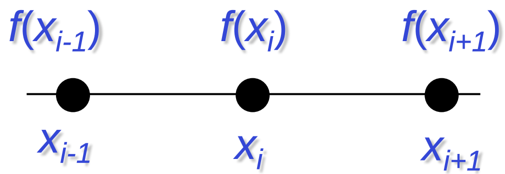
Taylor Series Expansion (continue)

- Rearranging the equation

$$f_i' = \frac{f_{i+1} - f_{i-1}}{2\Delta x} \underbrace{- \frac{(\Delta x)^2}{6} f_i''' - \frac{(\Delta x)^5}{120} f_i^{(5)} - \ldots}_{-\frac{(\Delta x)^2}{6} f_i'''(\xi) = O((\Delta x)^2)}$$

- 2nd central difference

$$\boxed{f_i' = \frac{f_{i+1} - f_{i-1}}{2\Delta x} + O((\Delta x)^2)}$$



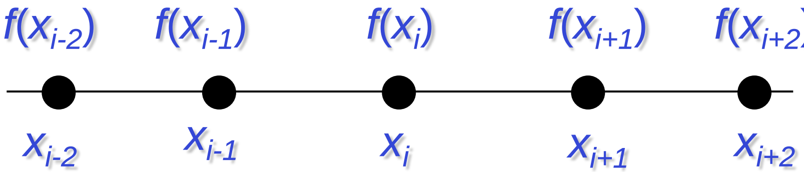
2nd Order Finite Difference

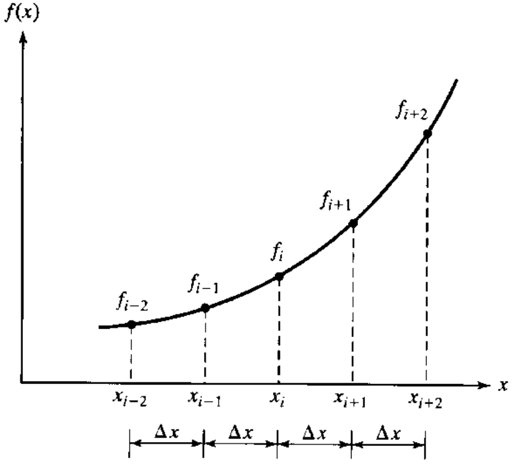
- Recalling Taylor Series Expansion

$$f_{i+1} = f_i + \Delta x f_i' + \frac{(\Delta x)^2}{2!} f_i'' + \frac{(\Delta x)^3}{3!} f_i''' + \frac{(\Delta x)^4}{4!} f_i^{(4)} + \ldots$$

- Using $f_{i+2} = f(x_{i+2}),\ 2\Delta x = x_{i+2} - x_i$ for uniform spacing
- We get

$$f_{i+2} = f_i + 2\Delta x f_i' + \frac{(2\Delta x)^2}{2!} f_i'' + \frac{(2\Delta x)^3}{3!} f_i''' + \frac{(2\Delta x)^4}{4!} f_i^{(4)} + \ldots$$





2nd Order Finite Difference (continue)

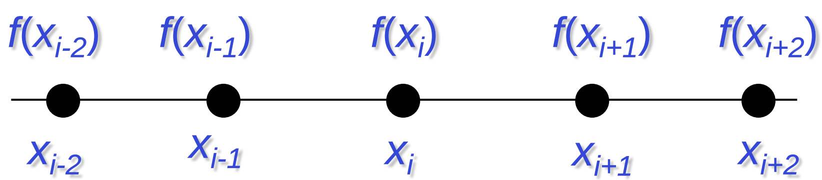
- Multiply by 2

$$\left[f_{i+1} = f_i + \Delta x f_i' + \frac{(\Delta x)^2}{2!} f_i'' + \frac{(\Delta x)^3}{3!} f_i''' + \frac{(\Delta x)^4}{4!} f_i^{(4)} + \dots \right] \quad \text{X 2}$$

- Subtracted from

$$f_{i+2} = f_i + 2\Delta x f_i' + \frac{(2\Delta x)^2}{2!} f_i'' + \frac{(2\Delta x)^3}{3!} f_i''' + \frac{(2\Delta x)^4}{4!} f_i^{(4)} + \dots$$

- We get $\quad f_{i+2} - 2 f_{i+1} = -f_i + (\Delta x)^2 f_i'' + (\Delta x)^3 f_i''' + \dots$



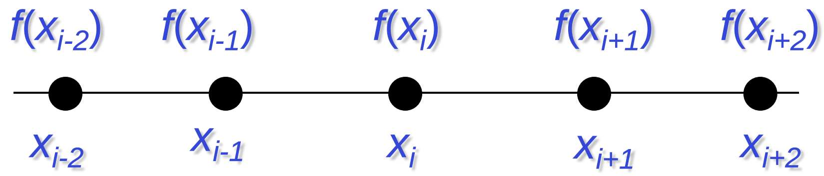
2nd Order Finite Difference (continue)

- Rearranging the equation

$$f_i'' = \frac{f_{i+2} - 2f_{i+1} + f_i}{(\Delta x)^2} \underbrace{-\Delta x\, f_i''' + \ldots}_{-\Delta x\, f'''(\xi) = O(\Delta x)}$$

- 1st forward difference

$$\boxed{f_i'' = \frac{f_{i+2} - 2f_{i+1} + f_i}{(\Delta x)^2} + O(\Delta x)}$$



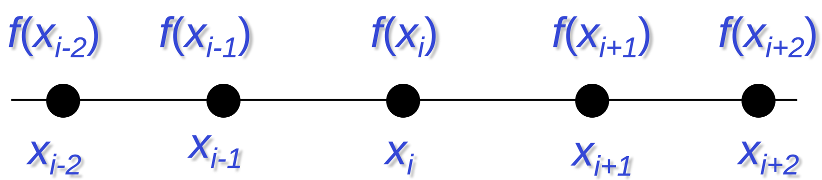
2nd Order Finite Difference (continue)

- Recalling Taylor Series Expansion

$$f_{i-1} = f_i - \Delta x\, f_i' + \frac{(\Delta x)^2}{2!} f_i'' - \frac{(\Delta x)^3}{3!} f_i''' + \frac{(\Delta x)^4}{4!} f_i^{(4)} - \dots$$

- Using $f_{i-2} = f(x_{i-2}),\ 2\Delta x = x_i - x_{i-2}$ for uniform spacing
- We get

$$f_{i-2} = f_i - 2\Delta x\, f_i' + \frac{(2\Delta x)^2}{2!} f_i'' - \frac{(2\Delta x)^3}{3!} f_i''' + \frac{(2\Delta x)^4}{4!} f_i^{(4)} - \dots$$



2nd Order Finite Difference (continue)

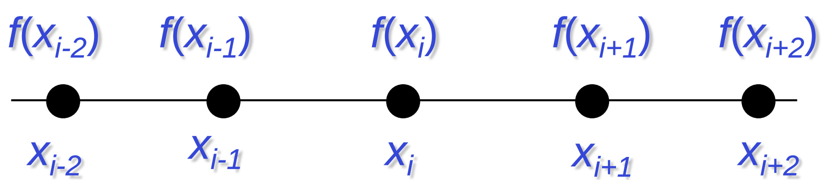
- Multiply by 2

$$\left[\; f_{i-1} = f_i - \Delta x\, f_i' + \frac{(\Delta x)^2}{2!} f_i'' - \frac{(\Delta x)^3}{3!} f_i''' + \frac{(\Delta x)^4}{4!} f_i^{(4)} - \dots \;\right] \quad \text{X 2}$$

- Subtracted from

$$f_{i-2} = f_i - 2\Delta x\, f_i' + \frac{(2\Delta x)^2}{2!} f_i'' - \frac{(2\Delta x)^3}{3!} f_i''' + \frac{(2\Delta x)^4}{4!} f_i^{(4)} - \dots$$

- We get $\quad f_{i-2} - 2 f_{i-1} = - f_i + (\Delta x)^2 f_i'' - (\Delta x)^3 f_i''' + \dots$



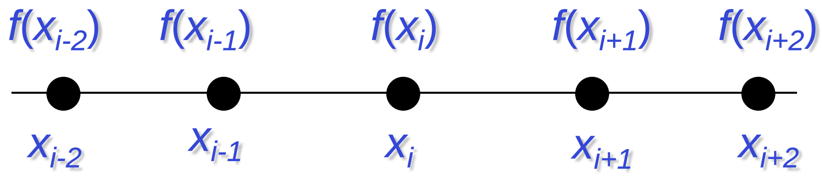
2nd Order Finite Difference (continue)

- Rearranging the equation

$$f_i'' = \frac{f_i - 2f_{i-1} + f_{i-2}}{(\Delta x)^2} \underbrace{-\Delta x\, f_i''' + \ldots}_{-\Delta x\, f'''(\xi) = O(\Delta x)}$$

- 1st backward difference

$$\boxed{f_i'' = \frac{f_i - 2f_{i-1} + f_{i-2}}{(\Delta x)^2} + O(\Delta x)}$$



2nd Order Finite Difference (continue)

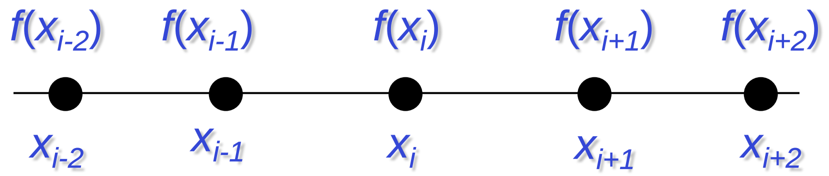
- Recapping that

$$f_{i+1} = f_i + \Delta x f_i' + \frac{(\Delta x)^2}{2!} f_i'' + \frac{(\Delta x)^3}{3!} f_i''' + \frac{(\Delta x)^4}{4!} f_i^{(4)} + \dots$$

$$f_{i-1} = f_i - \Delta x f_i' + \frac{(\Delta x)^2}{2!} f_i'' - \frac{(\Delta x)^3}{3!} f_i''' + \frac{(\Delta x)^4}{4!} f_i^{(4)} - \dots$$

- Adding the above two equations yields

$$f_{i+1} + f_{i-1} = 2 f_i + (\Delta x)^2 f_i'' + \frac{(\Delta x)^4}{12} f_i^{(4)} + \dots$$



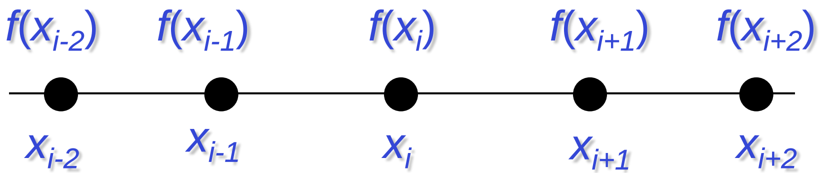
2nd Order Finite Difference (continue)

- Rearranging the equation

$$f_i'' = \frac{f_{i+1} - 2f_i + f_{i-1}}{(\Delta x)^2} \underbrace{- \frac{(\Delta x)^2}{12} f_i^{(4)} + \ldots}_{-\frac{(\Delta x)^2}{12} f^{(4)}(\xi) = O((\Delta x)^2)}$$

- 2nd central difference

$$f_i'' = \frac{f_{i+1} - 2f_i + f_{i-1}}{(\Delta x)^2} + O((\Delta x)^2)$$



Common Finite Difference Formulae

Type of approximation	Formula	Truncation error
Forward differences	$f_i' = (f_{i+1} - f_i)/(\Delta x)$ $f_i'' = (f_{i+2} - 2f_{i+1} + f_i)/(\Delta x)^2$ $f_i''' = (f_{i+3} - 3f_{i+2} + 3f_{i+1} - f_i)/(\Delta x)^3$ $f_i'''' = (f_{i+4} - 4f_{i+3} + 6f_{i+2} - 4f_{i+1} + f_i)/(\Delta x)^4$	$O(\Delta x)$
Backward differences	$f_i' = (f_i - f_{i-1})/(\Delta x)$ $f_i'' = (f_i - 2f_{i-1} + f_{i-2})/(\Delta x)^2$ $f_i''' = (f_i - 3f_{i-1} + 3f_{i-2} - f_{i-3})/(\Delta x)^3$ $f_i'''' = (f_i - 4f_{i-1} + 6f_{i-2} - 4f_{i-3} + f_{i-4})/(\Delta x)^4$	$O(\Delta x)$
Central differences	$f_i' = (f_{i+1} - f_{i-1})/(2\,\Delta x)$ $f_i'' = (f_{i+1} - 2f_i + f_{i-1})/(\Delta x)^2$ $f_i''' = (f_{i+2} - 2f_{i+1} + 2f_{i-1} - f_{i-2})/(2(\Delta x)^3)$ $f_i'''' = (f_{i+2} - 4f_{i+1} + 6f_i - 4f_{i-1} + f_{i-2})/(\Delta x)^4$	$O(\Delta x^2)$

Higher Order Finite Difference

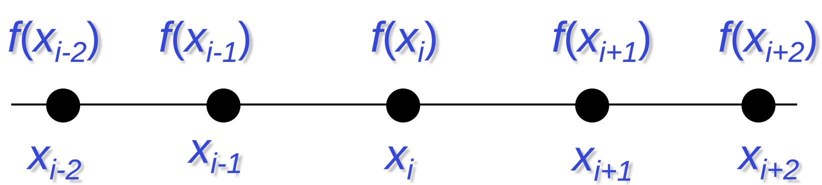
- Recalling Taylor Series Expansion

$$f_i'' = \frac{f_{i+2} - 2 f_{i+1} + f_i}{(\Delta x)^2} - \Delta x \, f_i''' + \ldots \qquad (1)$$

$$f_i' = \frac{f_{i+1} - f_i}{\Delta x} - \frac{\Delta x}{2!} f_i'' - \frac{(\Delta x)^2}{3!} f_i''' - \ldots \qquad (2)$$

- Replace f_i'' in (2), using (1), we get

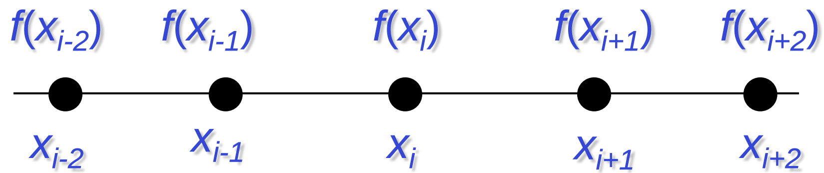
$$f_i' = \frac{f_{i+1} - f_i}{\Delta x} - \frac{\Delta x}{2!}\left[\frac{f_{i+2} - 2 f_{i+1} + f_i}{(\Delta x)^2} - \Delta x \, f_i''' + \ldots\right] - \frac{(\Delta x)^2}{3!} f_i''' - \ldots$$



Higher Order Finite Difference (continue)

- Rearranging the equation yields 2nd forward difference

$$\boxed{f_i' = \frac{-f_{i+2} + 4f_{i+1} - 3f_i}{2\Delta x} + O((\Delta x)^2)}$$



Higher Order Finite Difference (continue)

- Sum of all the coefficients of the function value (*f*) appearing in the numerator can be seen to be zero, implying that the derivative becomes zero if $f(x)$ is a constant
- Accuracy of the computed derivatives can be improved either by using a smaller step size or by using a higher accuracy formula
- Use of finite-difference approximation transforms an ordinary differential equation into algebraic equation, which is relatively simpler to solve

Example

- Formulate the boundary-value problem for an infinitely long hollow cylinder whose inner surface (r = 5″) is maintained at 200°F, while the outer surface (r = 10″) is maintained at 65°F. The radial heat transfer in a thick hollow cylinder is given by

$$\frac{d^2T}{dr^2} + \frac{1}{r}\frac{dT}{dr} = 0$$

- Solution

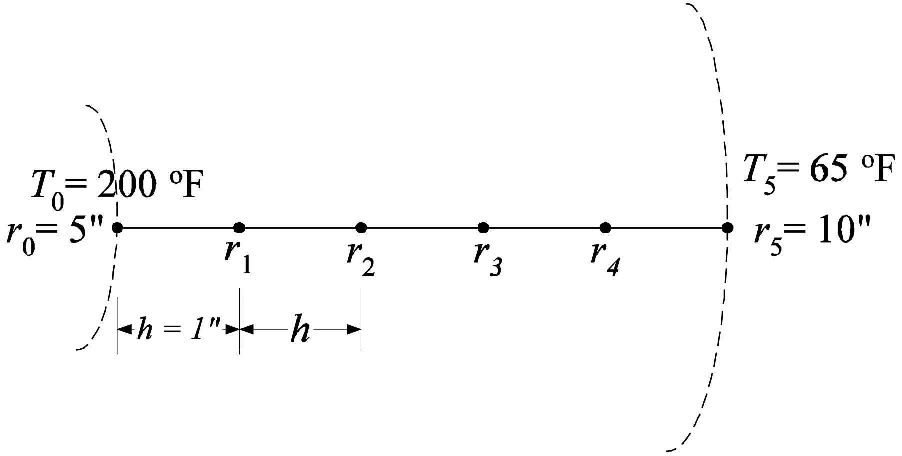
Using h = 1″, interval 5″ $\leq x \leq$ 10″ can be divided into N = 5

Example (continue)

- Employ the central difference formulae

$$\frac{d^2T}{dr^2} + \frac{1}{r}\frac{dT}{dr} = 0 \quad \Longrightarrow$$

$$\frac{T_{i+1} - 2T_i + T_{i-1}}{h^2} + \frac{1}{r_i}\frac{T_{i+1} - T_{i-1}}{2h} = 0$$



Higher Order Finite Difference Formulae

Type of formula	Formula	Truncation error
Forward differences	$f_i' = (-f_{i+2} + 4f_{i+1} - 3f_i)/(2(\Delta x))$	$O(\Delta x)^2$
	$f_i'' = (-f_{i+3} + 4f_{i+2} - 5f_{i+1} + 2f_i)/(\Delta x)^2$	
	$f_i''' = (-3f_{i+4} + 14f_{i+3} - 24f_{i+2} + 18f_{i+1} - 5f_i)/(2(\Delta x)^3)$	
	$f_i'''' = (-2f_{i+5} + 11f_{i+4} - 24f_{i+3} + 26f_{i+2} - 14f_{i+1} + 3f_i)/(\Delta x)^4$	
Backward differences	$f_i' = (3f_i - 4f_{i-1} + f_{i-2})/(2(\Delta x))$	$O(\Delta x^2)$
	$f_i'' = (2f_i - 5f_{i-1} + 4f_{i-2} - f_{i-3})/(\Delta x)^2$	
	$f_i''' = (5f_i - 18f_{i-1} + 24f_{i-2} - 14f_{i-3} + 3f_{i-4})/(2(\Delta x)^3)$	
	$f_i'''' = (3f_i - 14f_{i-1} + 26f_{i-2} - 24f_{i-3} + 11f_{i-4} - 2f_{i-5})/(\Delta x)^4$	
Central differences	$f_i' = (-f_{i+2} + 8f_{i+1} - 8f_{i-1} + f_{i-2})/(12(\Delta x))$	$O(\Delta x^4)$
	$f_i'' = (-f_{i+2} + 16f_{i+1} - 30f_i + 16f_{i-1} - f_{i-2})/(12(\Delta x)^2)$	
	$f_i''' = (-f_{i+3} + 8f_{i+2} - 13f_{i+1} + 13f_{i-1} - 8f_{i-2} + f_{i-3})/(8(\Delta x)^3)$	
	$f_i'''' = (-f_{i+3} + 12f_{i+2} - 39f_{i+1} + 56f_i - 39f_{i-1} + 12f_{i-2} - f_{i-3})/(6(\Delta x)^4)$	

Example

- Compute forward and backward difference approximations of $O(\Delta x)$ and $O(\Delta x)^2$, and central difference approximations of $O(\Delta x)^2$ and $O(\Delta x)^4$ for the first derivative of $f(x) = \sin x$ at $x = \pi/4$ using a value of $\Delta x = \pi/12$. Estimate the true percent relative error E_t for each approximation.

- Exact solution: $f'(\pi/4) = \cos \pi/4 = 0.707$

Example (continue)

- 1st forward difference $f_i' = (f_{i+1} - f_i)/\Delta x$
- 2nd forward difference $f_i' = (-f_{i+2} + 4f_{i+1} - 3f_i)/2\Delta x$
- 1st backward difference $f_i' = (f_i - f_{i-1})/\Delta x$
- 2nd backward difference $f_i' = (3f_i - 4f_{i-1} + f_{i-2})/2\Delta x$
- 2nd central difference $f_i' = (f_{i+1} - f_{i-1})/2\Delta x$
- 4th central difference $f_i' = (-f_{i+2} + 8f_{i+1} - 8f_{i-1} + f_{i-2})/12\Delta x$

notation	x	f(x) = sin(x)
i - 2	π / 4 - 2π / 12 = π / 12	0.259
i -1	π / 4 - π / 12 = π / 6	0.500
i	π / 4	0.707
i + 1	π / 4 + π / 12 = π / 3	0.866
i + 2	π / 4 + 2π / 12 = 5π / 12	0.966

Example (continue)

- 1st forward difference $f_i' = (f_{i+1} - f_i)/\Delta x = (0.866 - 0.707)/(\pi/12) = 0.607$ $E_t = 14.1\%$
- 2nd forward difference $f_i' = (-f_{i+2} + 4f_{i+1} - 3f_i)/2\Delta x = 0.72$ $E_t = -1.84\%$
- 1st backward difference $f_i' = (f_i - f_{i-1})/\Delta x = 0.791$ $E_t = -11.9\%$
- 2nd backward difference $f_i' = (3f_i - 4f_{i-1} + f_{i-2})/2\Delta x = 0.726$ $E_t = -2.69\%$
- 2nd central difference $f_i' = (f_{i+1} - f_{i-1})/2\Delta x = 0.699$ $E_t = 1.13\%$
- 4th central difference $f_i' = (-f_{i+2} + 8f_{i+1} - 8f_{i-1} + f_{i-2})/12\Delta x = 0.707$ $E_t = 0\%$

- E_t = (Actual – Approx)/Actual X 100%

$$f'(\pi/4) = \cos\pi/4 = 0.707$$

notation	x	f(x) = sin(x)
i - 2	π / 4 - 2π / 12 = π / 12	0.259
i -1	π / 4 - π / 12 = π / 6	0.500
i	π / 4	0.707
i + 1	π / 4 + π / 12 = π / 3	0.866
i + 2	π / 4 + 2π / 12 = 5π / 12	0.966

Differentiation of Interpolating Polynomials

- Power Series Type

$$f(x) = a_0 + a_1 x + a_2 x^2$$

$$f(x_i) = f_i = a_0 + a_1 x_i + a_2 x_i^2$$

$$f(x_{i+1} = x_i + h) = f_{i+1} = a_0 + a_1\left(x_i + h\right) + a_2\left(x_i + h\right)^2$$

$$f(x_{i+2} = x_i + 2h) = f_{i+2} = a_0 + a_1\left(x_i + 2h\right) + a_2\left(x_i + 2h\right)^2$$

- Simplifying

$$\begin{array}{l} x_i = 0, \\ x_{i+1} = h, \\ x_{i+2} = 2h \end{array} \quad \Rightarrow \quad \left. \begin{array}{l} f_i = a_0 \\ f_{i+1} = a_0 + a_1 h + a_2 h^2 \\ f_{i+2} = a_0 + 2a_1 h + 4a_2 h^2 \end{array} \right\} \quad \begin{array}{l} a_0 = f_i \\ a_1 = \dfrac{-f_{i+2} + 4f_{i+1} - 3f_i}{2h} \\ a_2 = \dfrac{f_{i+2} - 2f_{i+1} + f_i}{2h^2} \end{array}$$

$$f_i' = f'(x_i = 0) = a_1 + 2a_2 x_i = a_1 = \frac{-f_{i+2} + 4f_{i+1} - 3f_i}{2h} \qquad f_i'' = f''(x_i = 0) = 2a_2 = \frac{f_{i+2} - 2f_{i+1} + f_i}{h^2}$$

Observations

- Finite-difference approximations are the same as those derived by Taylor Series Expansion without error terms
- Derivation of finite-difference approximations from interpolating polynomials is particularly useful when the data points have **non-uniform** spacing

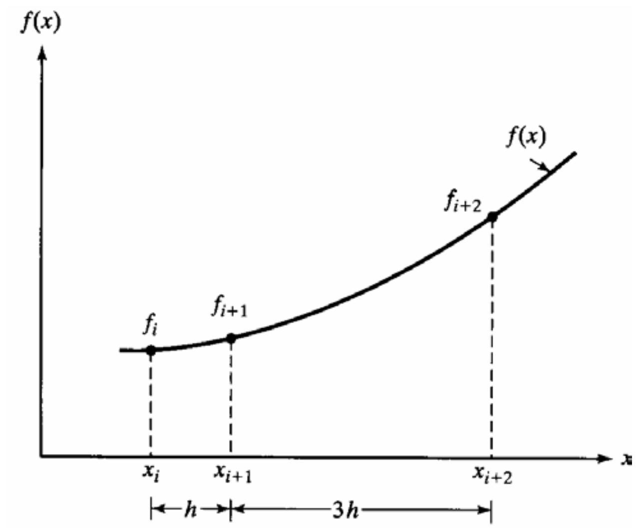
Example 1

- If $x_i = 0, \quad x_{i+1} = h, \quad x_{i+2} = 4h$

$$f(x_i) = f_i = a_0 + a_1 x_i + a_2 x_i^2$$

$$f(x_{i+1} = x_i + h) = f_{i+1} = a_0 + a_1 (x_i + h) + a_2 (x_i + h)^2$$

$$f(x_{i+2} = x_i + 4h) = f_{i+2} = a_0 + a_1 (x_i + 4h) + a_2 (x_i + 4h)^2$$



- Then

$$f_i = a_0$$

$$f_{i+1} = a_0 + a_1 h + a_2 h^2$$

$$f_{i+2} = a_0 + 4a_1 h + 16 a_2 h^2$$

$$a_0 = f_i$$

$$a_1 = \frac{-f_{i+2} + 16 f_{i+1} - 15 f_i}{12h}$$

$$a_2 = \frac{f_{i+2} - 4 f_{i+1} + 3 f_i}{12h^2}$$

$$f_i' = a_1 = \frac{-f_{i+2} + 16 f_{i+1} - 15 f_i}{12h}$$

$$f_i'' = 2a_2 = \frac{f_{i+2} - 4 f_{i+1} + 3 f_i}{6h^2}$$

Example 2

- Heat flux at the soil-air interface can be computed with Fourier's law

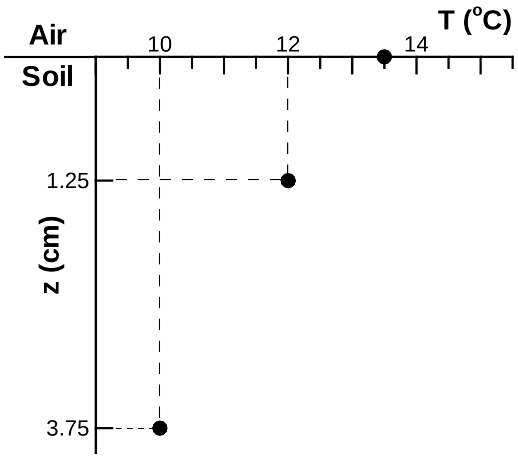
$$q(z=0) = -\alpha \rho C \left.\frac{dT}{dz}\right|_{z=0}$$

  - α = soil thermal diffusivity ($\cong 3.5 \times 10^{-7}$ m^2/s)
  - ρ = soil density ($\cong$ 1800 kg/m^3)
  - C = soil specific heat ($\cong$ 840 J/(kg · °C))

- Use numerical differentiation to evaluate the gradient at the soil-air interface and employ this estimate to determine the heat flux into ground

Example 2 (continue)

- Problem definition



z (cm)	T (°C)
0	13.5
1.25	12
3.75	10

- Non-uniform data spacing. Use Power Series Type Interpolation based on polynomial

$$T(z) = a_0 + a_1 z + a_2 z^2$$

Example 2 (continue)

- With $h = 1.25 \text{ cm}, z_i = 0, z_{i+1} = h, z_{i+2} = 3h$ $\quad T(z) = a_0 + a_1 z + a_2 z^2$

$$T_i = a_0$$

$$T_{i+1} = a_0 + a_1 h + a_2 h^2$$

$$T_{i+2} = a_0 + 3a_1 h + 9a_2 h^2$$

z (cm)	T (°C)
0	13.5
1.25	12
3.75	10

- Since

$$\left.\frac{dT}{dz}\right|_{z=0} = a_1 + 2a_2(0) = a_1$$

$$a_1 = \frac{-T_{i+2} + 9T_{i+1} - 8T_i}{6h} = \frac{-10 + 9(12) - 8(13.5)}{6(1.25)}$$ = -1.333°C/cm = -133.3°C/m

$$q(z=0) = -\alpha \rho C \left.\frac{dT}{dz}\right|_{z=0}$$ = (3.5 × 10^{-7})(1800)(840)(133.3) = 70.56 W/m^2

DERIVATIVES FOR DATA WITH ERRORS

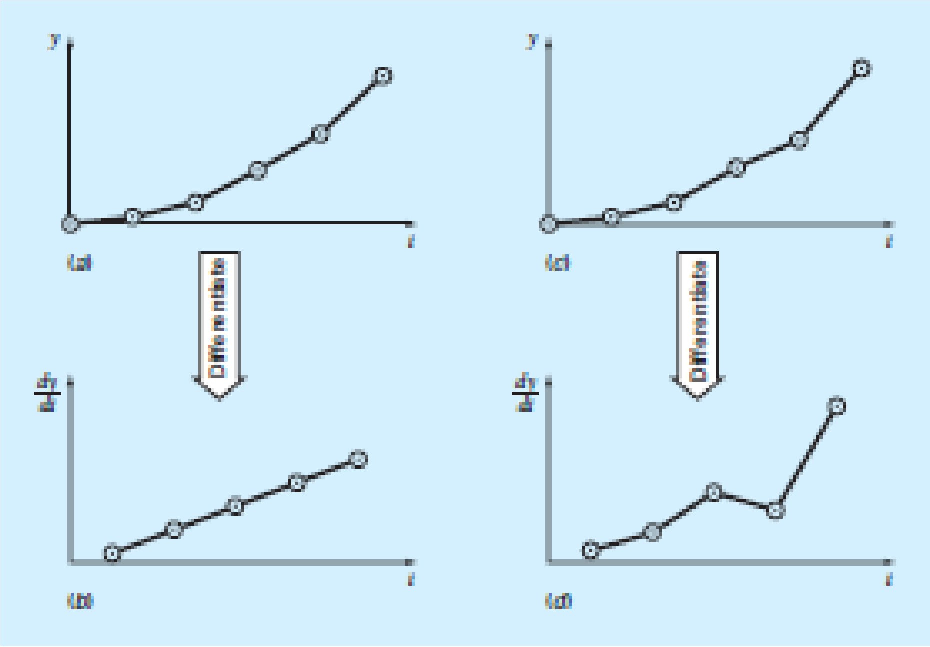


Illustration of how small data errors are amplified by numerical differentiation: (*a*) data with no
error, (*b*) the resulting numerical differentiation of curve (*a*), (*c*) data modified slightly, and (*d*) the
resulting differentiation of curve (*c*) manifesting increased variability.

Richardson's Extrapolation for Differentiation

- Represents another way of improving the accuracy of the estimates of the derivatives
- Truncation error $E = O(h^n) \approx ch^n$
- If D_1 and D_2 are the approximated derivatives with a step size h_1 and h_2

$$\left.\begin{aligned} D &= D_1 + O(h_1^n) = D_1 + E_1 \approx D_1 + ch_1^n \\ D &= D_2 + O(h_2^n) = D_2 + E_2 \approx D_2 + ch_2^n \end{aligned}\right\} \quad D_1 + ch_1^n \approx D_2 + ch_2^n \quad \Rightarrow \quad c = \frac{D_2 - D_1}{h_1^n - h_2^n}$$

$$D \approx D_2 + \frac{D_2 - D_1}{\left\{\left(\dfrac{h_1}{h_2}\right)^n - 1\right\}}$$

- Using $h_2 = h_1 / 2$ $\quad D \approx D_2 + \dfrac{D_2 - D_1}{2^n - 1} + O(h^{n+2})$
- The more accurate is the one computed with smaller *h*

Example

- Estimate the 1st derivative $f(x) = x^4 + 1.5x^3 + 5x^2 + 2.5x - 12$ at *x* = 0.5 using central difference approximation of $O(h^2)$ employing a step size of $h_1 = 0.5$ and $h_2 = 0.25$. Then use Richardson extrapolation to compute an improved estimate. Compare solution with exact solution and estimated solution using central difference approximation of $O(h^4)$ with $h = 0.25$.

Example (continue)

- Exact solution is

$$f'(x) = 4x^3 + 4.5x^2 + 10x^2 + 2.5$$

$$f'(0.5) = 4(0.5)^3 + 4.5(0.5)^2 + 10(0.5) + 2.5 = 9.125$$

x	f(x)
0	-12
0.25	-11.0352
0.5	-9.25
0.75	-6.36328
1	-2

$$f_i' = (f_{i+1} - f_{i-1})/2\Delta x$$

- $h_1 = 0.5$ $\quad f'(0.5) = \dfrac{-2+12}{2(0.5)} = 10$

- $h_2 = 0.25$ $\quad f'(0.5) = \dfrac{-6.36328+11.0352}{2(0.25)} = 9.34375$

compare

- For $h_2 = h_1/2$ and $n = 2$, $D_1 = 10$ and $D_2 = 9.34375$

- Then $D \approx D_2 + \dfrac{D_2 - D_1}{2^n - 1} + O(h^{n+2}) = 9.34375 + \dfrac{9.34375 - 10}{2^2 - 1} + O(h^4) = 9.125$

Example (continue)

- Using central difference of $O(h^4)$, $h = 0.25$

x	f(x)
0	-12
0.25	-11.0352
0.5	-9.25
0.75	-6.36328
1	-2

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

$$f'(0.5) = \frac{2 + 8(-6.36328) - 8(-11.0352) - 11.0352}{12(0.25)} = 9.125$$

- Estimates of $O(h^4)$ is the same as exact solution! Recalling Richardson Extrapolation in previous slide