

Computational Hydraulics
Professor Anirban Dhar
Department of Civil Engineering
Indian Institute of Technology Kharagpur
Lecture 6
Finite Difference Approximation

Welcome to this lecture number 6 of the course computational hydraulics. We are in module number 2 numerical methods and this is unit number 2, finite difference approximations.

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The image shows a presentation slide with a white background and a red header bar at the top. The header bar contains the text: "Numerical Approximation of First Derivative", "Numerical Approximation of Second Derivative", and "Non-uniform Grid". Below the header bar, there is a red rectangular box containing the text: "Module 02: Numerical Methods" and "Unit 02: Finite Difference Approximation". Below this box, the name "Anirban Dhar" is displayed, followed by "Department of Civil Engineering" and "Indian Institute of Technology Kharagpur, Kharagpur". Below that, it says "National Programme for Technology Enhanced Learning (NPTEL)". At the bottom of the slide, there is a footer bar with the text: "Dr. Anirban Dhar", "NPTEL", "Computational Hydraulics", and "1 / 25".

So what is the learning objective of this particular module? At the end of this module at the end of this unit students will be able to discretize the derivative of single valued one-dimensional functions using finite difference approximation.

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Numerical Approximation of First Derivative
Numerical Approximation of Second Derivative
Non-uniform Grid

Learning Objectives

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

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So let us consider derivative of function and phi is a single valued, finite and continuous function of x . So this is one dimensional function and its derivatives and function both are continuous.

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Numerical Approximation of First Derivative
Numerical Approximation of Second Derivative
Non-uniform Grid

Derivative of a Function

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

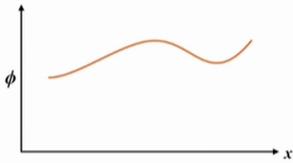
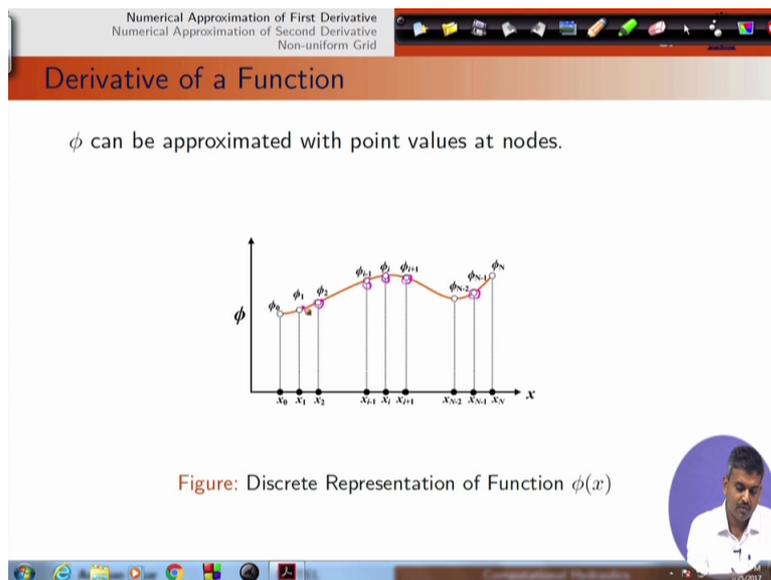


Figure: Single-valued Continuous Function $\phi(x)$

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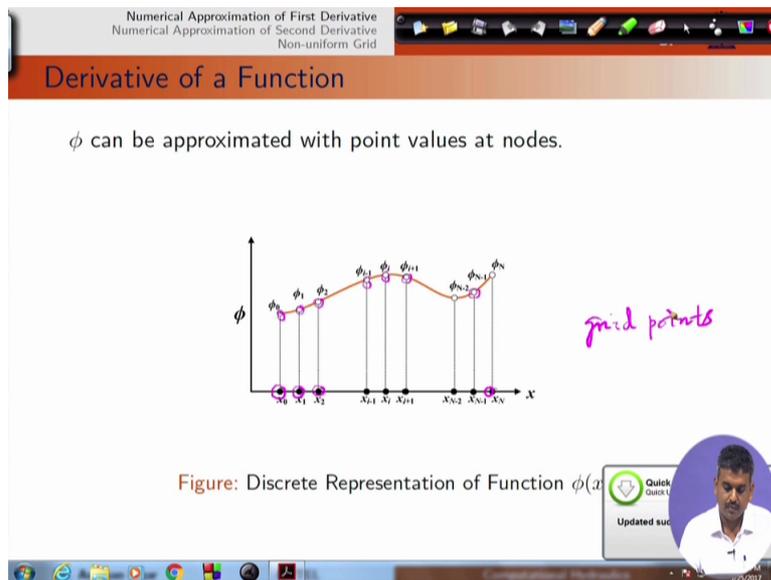
Phi can be approximated with point values at nodes. So these are actually point values. Individual point values for the function.

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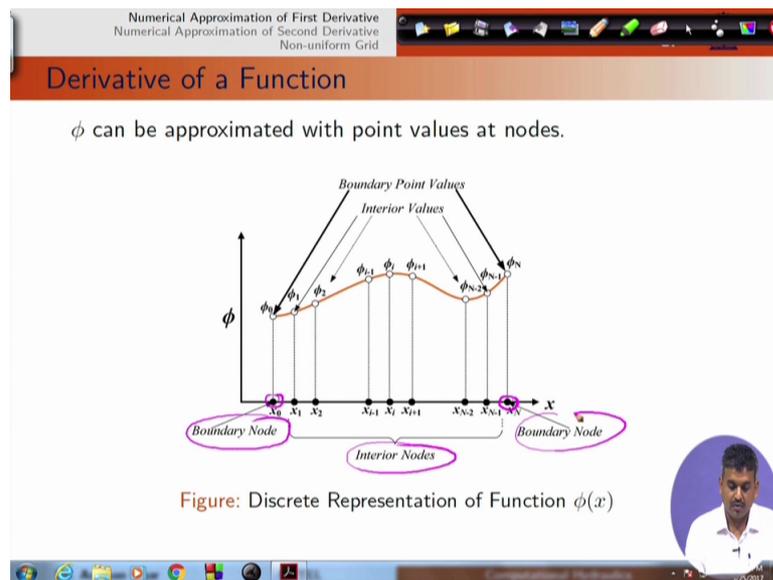
And these are corresponding to nodes x_0 to x_N . And sometimes these are also called as grid points.

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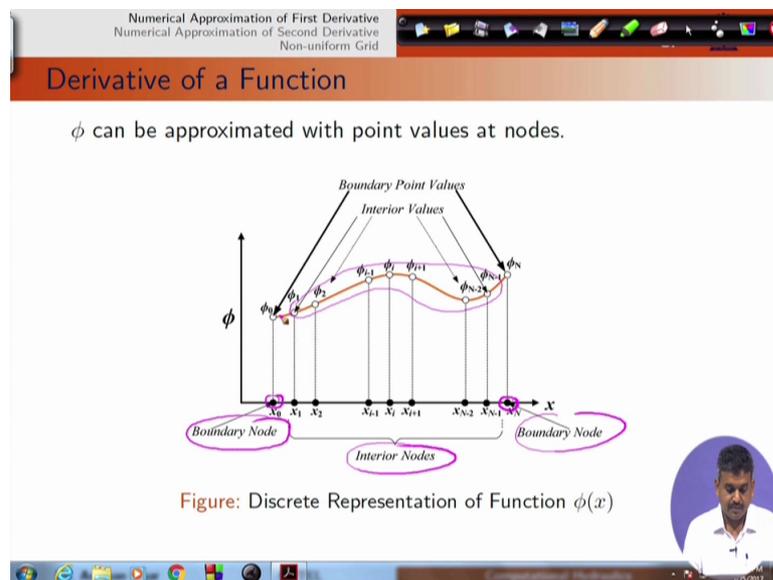
So in this one we represent the function with discrete points. So this is the discrete representation of function phi. So phi can be approximated with points at nodal values. So we have two boundary points in one dimension. And these are actually interior nodes and boundary nodes.

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So at boundary points values can be specified in terms of boundary conditions and within the interior the point it should be with governing equation. So this is the total discrete representation of the single valued function phi.

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Let us consider this forward difference. In forward difference first derivative at node x_0 can be calculated with limit definition. So x_0' can be written in terms of this limit definition that $\phi(x_0 + \Delta x) - \phi(x_0)$ divided by Δx when the limiting value of Δx is tends to zero. this represents the first order derivative.

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Numerical Approximation of First Derivative
Numerical Approximation of Second Derivative
Non-uniform Grid

Forward Difference

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

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

A small circular inset in the bottom right corner shows a man in a white shirt speaking.

Now in this case this limit definition can be approximated and with this approximation for finite value of Δx we can write that $\phi(x_0 + \Delta x) - \phi(x_0)$ divided by Δx is representing the approximated value of first derivative.

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Numerical Approximation of First Derivative
Numerical Approximation of Second Derivative
Non-uniform Grid

Forward Difference

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

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

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

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

A small circular inset in the bottom right corner shows a man in a white shirt speaking.

So we can apply the same approach for x_1 which is interior point, x_i which is general interior point for the function. And for points $n-2$, $n-1$ and n . However we cannot compute this ϕ'_n with this forward difference approach. Why? Because we do not have information about the point $n+1$.

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Numerical Approximation of First Derivative
Numerical Approximation of Second Derivative
Non-uniform Grid

Forward Difference

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

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

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

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

Similarly,

$$\phi'_1 = \frac{\phi_2 - \phi_1}{x_2 - x_1} \quad (3)$$

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

$$\phi'_{N-2} = \frac{\phi_{N-1} - \phi_{N-2}}{x_{N-1} - x_{N-2}}$$

$$\phi'_{N-1} = \frac{\phi_N - \phi_{N-1}}{x_{N-1} - x_N}$$

ϕ'_N cannot be computed with this approach.

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So in this case we can use alternate definition of limit and we can write this phi N prime with backward difference where this is written as x_N minus x_N minus delta x. So it is moving in the backward direction.

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Numerical Approximation of First Derivative
Numerical Approximation of Second Derivative
Non-uniform Grid

Backward Difference

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

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

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Now if we approximate this with the backward difference thing again we can write for finite value of delta x this is representing the first order derivative.

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Numerical Approximation of First Derivative
Numerical Approximation of Second Derivative
Non-uniform Grid

Backward Difference

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

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

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

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

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

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


For interior points we can approximate it using this center difference approach. In central difference approximation we take difference of x_1 plus delta x and x_1 minus delta x divided by $2 \Delta x$, $2 \Delta x$ is the distance between two nodes x_2 and x_0 in this case.

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Numerical Approximation of First Derivative
Numerical Approximation of Second Derivative
Non-uniform Grid

Backward Difference

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

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

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

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

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

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


So in general if we write for any point I , then we can write this forward difference as $\Delta x + x_I$ which is $\phi_{I+1} - \phi_I$ and Δx . Backward difference $\phi_I - \phi_{I-1}$ divided by Δx . If we use center difference then $I + 1$ minus ϕ_{I-1} divided by $2 \Delta x$. This is represented in short forms for the center difference and which is average value of this forward and backward difference.

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Numerical Approximation of First Derivative
Numerical Approximation of Second Derivative
Non-uniform Grid

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)

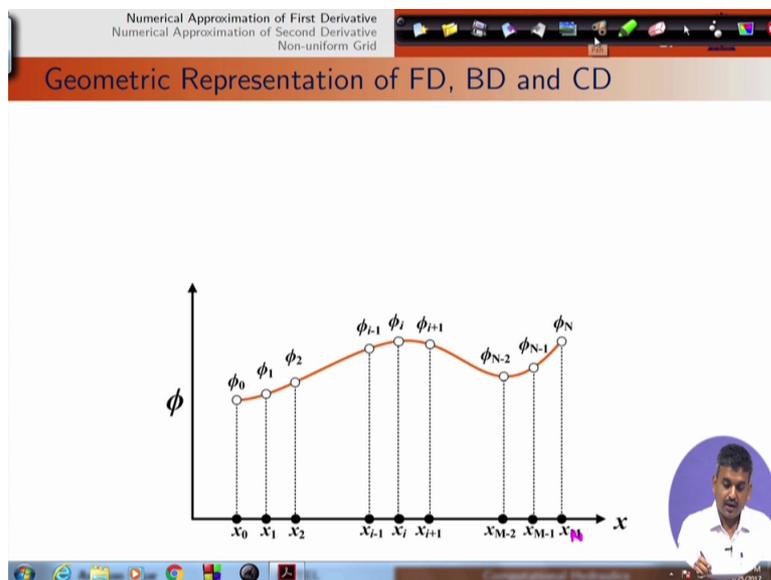
$$\phi'(x_i)|_{BD} = \delta_- \phi_i = \frac{\phi_i - \phi_{i-1}}{x_i - x_{i-1}} = \frac{\phi_i - \phi_{i-1}}{\Delta x}$$

Center Difference (CD)

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

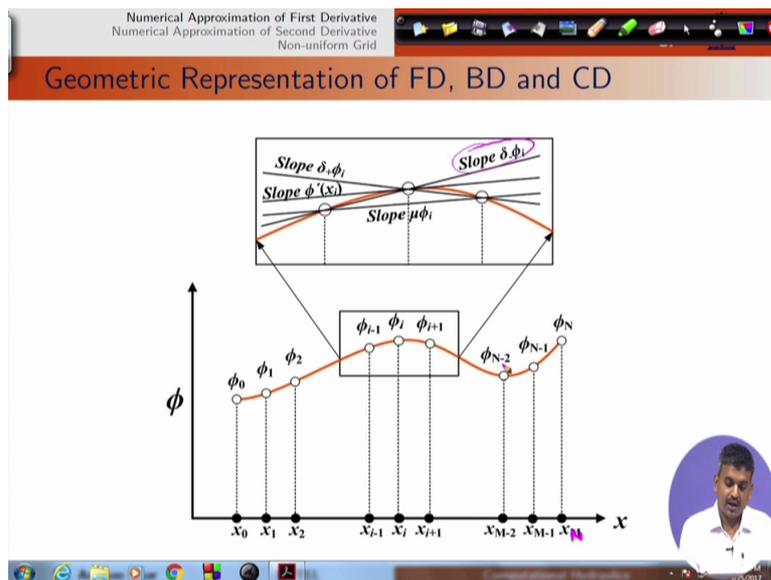
Now if we geometrical say this forward difference, backward difference and center difference representation, then for this discretized one dimensional grid we have distinct grid points from x_0 to x_N .

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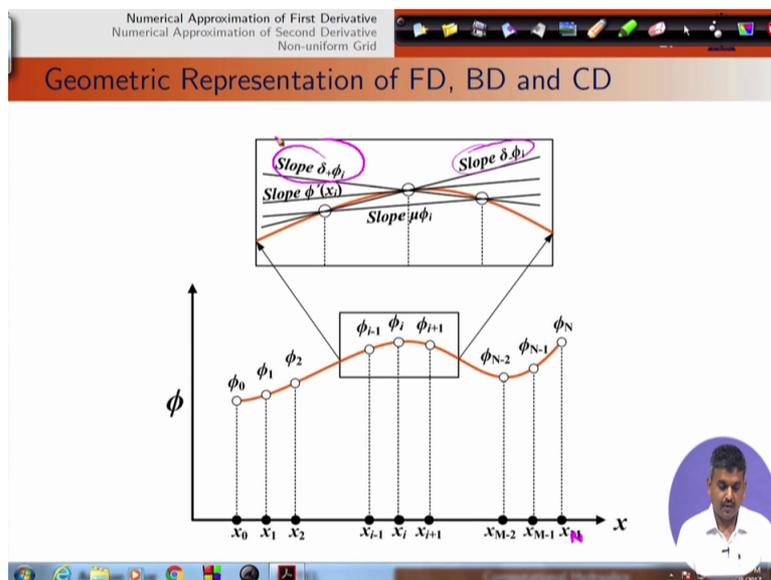
And in this case we can see that the slope between the point x_{i-1} to x_{i+1} that is representing the center difference the slope which is between $i-1$ and i that is representing the backward difference thing.

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And this slope between the points ϕ_{i+1} and ϕ_i that is representing the forward difference.

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So what are the observations? Same derivative can be approximated with different forms of finite difference. Different approximation will give different results for finite value of Δx . Results should converge to the same value as Δx tends to zero. This property is called as consistency of the discretization. And forward backward and center difference approximations are consistent. However, they will not produce same value for finite Δx due to associated truncation error.

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Numerical Approximation of First Derivative
Numerical Approximation of Second Derivative
Non-uniform Grid

FD, BD and CD

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 $\Delta x \rightarrow 0$. 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.

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Now we will talk about this truncation error thing. Although these schemes are consistent but there will be some difference in values.

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Numerical Approximation of First Derivative
Numerical Approximation of Second Derivative
Non-uniform Grid

FD, BD and CD

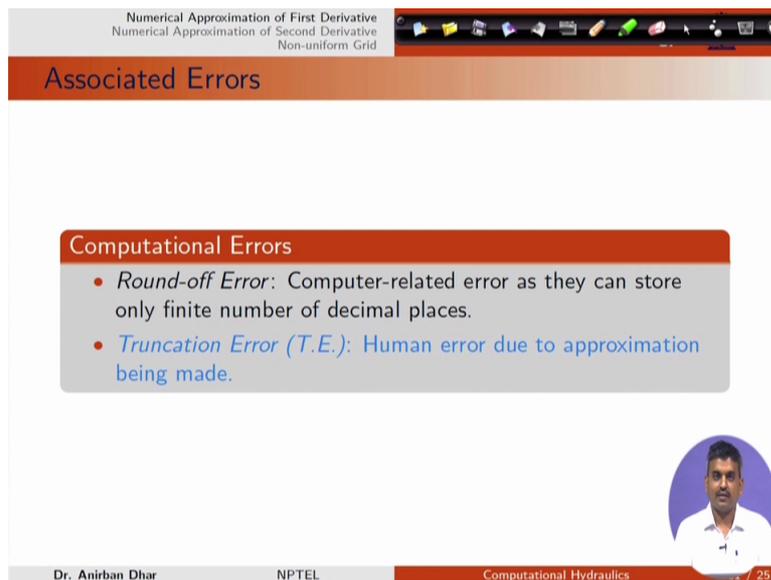
Observations

- 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 $\Delta x \rightarrow 0$. 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.

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So associated errors, one is computational error that is round off error. Computer related error as they cannot they can store only finite number of decimal places. Then comes this truncation error. Human error due to approximation being made.

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Numerical Approximation of First Derivative
Numerical Approximation of Second Derivative
Non-uniform Grid

Associated Errors

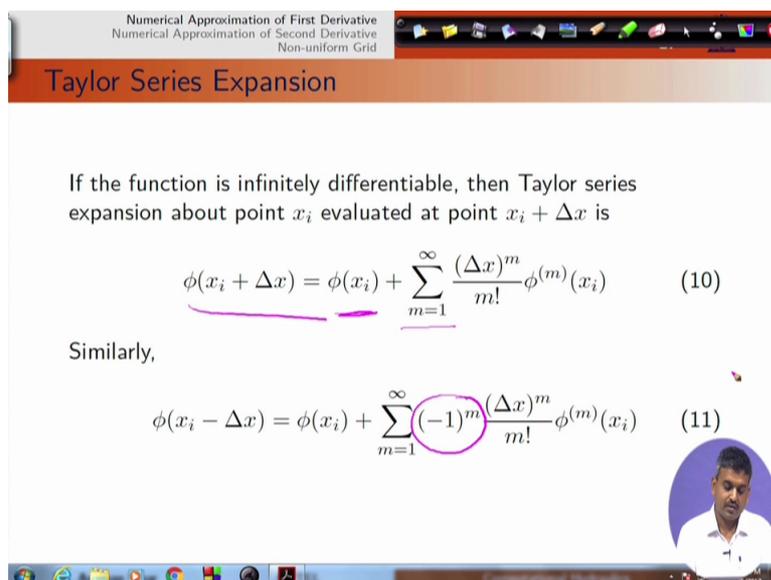
Computational Errors

- **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.

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So if we consider Taylor series expansion and this is for infinitely differentiable function then Taylor series expansion about point x_i evaluated at point $x_i + \Delta x$ is represented as this form. Where m equals to 1 to infinity uhh. This is representing the higher order terms. And around x_i we are expanding this. Similarly if we take $x_i - \Delta x$ again we can expand it using Taylor series and only difference is minus one to the power m . That will determine the sign of this higher order terms.

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Numerical Approximation of First Derivative
Numerical Approximation of Second Derivative
Non-uniform Grid

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

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

Similarly,

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

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Now approximation, forward difference approximation. So we have approximated the forward difference using this expression. Now if we use the Taylor series for this term then

we can write it this format where phi I prime is exact value plus some higher order terms available there. And these terms all total these are called as truncation error.

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Numerical Approximation of First Derivative
Numerical Approximation of Second Derivative
Non-uniform Grid

Approximation

Forward Difference Approximation

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

And in this one the term with lowest order of this delta x is called leading error term. And this determines the order of truncation error. In this case we can say that truncation error is of the order delta x. So in forward difference we have exact value plus some amount of truncation error which is of the order delta x.

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Numerical Approximation of First Derivative
Numerical Approximation of Second Derivative
Non-uniform Grid

Approximation

Forward Difference Approximation

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

TE ~ O(dx)

Now if we see the backward difference again we can use the Taylor series expansion. And with this one again the leading other term is having delx which is the lowest power of delta x.

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Numerical Approximation of First Derivative
Numerical Approximation of Second Derivative
Non-uniform Grid

Approximation

Backward Difference Approximation

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


And this is giving again first order error or truncation error is again of the order delta x.

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Numerical Approximation of First Derivative
Numerical Approximation of Second Derivative
Non-uniform Grid

Approximation

Backward Difference Approximation

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

TE ~ O(Δx)



Now if we repeat the same thing for center difference the result is somewhat different. In this case we are getting this term as truncation error.

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Numerical Approximation of First Derivative
Numerical Approximation of Second Derivative
Non-uniform Grid

Approximation

Center Difference Approximation

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


And we can see that leading error term is having delx square term. And in this case truncation error is of the order delx square.

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Numerical Approximation of First Derivative
Numerical Approximation of Second Derivative
Non-uniform Grid

Approximation

Center Difference Approximation

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


So truncation error is of the order delx square. So in this case lower the order more is the error. So in this case if you have high order truncation error that means this approximation is more accurate compared to forward or backward difference.

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Numerical Approximation of First Derivative
Numerical Approximation of Second Derivative
Non-uniform Grid

Approximation

Center Difference Approximation

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

$TE \sim \mathcal{O}(\Delta x^2)$

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So what are the observations? Forward difference approximation for phi prime x is a first order discretization. Backward difference is of first order. Center difference is of second order discretization.

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Numerical Approximation of First Derivative
Numerical Approximation of Second Derivative
Non-uniform Grid

Approximation

Observations

- FD approximation for $\phi'(x) \Rightarrow TE \sim \mathcal{O}(\Delta x) \Rightarrow 1^{st}$ order discretization
- BD approximation for $\phi'(x) \Rightarrow TE \sim \mathcal{O}(\Delta x) \Rightarrow 1^{st}$ order discretization
- CD approximation for $\phi'(x) \Rightarrow TE \sim \mathcal{O}(\Delta x^2) \Rightarrow 2^{nd}$ order discretization

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And if we take the same problem and discretize with delta x which is equal spacing of the node points. And in this case second case if we divide it with delx by 2 distance between the grid points. So obviously the second grid is much more finer. So if we compare the error between this one and the second one then we can see if we reduce the size of the grid then your delx in case of forward or backward difference the error will be half. But in case of center difference it will be one fourth because we have squared terms present there.

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Numerical Approximation of First Derivative
Numerical Approximation of Second Derivative
Non-uniform Grid

Approximation

Observations

- FD approximation for $\phi'(x) \Rightarrow TE \sim \mathcal{O}(\Delta x) \Rightarrow 1^{st}$ order discretization
- BD approximation for $\phi'(x) \Rightarrow TE \sim \mathcal{O}(\Delta x) \Rightarrow 1^{st}$ order discretization
- CD approximation for $\phi'(x) \Rightarrow TE \sim \mathcal{O}(\Delta x^2) \Rightarrow 2^{nd}$ order discretization

So higher order discretization of the first order derivative. So we have seen that forward difference and backward difference is giving first order discretization. So if we associate one extra point in same side maybe this is on the backward direction.

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Numerical Approximation of First Derivative
Numerical Approximation of Second Derivative
Non-uniform Grid

Higher Order Discretization for First-order Derivative

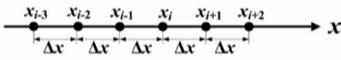
$$\begin{aligned} \phi'_i &= \alpha_{i-2}\phi_{i-2} + \alpha_{i-1}\phi_{i-1} + \alpha_i\phi_i \\ &= \alpha_{i-2} \left[\phi_i + \sum_{m=1}^{\infty} (-1)^m \frac{(2\Delta x)^m}{m!} \phi^{(m)}(x_i) \right] \\ &+ \alpha_{i-1} \left[\phi_i + \sum_{m=1}^{\infty} (-1)^m \frac{(\Delta x)^m}{m!} \phi^{(m)}(x_i)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

We have ϕ_i , ϕ_{i-1} , ϕ_{i-2} with associated coefficient α_{i-2} , α_{i-1} , α_i then with Taylor series expansion around point ϕ_i we can write like this.

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Numerical Approximation of First Derivative
 Numerical Approximation of Second Derivative
 Non-uniform Grid

Higher Order Discretization for First-order Derivative



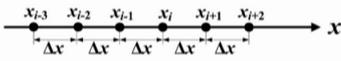
$$\begin{aligned} \phi'_i &= \alpha_{i-2}\phi_{i-2} + \alpha_{i-1}\phi_{i-1} + \alpha_i\phi_i \\ &= \alpha_{i-2} \left[\phi_i + \sum_{m=1}^{\infty} (-1)^m \frac{(2\Delta x)^m}{m!} \phi^{(m)}(x_i) \right] \\ &\quad + \alpha_{i-1} \left[\phi_i + \sum_{m=1}^{\infty} (-1)^m \frac{(\Delta x)^m}{m!} \phi^{(m)}(x_i)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


And we can check the coefficient of phi I, phi I prime, phi I double prime. So in this case we do not have any phi I term in the left hand side. So obviously this should be zero and the coefficient of phi I prime that should be one. And again we do not have any second order derivative on the left hand side so this will be zero.

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Numerical Approximation of First Derivative
 Numerical Approximation of Second Derivative
 Non-uniform Grid

Higher Order Discretization for First-order Derivative



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


So with this information we can construct the linear algebraic equation. And if you solve this we can get the values for the coefficient. So in this case we have first order derivative with second order discretization.

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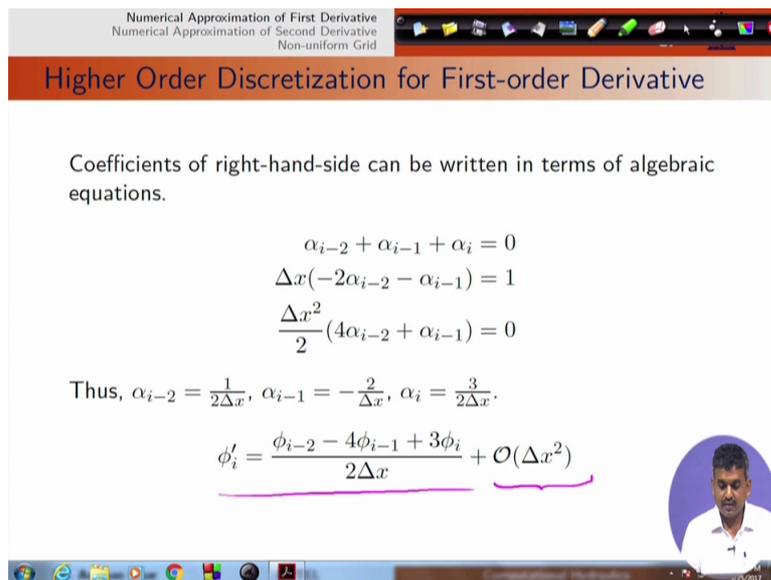
Numerical Approximation of First Derivative
Numerical Approximation of Second Derivative
Non-uniform Grid

Higher Order Discretization for First-order Derivative

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

$$\begin{aligned}\alpha_{i-2} + \alpha_{i-1} + \alpha_i &= 0 \\ \Delta x(-2\alpha_{i-2} - \alpha_{i-1}) &= 1 \\ \frac{\Delta x^2}{2}(4\alpha_{i-2} + \alpha_{i-1}) &= 0\end{aligned}$$

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

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


So let us consider the case for second order derivative. Like forward difference we can apply this approximation. So with forward difference we can write this again if we use backward difference for ϕ_{i+1} and ϕ_i we can get this approximated form of forward difference.

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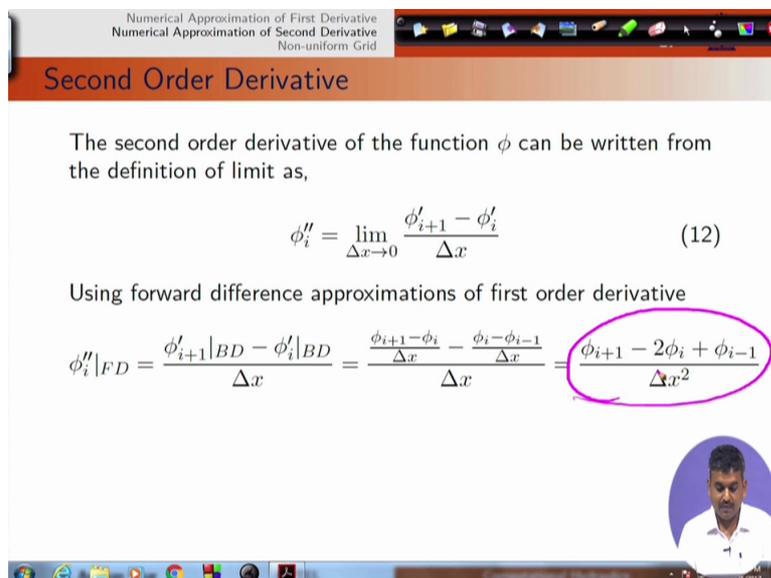
Numerical Approximation of First Derivative
Numerical Approximation of Second Derivative
Non-uniform Grid

Second Order Derivative

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

$$\phi''_i = \lim_{\Delta x \rightarrow 0} \frac{\phi'_{i+1} - \phi'_i}{\Delta x} \quad (12)$$

Using forward difference approximations of first order derivative

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


Now if we check the backward difference approach again we can start with backward differences and we can get the same expression.

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Numerical Approximation of First Derivative
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Non-uniform Grid

Second Order Derivative

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

$$\phi''_i = \lim_{\Delta x \rightarrow 0} \frac{\phi'_{i+1} - \phi'_i}{\Delta x} \quad (12)$$

Using forward difference approximations of first order derivative

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

Similarly,

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

So now if we check the order of accuracy or truncation error for this second order derivative, then we can see that with this Taylor series expansion for ϕ_{i+1} and ϕ_{i-1} we are getting this truncation error.

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Numerical Approximation of First Derivative
Numerical Approximation of Second Derivative
Non-uniform Grid

Second Order Derivative

$$\phi''_i|_{FD} = \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2} \quad (13)$$

$$= \frac{1}{\Delta x^2} \left(\phi(x_i) + \sum_{m=1}^{\infty} \frac{(\Delta x)^m}{m!} \phi^{(m)}(x_i) \right) - \frac{2}{\Delta x^2} \phi(x_i)$$

$$+ \frac{1}{\Delta x^2} \left(\phi(x_i) + \sum_{m=1}^{\infty} (-1)^m \frac{(\Delta x)^m}{m!} \phi^{(m)}(x_i) \right) \quad (14)$$

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

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

And this is the order of accuracy for the second order discretization.

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Numerical Approximation of First Derivative
Numerical Approximation of Second Derivative
Non-uniform Grid

Second Order Derivative

$$\phi_i''|_{FD} = \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2} \quad (13)$$

$$= \frac{1}{\Delta x^2} \left(\phi(x_i) + \sum_{m=1}^{\infty} \frac{(\Delta x)^m}{m!} \phi^{(m)}(x_i) \right) - \frac{2}{\Delta x^2} \phi(x_i)$$

$$+ \frac{1}{\Delta x^2} \left(\phi(x_i) + \sum_{m=1}^{\infty} (-1)^m \frac{(\Delta x)^m}{m!} \phi^{(m)}(x_i) \right) \quad (14)$$

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

$$= \underbrace{\phi_i''}_{\text{Exact Value}} + \underbrace{\mathcal{O}(\Delta x^2)}_{\text{Truncation Error}}$$


Now second order derivative in previous case we have estimated with a symmetric stencil or arrangement of nodes. In that case we have considered I minus one, I, I plus one.

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Numerical Approximation of First Derivative
Numerical Approximation of Second Derivative
Non-uniform Grid

Second Order Derivative

Second Order Derivative can be estimated as,

$$\phi_i'' = \alpha_{i-1}\phi_{i-1} + \alpha_i\phi_i + \alpha_{i+1}\phi_{i+1} \quad (15)$$

$$\alpha_i\phi_i = \alpha_i\phi_i$$

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

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

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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So if we apply the same thing here with coefficient approach then we can right using Taylor series expansion these three expressions.

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Numerical Approximation of First Derivative
Numerical Approximation of Second Derivative
Non-uniform Grid

Second Order Derivative

Second Order Derivative can be estimated as,

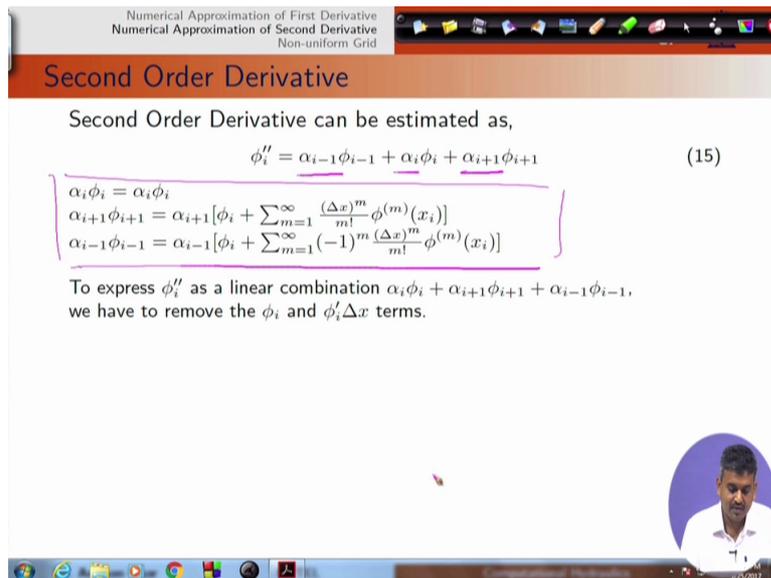
$$\phi_i'' = \alpha_{i-1}\phi_{i-1} + \alpha_i\phi_i + \alpha_{i+1}\phi_{i+1} \quad (15)$$

$$\alpha_i\phi_i = \alpha_i\phi_i$$

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

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

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.



Now ϕ_i'' we can write as linear combination. So we have to remove the ϕ_i and $\phi_i'\Delta x$ term.

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Numerical Approximation of First Derivative
Numerical Approximation of Second Derivative
Non-uniform Grid

Second Order Derivative

Second Order Derivative can be estimated as,

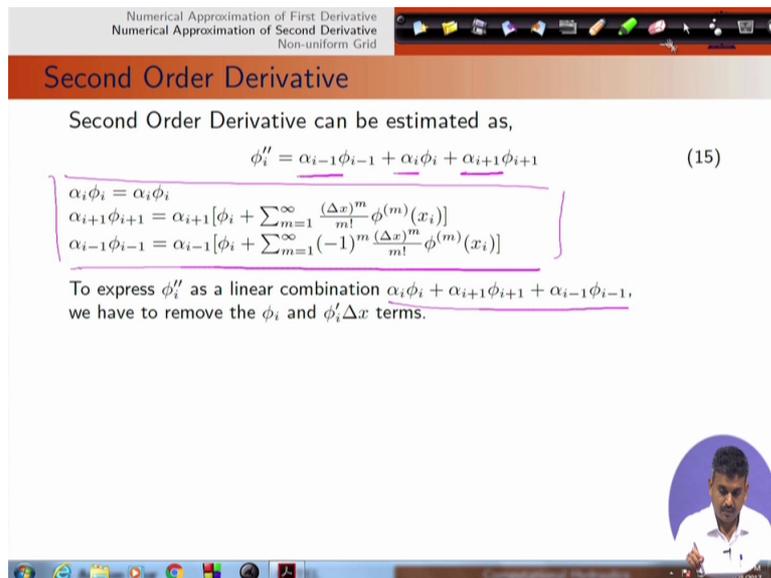
$$\phi_i'' = \alpha_{i-1}\phi_{i-1} + \alpha_i\phi_i + \alpha_{i+1}\phi_{i+1} \quad (15)$$

$$\alpha_i\phi_i = \alpha_i\phi_i$$

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

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

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.



So in this case we can write these three equations. And if you solve this we will get again the approximation in terms of our second order derivative which is coming similar to or same as our previous expression.

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Numerical Approximation of First Derivative
Numerical Approximation of Second Derivative
Non-uniform Grid

Second Order Derivative

Second Order Derivative can be estimated as,

$$\phi_i'' = \alpha_{i-1}\phi_{i-1} + \alpha_i\phi_i + \alpha_{i+1}\phi_{i+1} \quad (15)$$

$$\alpha_i\phi_i = \alpha_i\phi_i$$

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

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

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.

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

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

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

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

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

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Now one sided three point second order derivative. If we consider one sided derivative, in previous case we have considered symmetric one. I minus one, I, I plus one. In this case let us consider one sided that means, first case I minus 2, I minus 3 I, I minus 1 I. And next case we are getting this order of accuracy which is Δx in this case.

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Numerical Approximation of First Derivative
Numerical Approximation of Second Derivative
Non-uniform Grid

One-sided Three-point Second-order Derivative

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

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

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So if we apply the same approach for non-uniform grids then we can write this as with non-uniform spacing. That means I, I minus 1, x_i , Δx_i . So with this information if we expand and utilize the Taylor series expansion then we can get the desired expression for second order derivative.

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Numerical Approximation of First Derivative
Numerical Approximation of Second Derivative
Non-uniform Grid

Non-uniform Grid

x_{i-3} x_{i-2} x_{i-1} x_i x_{i+1} x_{i+2}

Δx_{i-3} Δx_{i-2} Δx_{i-1} Δx_i Δx_{i+1}

x

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

$$\phi''(x_i) = \alpha_{i-1}\phi_{i-1} + \alpha_i\phi_i + \alpha_{i+1}\phi_{i+1}$$
$$= \alpha_{i-1}\phi(x_i - \Delta x_{i-1}) + \alpha_i\phi(x_i) + \alpha_{i+1}\phi(x_i + \Delta x_i) \quad (16)$$

So what are the observations? One sided m point stencil provides m minus 1 order accurate first derivative. This is valid for forward difference and backward difference because I , I minus 1 or I plus 1 I . In that case we are getting first order accurate scheme. And second case you are getting m minus 2 order accurate for second order case second order derivative

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Numerical Approximation of First Derivative
Numerical Approximation of Second Derivative
Non-uniform Grid

Observations

- One-sided m point stencil provides
 - $m - 1$ order accurate first order derivative.
 - $m - 2$ order accurate second order accurate.

And to approximate n th order derivative we need at least N plus 1 neighboring points. In accuracy of solution of a problem depends on accuracy of discretization of differential equation and accuracy of discretization of boundary condition. Thank you. (27:10 – 29:43)