Introuction To numerical methods

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Introduction to numerical methods

- Numerical methods are those in which the mathematical problem is reformulated so it can be solved by arithmetic operations.
- We use numerical methods when:
  - Geometry is very complex
  - There is no way to find exact solution
- Mathematical model general form:

$$\begin{matrix} Dependent \\ Variable \end{matrix} = f\begin{pmatrix} Independent \\ Variable \end{pmatrix}, Parameters, \begin{matrix} Forcing \\ Function \end{matrix}\Bigg)$$

Introduction to numerical methods

Problem Definition: Physical problem + Assumptions + Boundary or Initial Conditions

Mathematical Model: Transform the physical problem into mathematical equation or equations and define the solution desired to be obtained

Numeric Or Graphic Results: Solve the Mathematical model to find the desired solution and represent in by numeric or graphic means

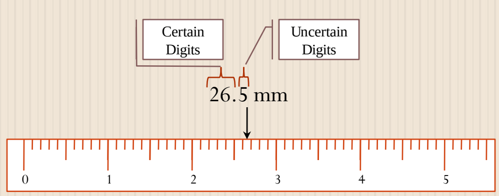
Implementation: Explain and discus the mathematical solution and refer it back to the physical problem

Introduction to numerical methods

Significant Figures

- Significant Figures: are the digits of a number we can use with confidence.
- Significant Figures = number of certain digits + one digit
- Examples:

3 Sign. Figs



Introduction to numerical methods

Significant Figures

- **Special Cases:**
  - 2.55 & 25.5 & 255 & 2550 & 25500 have 3 Sig. Figs.

    Representation : $2.55 \times 10^{1\ \&\ 2\ \&\ 3\ \&\ 4}$
  - 2.55 & 0.255 & 0.0255 & 0.00255 have 3 Sig. Figs.

    Representation : $2.55 \times 10^{-1\ \&\ -2\ \&\ -3\ \&\ -4}$

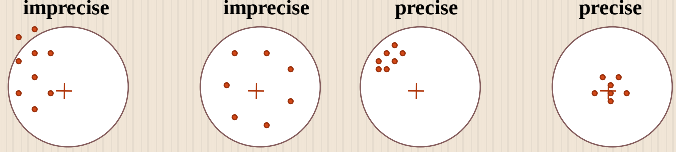
Introduction to numerical methods

Accuracy and Precision

- **Accuracy** refers to how closely a computed or measured value agree with the true value.
- **Precision** refers to how closely individual computed or measured value agree with each other.
- **Bias** (inaccuracy) is the opposite of accuracy. Systematic deviation from true value
- **Uncertainty** (imprecision) is the opposite of precision. Magnitude of scatter.
- **Example:**

Numerical methods must be

Inaccurate & imprecise	accurate & imprecise	Inaccurate & precise	accurate & precise



Introduction to numerical methods

Errors Definitions

- Error represents the deviation from the truth or true value
- There are two types of error may appear when numerical methods are used: Round – off error and Truncation error.
- Both errors can be represented mathematically by:

$$E_t = TrueValue - Approximation$$

$$\varepsilon_t = \left|\frac{TrueValue - Approximation}{TrueValue}\right| x100\%$$

$$E_a = Current\ Approximation - Previous\ Approximation$$

$$\varepsilon_t = \left|\frac{Current\ Approximation - Previous\ Approximation}{Current\ Approximation}\right| x100\%$$

E_t = True error

ε_t = relative true error

E_a = Approximate error

ε_a = relative Approximate error

Introduction to numerical methods

Round – off error

- Round – off error: Results form chopping off some significant figures. This type of error is found in computer processes.

Example:

$\pi = 3.14159265....$

Round – off error

- Computer limitations in representation of numeral quantity create such error.
- Computer reduce such problem by rearranging number presentation : 25560000 → $2.556\ x10^7$

Introduction to numerical methods

Truncation error

- **Truncation error: Results form using approximation methods instead of exact mathematical procedures to find the solution**

Example:

Assume $f(x) = x^2+x+1$, then $f(5) = 5^2 +5+1 = 31$

Assume you used the 1st order Taylor series for example to find the value of $f(5)$ and the results was:

$f(5) = f(4)+f'(4)(5-4) = 30$ assume $x_i = 4$, $x_{i+1} = 5$

Error = 31 – 30 = 1 (this is a truncation error)

Truncation Error

Taylor series

- **Taylor series formula:**

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

$$R_n = \frac{f^{(n+1)}(\xi)h^{n+1}}{(n+1)!}$$: **the reminder of Taylor series**

Where:

$h = x_{i+1} - x_i$ *(step size)*

x_i *: initial independent value*

x_{i+1}*: next independent value*

ζ: is a value lies somewhere between x_{i+1} and x_i

n: Taylor series approximation order

Truncation Error

Taylor series

❖**Example#1:**

If $f(x) = 5x^4 + 3x^3 + 6x^2 + 2x + 5$ and $x_i = 0$ $x_{i+1} = 1$

Then the Taylor series expansion for

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)h^2}{2!} + \frac{f'''(x_i)h^3}{3!} + \frac{f^4(x_i)h^4}{4!}$$

❖Note: when applying Taylor series to estimate polynomials, the number of terms that gives the exact solution equals the order of approximation and the rest term will be equal zero (ie. $f^{(n+1)} = 0$)

Truncation Error

Taylor series

❖**Example#1**$^{(cont)}$**:**

$$f(x) = 5x^4 + 3x^3 + 6x^2 + 2x + 5 \quad x_i = 0 \; \& \; x_{i+1} = 1$$

$$f(x_i = 0) = 5 \qquad f(x_{i+1} = 1) = 21$$

$f^{(1)}(x) = 20x^3 + 9x^2 + 12x + 2$ $\quad f^{(1)}(0) = 2$

$f^{(2)}(x) = 60x^2 + 18x + 12$ $\quad f^{(2)}(0) = 12$

$f^{(3)}(x) = 120x + 18$ $\quad f^{(3)}(0) = 18$

$f^{(4)}(x) = 120$ $\quad f^{(4)}(0) = 120$

0^{th} order : $f(1) = f(0) = 5$

1^{st} order : $f(1) = f(0) + f^{(1)}(0)h = 7$

2^{nd} order : $f(1) = f(0) + f^{(1)}(0)h + \frac{f^{(2)}(0)h^{(2)}}{2!} = 13$

3^{rd} order. : $(1) = f(0) + f^{(1)}(0)h + \frac{f^{(2)}(0)h^{(2)}}{2!} + \frac{f^{(3)}(0)h^{(3)}}{3!} = 16$

4^{th} order : $f(1) = f(0) + f^{(1)}(0)h + \frac{f^{(2)}(0)h^{(2)}}{2!} + \frac{f^{(3)}(0)h^{(3)}}{3!} + \frac{f^{(4)}(0)h^{(4)}}{4!} = 21$

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)h^2}{2!} + \frac{f'''(x_i)h^3}{3!} + \frac{f^4(x_i)h^4}{4!}$$

Truncation Error

Taylor series

Example#1(cont):

$f(x_{i+1}=1)=21$

$$0^{th} \text{ order}: \varepsilon_t = \frac{21-5}{21} x100\% = 76.19\%$$

$$1^{st} \text{ order}: \varepsilon_t = \frac{21-7}{21} x100\% = 66.67\%$$

$$2^{nd} \text{ order}: \varepsilon_t = \frac{21-13}{21} x100\% = 38.09\%$$

$$3^{rd} \text{ order.}: \varepsilon_t = \frac{21-16}{21} x100\% = 23.81\%$$

$$4^{th} \text{ order}: \varepsilon_t = \frac{21-21}{21} x100\% = 0\%$$

Note : as the order of Taylor approximation increase, the accuracy increase too

Truncation Error

Taylor series

Example#2:

$f(x)=\cos(x)$ and $x_i = \pi/4$ $x_{i+1} = \pi/3$

Solution:

Order (n)	$f^{(n)}(x)$	$f(\pi/3)$	ε_t
0	Cos(x)	0.707106781	41.4
1	-sin(x)	0.521986659	4.4
2	-cos(x)	0.497754491	0.449
3	Sin(x)	0.499869147	$2.62x10^{-2}$
4	Cos(x)	0.500007551	$1.51x10^{-3}$
5	-sin(x)	0.500000304	$6.08x10^{-5}$
6	-cos(x)	0.499999988	$2.44x10^{-6}$

Truncation Error

Taylor series reminder

❖ **Taylor series reminder:**

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)h^2}{2!} + \ldots + \frac{f^{(n)}(x_i)h^n}{n!} + \underbrace{\frac{f^{(n+1)}(\xi)h^{n+1}}{(n+1)!}}_{R_n}$$

❖ **Assume 0^{th} order T.S:**

$$f(x_{i+1}) = f(x_i), \quad R_n = f'(x_i)h + \frac{f''(x_i)h^2}{2!} + \frac{f'''(x_i)h^3}{3!} + \ldots$$

❖ It is inconvenient to deal with the remainder as infinite series . So, let us start with the 1^{st} term of the remainder : $R_n = f'(x_i)h$

❖ derivative mean – value theorem states that if a function $f(x)$ and its derivative are continues over an interval from xi and $xi+1$, then there exists at least one point on the function has a slope, designated by $f'(\xi)$, that is parallel to the line joining $f(x_i)$ and $f(x_{i+1})$.

Truncation Error

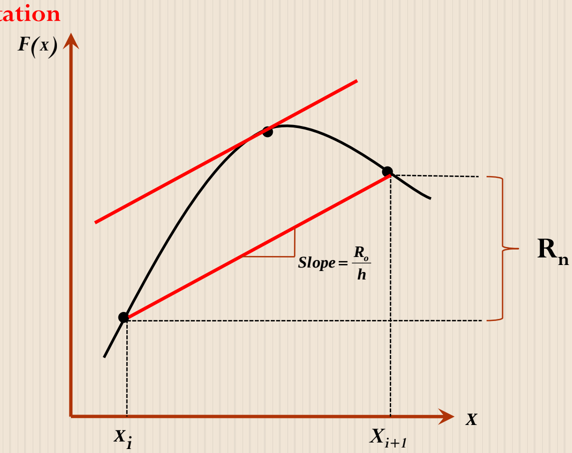
Taylor series reminder

❖ **Graphical Presentation**

$$f'(\xi) = \frac{R_o}{h}$$

$$\Rightarrow R_o = f'(\xi)h$$

$$\Rightarrow R_1 = \frac{f''(\xi)}{2!}h^2$$



Truncation Error

Using Taylor series to estimate truncation error

Example:

Let us take the 1st order approximation in Taylor series:

$$f(x_{i+1}) = f(x_i) + f'(x_i)(x_{i+1} - x_i) + R_1$$

Rearrange the terms :

$$f'(x_i) = \underbrace{\frac{f(x_{i+1}) - f(x_i)}{(x_{i+1} - x_i)}}_{\text{First-order Approximation}} + \underbrace{\frac{R_1}{(x_{i+1} - x_i)}}_{\text{Truncation Error}}$$

Note that the 1st part is used to approximate the 1st derivative in numerical methods

Truncation Error

Using Taylor series to estimate truncation error

Example(cont):

The reminder represents the truncation error and equal to

$$\frac{R_1}{(x_{i+1} - x_i)} = \frac{f''(\xi)}{2!}(x_{i+1} - x_i)$$

Or:

$$\frac{R_1}{(x_{i+1} - x_i)} = O(x_{i+1} - x_i)$$

$O(x_{i+1}-x_i)$: error order notification and it means that the error is in the order of h so, if h is halve, then the error is halve too. In similar way, if the error was in order $O(h^2)$, its mean if the step h is halve the error will be reduced to 1/4th of its previous value.

Numerical Differentiation

Forward Difference

- First derivative
- Formula derivation
- Assume we take the 1st order Taylor series terms

$$f(x_{i+1}) = f(x_i) + f'(x_i)(x_{i+1} - x_i) + R_1$$

- Rearrange to separate the first derivative:

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{(x_{i+1} - x_i)} + O(x_{i+1} - x_i) = \frac{\Delta f_i}{h} + O(h)$$

- Δf_i : 1st forward difference.
- $\Delta f/h$: 1st finite forward divided difference.

Numerical Differentiation

Backward Difference

- First derivative
- Formula derivation
- Expand 2nd order Taylor series terms backward to get:

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

- Truncate above equation after the 1st term and rearrange to separate the first derivative:

$$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{(h)} + O(x_{i+1} - x_i) = \frac{\nabla f_1}{h} + O(h)$$

- ∇f_1 : 1st Backward difference.
- $\nabla f_1 / h$: 1st finite backward divided difference.

Numerical Differentiation

Centered Difference

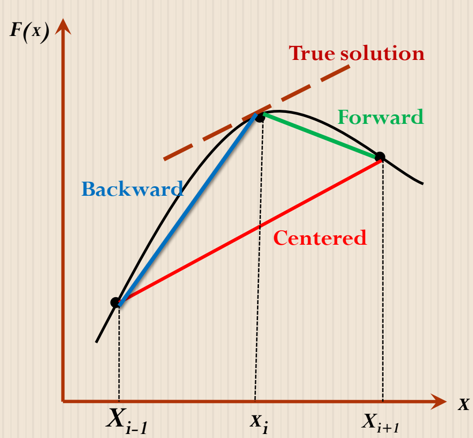
- **First derivative**
- **Formula derivation**

$$f(x_{i+1}) = f(x_i) + f'(x_i)(h) + \frac{f''(x_i)}{2!}h^2 + \ldots \qquad f(x_{i-1}) = f(x_i) - f'(x_i)(h) + \frac{f''(x_i)}{2!}h^2 + \ldots$$

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{(2h)} - \frac{f^{(3)}(x_i)}{6} - \ldots = \frac{f(x_{i+1}) - f(x_{i-1})}{(2h)} + O(h^2)$$

Numerical Differentiation

Graphical representation



Examples

Taylor series

❖ **Example #1**

❖ **Given information**

❖ **assume you have the following functions :**

$$a.\ \ f(x) = \frac{x^4 - x^3 + 1}{x^2 - 1}$$

$$b.\ \ f(x) = \sqrt{x^4 - x^3 + 1}$$

$$c.\ \ f(x) = \frac{x^4 - x^3 + 1}{\sqrt{x^3 + 1}}$$

❖ **Find the value of** $f(2)$ **using Taylor series 3rd order expansion. Let** $h=0.5$ **and find the relative true error (**ε_t**)**

Examples

Taylor series

❖ **Example #1**

❖ **Solution**

❖ **Taylor series 3rd order expansion (n=3) is obtained as:**

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

❖ **The exact solution is found as:**

$$a.\ \ f(2) = \frac{2^4 - 2^3 + 1}{2^2 - 1} = 3$$

$$b.\ \ f(2) = \sqrt{2^4 - 2^3 + 1} = 3$$

$$c.\ \ f(2) = \frac{2^4 - 2^3 + 1}{\sqrt{2^3 + 1}} = 3$$

Examples

Taylor series

- **Example #1**
- **Solution**
- $a.\ f_1(2) = f_1(1.5) + f_1^{'}(1.5)*0.5 + \frac{f_1^{''}(1.5)*0.5^2}{2!} + \frac{f_1^{'''}(1.5)*0.5^3}{3!} = 2.5008$

$$b.\ f_2(2) = f_2(1.5) + f_2^{'}(1.5)*0.5 + \frac{f_2^{''}(1.5)*0.5^2}{2!} + \frac{f_2^{'''}(1.5)*0.5^3}{3!} = 2.9944$$

$$c.\ f_3(2) = f_3(1.5) + f_3^{'}(1.5)*0.5 + \frac{f_3^{''}(1.5)*0.5^2}{2!} + \frac{f_3^{'''}(1.5)*0.5^3}{3!} = 3.0027$$

function	$f^{(1)}(1.5)$	$f^{(2)}(1.5)$	$f^{(3)}(1.5)$	$f(2)$
a	0.2400	9.8080	0.2400	2.5008
b	2.0587	2.9046	2.0587	2.9944
c	2.2359	4.5990	2.2359	3.0027

Examples

Finite divided difference

- **Example #2**
- **Given information**
- **assume you have the following functions :**

$$a.\ f(x) = \frac{x^4 - x^3 + 1}{x^2 - 1}$$

$$b.\ f(x) = \sqrt{x^4 - x^3 + 1}$$

$$c.\ f(x) = \frac{x^4 - x^3 + 1}{\sqrt{x^3 + 1}}$$

- **Find the value of $f'(2)$ using forward, backward and centered finite divided difference**
- **Assume $x_{i-1} = 1.5$ $x_i = 2$ $x_{i+1} = 2.5$**

Examples

Finite divided difference

- **Example #2**
- **Solution**
- **forward finite divided difference:**

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{(x_{i+1} - x_i)}$$

- **Assume:** $x_i = 2$ $x_{i+1} = 2.5$

$$a.\ \ f'(2) = \frac{f(2.5) - f(2)}{2.5 - 2} = 3.3095$$

$$b.\ \ f'(2) = \frac{f(2.5) - f(2)}{2.5 - 2} = 3.8869$$

$$c.\ \ f'(2) = \frac{f(2.5) - f(2)}{2.5 - 2} = 5.9869$$

Examples

Finite divided difference

- **Example #2**
- **Solution**
- **backward finite divided difference:**

$$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{(h)}$$

- **Assume:** $x_{i-1} = 1.5$ $x_i = 2$

$$a.\ \ f'(2) = \frac{f(2) - f(1.5)}{2.5 - 2} = 1.7000$$

$$b.\ \ f'(2) = \frac{f(2) - f(1.5)}{2.5 - 2} = 2.7213$$

$$c.\ \ f'(2) = \frac{f(2) - f(1.5)}{2.5 - 2} = 3.4303$$

Examples

Finite divided difference

❖ **Example #2**

❖ **Solution**

❖ **centered finite divided difference:**

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

❖ **Assume:** $x_{i-1} = 1.5$ $x_{i+1} = 2.5$

$$a.\quad f'(2) = \frac{f(2.5) - f(1.5)}{2(2.5-2)} = 2.5048$$

$$b.\quad f'(2) = \frac{f(2.5) - f(1.5)}{2(2.5-2)} = 3.3041$$

$$c.\quad f'(2) = \frac{f(2.5) - f(1.5)}{2(2.5-2)} = 4.7086$$