Module 02: Numerical Methods

Unit 02: Finite Difference Approximation

Anirban Dhar

Department of Civil Engineering
Indian Institute of Technology Kharagpur, Kharagpur

National Programme for Technology Enhanced Learning (NPTEL)

Learning Objectives

- To discretize the derivatives of single-valued one-dimensional functions using finite difference approximations.

Derivative of a Function

Let us consider a function ϕ such that its derivatives are single-valued, finite and continuous functions of x.

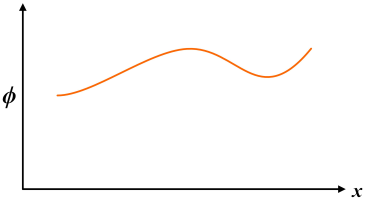

Figure: Single-valued Continuous Function $\phi(x)$

Derivative of a Function

ϕ can be approximated with point values at nodes.

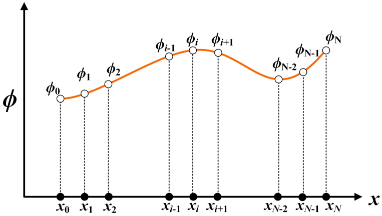

Figure: Discrete Representation of Function $\phi(x)$

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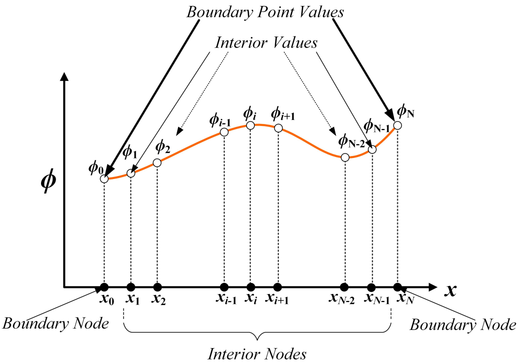

Figure: Discrete Representation of Function $\phi(x)$

Forward Difference

The first derivative at node x_0 can be calculated with limit definition

$$\phi'_0 = \lim_{\Delta x \to 0} \frac{\phi(x_0 + \Delta x) - \phi(x_0)}{\Delta x} \tag{1}$$

Forward Difference

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This can be approximated for *Forward Difference* with finite Δx as

$$\phi'_0 \cong \frac{\phi(x_0 + \Delta x) - \phi(x_0)}{\Delta x} = \frac{\phi(x_1) - \phi(x_0)}{x_1 - x_0} \tag{2}$$

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The first derivative at node x_0 can be calculated with limit definition

$$\phi_0' = \lim_{\Delta x \to 0} \frac{\phi(x_0 + \Delta x) - \phi(x_0)}{\Delta x} \tag{1}$$

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Similarly,

$$\phi_1' = \frac{\phi_2 - \phi_1}{x_2 - x_1} \tag{3}$$

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$$\phi'_1 = \frac{\phi_2 - \phi_1}{x_2 - x_1} \tag{3}$$

$$\phi'_i = \frac{\phi_{i+1} - \phi_i}{x_{i+1} - x_i} \tag{4}$$

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$$\phi_i' = \frac{\phi_{i+1} - \phi_i}{x_{i+1} - x_i} \tag{4}$$

$$\phi_{N-2}' = \frac{\phi_{N-1} - \phi_{N-2}}{x_{N-1} - x_{N-2}} \tag{5}$$

$$\phi_{N-1}' = \frac{\phi_N - \phi_{N-1}}{x_N - x_{N-1}} \tag{6}$$

ϕ_N' cannot be computed with this approach.

Backward Difference

Alternate definition of limit can be used for ϕ'_N as,

$$\phi'_N = \lim_{\Delta x \to 0} \frac{\phi(x_N) - \phi(x_N - \Delta x)}{\Delta x} \tag{7}$$

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This can be approximated for *Backward Difference* with finite Δx as

$$\phi'_N \cong \frac{\phi(x_N) - \phi(x_N - \Delta x)}{\Delta x} = \frac{\phi_N - \phi_{N-1}}{x_N - x_{N-1}} \tag{8}$$

ϕ'_0 cannot be computed with this approach.
For interior nodes, x_1 to x_{N-1} *Center Difference* approximation can be utilized as,

$$\phi'_1 \cong \frac{\phi(x_1 + \Delta x) - \phi(x_1 - \Delta x)}{\Delta x + \Delta x} = \frac{\phi(x_2) - \phi(x_0)}{x_2 - x_0} \tag{9}$$

FD, BD and CD

Forward Difference (FD)

$$\phi'(x_i)|_{FD} = \delta_+\phi_i = \frac{\phi_{i+1} - \phi_i}{x_{i+1} - x_i} = \frac{\phi_{i+1} - \phi_i}{\Delta x}$$

FD, BD and CD

Forward Difference (FD)

$$\phi'(x_i)|_{FD} = \delta_+\phi_i = \frac{\phi_{i+1} - \phi_i}{x_{i+1} - x_i} = \frac{\phi_{i+1} - \phi_i}{\Delta x}$$

Backward Difference (BD)

$$\phi'(x_i)|_{BD} = \delta_-\phi_i = \frac{\phi_i - \phi_{i-1}}{x_i - x_{i-1}} = \frac{\phi_i - \phi_{i-1}}{\Delta x}$$

FD, BD and CD

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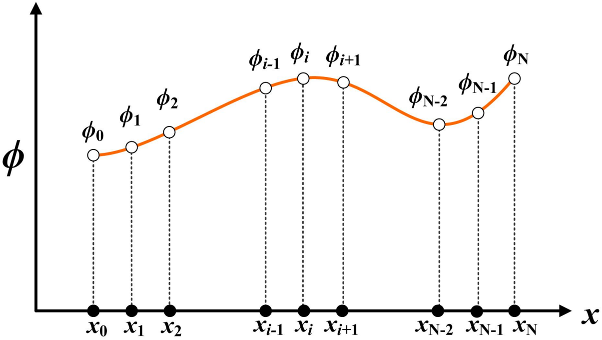
Center Difference (CD)

$$\phi'(x_i)|_{CD} = \mu\phi_i = \frac{1}{2}\left(\delta_+ + \delta_-\right)\phi_i = \frac{\phi_{i+1} - \phi_{i-1}}{x_{i+1} - x_{i-1}} = \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x}$$

Geometric Representation of FD, BD and CD



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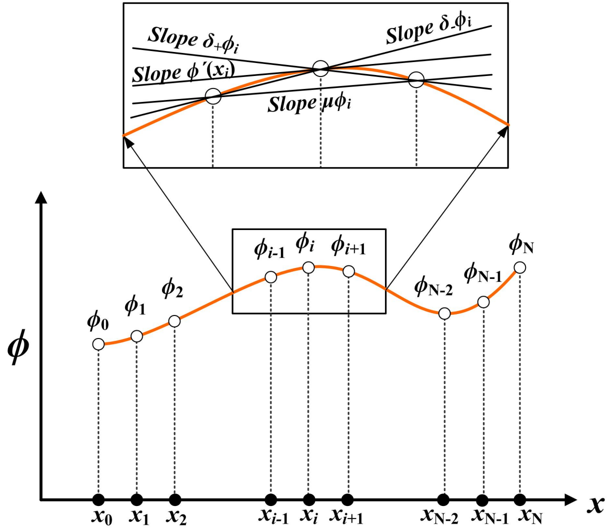

FD, BD and CD

Observations

- Same derivative can be approximated with different forms of finite difference.

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- Results should converge to the same value as $\Delta x \to 0$. This property is called *Consistency* of the discretization.

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Observations

- Same derivative can be approximated with different forms of finite difference.
- Different approximations will give different results for finite value of Δx.
- Results should converge to the same value as $\Delta x \to 0$. This property is called *Consistency* of the discretization.
- Forward, Backward and Center difference approximations are consistent. However, they will not produce same value for finite Δx due to associated truncation error.

Associated Errors

Computational Errors

- *Round-off Error*: Computer-related error as they can store only finite number of decimal places.

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Computational Errors

- *Round-off Error*: Computer-related error as they can store only finite number of decimal places.
- *Truncation Error (T.E.)*: Human error due to approximation being made.

Taylor Series Expansion

If the function is infinitely differentiable, then Taylor series expansion about point x_i evaluated at point $x_i + \Delta x$ is

$$\phi(x_i + \Delta x) = \phi(x_i) + \sum_{m=1}^{\infty} \frac{(\Delta x)^m}{m!} \phi^{(m)}(x_i) \tag{10}$$

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Similarly,

$$\phi(x_i - \Delta x) = \phi(x_i) + \sum_{m=1}^{\infty} (-1)^m \frac{(\Delta x)^m}{m!} \phi^{(m)}(x_i) \tag{11}$$

Approximation

Forward Difference Approximation

$$
\begin{aligned}
\phi'(x_i)|_{FD} &= \frac{\phi(x_i+\Delta x)-\phi(x_i)}{\Delta x} \\
&= \underbrace{\phi'(x_i)}_{Exact\ Value} + \underbrace{\sum_{m=2}^{\infty}\frac{(\Delta x)^{m-1}}{m!}\phi^{(m)}(x_i)}_{Truncation\ Error} \\
&= \underbrace{\phi'(x_i)}_{Exact\ Value} + \underbrace{\underbrace{\frac{\Delta x}{2}\phi''(x_i)}_{Leading\ Error} + \sum_{m=3}^{\infty}\frac{(\Delta x)^{m-1}}{m!}\phi^{(m)}(x_i)}_{Truncation\ Error} \\
&= \underbrace{\phi'(x_i)}_{Exact\ Value} + \mathcal{O}(\Delta x)
\end{aligned}
$$

Approximation

Backward Difference Approximation

$$\phi'(x_i)|_{BD} = \frac{\phi(x_i) - \phi(x_i - \Delta x)}{\Delta x}$$

$$= \underbrace{\phi'(x_i)}_{Exact\ Value} \underbrace{- \sum_{m=2}^{\infty} (-1)^m \frac{(\Delta x)^{m-1}}{m!} \phi^{(m)}(x_i)}_{Truncation\ Error}$$

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$$= \underbrace{\phi'(x_i)}_{Exact\ Value} + \mathcal{O}(\Delta x)$$

Approximation

Center Difference Approximation

$$\phi'(x_i)|_{CD} = \frac{\phi(x_i + \Delta x) - \phi(x_i - \Delta x)}{2\Delta x}$$

$$= \underbrace{\phi'(x_i)}_{Exact\ \ Value} + \underbrace{\sum_{m=1}^{\infty} \frac{(\Delta x)^{2m}}{(2m+1)!}\phi^{(2m+1)}(x_i)}_{Truncation\ \ Error}$$

$$= \underbrace{\phi'(x_i)}_{Exact\ \ Value} + \underbrace{\underbrace{\frac{(\Delta x)^2}{3!}\phi'''(x_i)}_{Leading\ \ Error} + \sum_{m=2}^{\infty} \frac{(\Delta x)^{2m}}{(2m+1)!}\phi^{(2m+1)}(x_i)}_{Truncation\ \ Error}$$

$$= \underbrace{\phi'(x_i)}_{Exact\ \ Value} + \mathcal{O}(\Delta x^2)$$

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- FD approximation for $\phi'(x) \Rightarrow TE \sim \mathcal{O}(\Delta x) \Rightarrow 1^{st}$ order discretization

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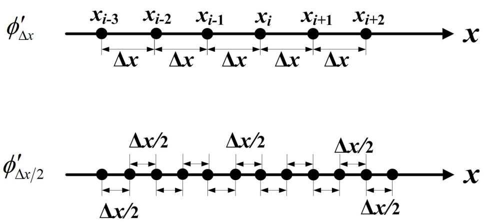
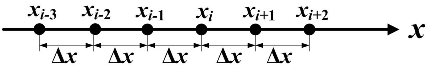


Higher Order Discretization for First-order Derivative



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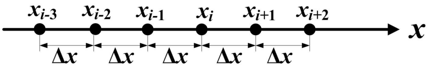

$$
\begin{aligned}
\phi_i' &= \alpha_{i-2}\phi_{i-2} + \alpha_{i-1}\phi_{i-1} + \alpha_i\phi_i \\
&= \alpha_{i-2}\left[\phi_i + \sum_{m=1}^{\infty}(-1)^m \frac{(2\Delta x)^m}{m!}\phi^{(m)}(x_i)\right] \\
&+ \alpha_{i-1}\left[\phi_i + \sum_{m=1}^{\infty}(-1)^m \frac{(\Delta x)^m}{m!}\phi^{(m)}(x_i)\right] + \alpha_i\phi_i \\
&= \phi_i(\alpha_{i-2} + \alpha_{i-1} + \alpha_i) + \phi_i'\Delta x(-2\alpha_{i-2} - \alpha_{i-1}) \\
&+ \phi_i''\frac{\Delta x^2}{2}(4\alpha_{i-2} + \alpha_{i-1}) + \cdots
\end{aligned}
$$

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Coefficients of right-hand-side can be written in terms of algebraic equations.

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Thus, $\alpha_{i-2} = \frac{1}{2\Delta x}$, $\alpha_{i-1} = -\frac{2}{\Delta x}$, $\alpha_i = \frac{3}{2\Delta x}$.

$$\phi_i' = \frac{\phi_{i-2} - 4\phi_{i-1} + 3\phi_i}{2\Delta x} + \mathcal{O}(\Delta x^2)$$

Second Order Derivative

The second order derivative of the function ϕ can be written from the definition of limit as,

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Using forward difference approximations of first order derivative

$$\phi_i''|_{FD} = \frac{\phi_{i+1}'|_{BD} - \phi_i'|_{BD}}{\Delta x} = \frac{\frac{\phi_{i+1}-\phi_i}{\Delta x} - \frac{\phi_i-\phi_{i-1}}{\Delta x}}{\Delta x} = \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2}$$

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Similarly,

$$\phi_i''|_{BD} = \frac{\phi_i'|_{FD} - \phi_{i-1}'|_{FD}}{\Delta x} = \frac{\frac{\phi_{i+1}-\phi_i}{\Delta x} - \frac{\phi_i - \phi_{i-1}}{\Delta x}}{\Delta x} = \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2}$$

Second Order Derivative

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$$\begin{aligned}
&= \frac{1}{\Delta x^2}\left(\phi(x_i) + \sum_{m=1}^{\infty}\frac{(\Delta x)^m}{m!}\phi^{(m)}(x_i)\right) - \frac{2}{\Delta x^2}\phi(x_i) \\
&+ \frac{1}{\Delta x^2}\left(\phi(x_i) + \sum_{m=1}^{\infty}(-1)^m\frac{(\Delta x)^m}{m!}\phi^{(m)}(x_i)\right) \\
&= \underbrace{\phi_i''}_{Exact\ Value} + \underbrace{\sum_{m=2}^{\infty}\frac{(\Delta x)^{(2m-2)}}{2m!}\phi^{(2m)}(x_i)}_{Truncation\ Error} \\
&= \underbrace{\phi_i''}_{Exact\ Value} + \underbrace{\mathcal{O}(\Delta x^2)}_{Truncation\ Error}
\end{aligned} \tag{14}$$

Second Order Derivative

Second Order Derivative can be estimated as,

$$\phi_i'' = \alpha_{i-1}\phi_{i-1} + \alpha_i\phi_i + \alpha_{i+1}\phi_{i+1} \tag{15}$$

$$\alpha_i\phi_i = \alpha_i\phi_i$$
$$\alpha_{i+1}\phi_{i+1} = \alpha_{i+1}[\phi_i + \textstyle\sum_{m=1}^{\infty} \frac{(\Delta x)^m}{m!}\phi^{(m)}(x_i)]$$
$$\alpha_{i-1}\phi_{i-1} = \alpha_{i-1}[\phi_i + \textstyle\sum_{m=1}^{\infty}(-1)^m \frac{(\Delta x)^m}{m!}\phi^{(m)}(x_i)]$$

To express ϕ_i'' as a linear combination $\alpha_i\phi_i + \alpha_{i+1}\phi_{i+1} + \alpha_{i-1}\phi_{i-1}$, we have to remove the ϕ_i and $\phi_i'\Delta x$ terms.

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$$\alpha_i + \alpha_{i+1} + \alpha_{i-1} = 0$$

$$\alpha_{i+1}\Delta x - \alpha_{i-1}\Delta x = 0$$

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$$\alpha_{i+1}\Delta x - \alpha_{i-1}\Delta x = 0$$

$$\alpha_{i+1}\frac{\Delta x^2}{2!} + \alpha_{i-1}\frac{\Delta x^2}{2!} = 1$$

Thus, $\alpha_i = -\frac{2}{\Delta x^2}$ $\alpha_{i+1} = \alpha_{i-1} = \frac{1}{\Delta x^2}$

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To express ϕ_i'' as a linear combination $\alpha_i\phi_i + \alpha_{i+1}\phi_{i+1} + \alpha_{i-1}\phi_{i-1}$, we have to remove the ϕ_i and $\phi_i'\Delta x$ terms.

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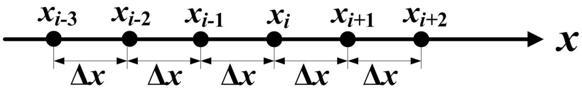
Thus, $\alpha_i = -\frac{2}{\Delta x^2}$ $\alpha_{i+1} = \alpha_{i-1} = \frac{1}{\Delta x^2}$

$$\phi_i'' = \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2}$$

One-sided Three-point Second-order Derivative



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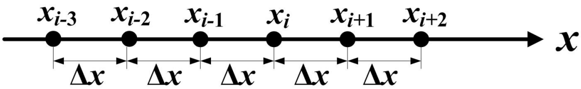
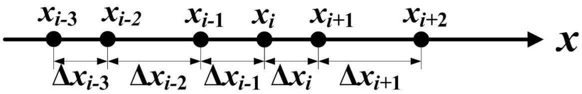


$$\phi_i'' = \frac{\phi_{i-2} - 2\phi_{i-1} + \phi_i}{\Delta x^2} + \mathcal{O}(\Delta x)$$

$$\phi_i'' = \frac{\phi_i - 2\phi_{i+1} + \phi_{i+2}}{\Delta x^2} + \mathcal{O}(\Delta x)$$

Non-uniform Grid



In case of non-uniform grid, second order derivative can be approximated as,

$$\begin{aligned}\phi''(x_i) &= \alpha_{i-1}\phi_{i-1} + \alpha_i\phi_i + \alpha_{i+1}\phi_{i+1} \\ &= \alpha_{i-1}\phi(x_i - \Delta x_{i-1}) + \alpha_i\phi(x_i) + \alpha_{i+1}\phi(x_i + \Delta x_i)\end{aligned} \tag{16}$$

Observations

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- Accuracy of any solution of a problem depends on
  - accuracy of discretization of differential equation.
  - accuracy of discretization of boundary condition.

Thank You