Numerical Methods for Engineers

SEVENTH EDITION

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Introduction

Mathematical Preliminaries

Numerical Methods, Mechanical Engineering

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1. **Taylor Series:** Approximates the function $f(x \pm \Delta x)$ knowing the value of *f*(x) and its derivatives. The first term is the largest term. Each subsequent term is smaller than the preceding one.

$$f(x \pm \Delta x) = f(x) \pm f'(x)\Delta x + \frac{f''(x)(\Delta x)^2}{2} \pm \frac{f'''(x)(\Delta x)^3}{6} + \dots\dots\dots$$

Thus,

$$f(x + \Delta x) = f(x) + f'(x)\Delta x + \frac{f''(x)(\Delta x)^2}{2} + \frac{f'''(x)(\Delta x)^3}{6} + \dots\dots\dots$$

$$f(x - \Delta x) = f(x) - f'(x)\Delta x + \frac{f''(x)(\Delta x)^2}{2} - \frac{f'''(x)(\Delta x)^3}{6} + \dots\dots\dots$$

Note: The series is very important as many of the Numerical methods and numerical representations are based on it.

The following are some of the uses of Taylor' Series:

A. Approximation of the function value:

Example: Given $f(x)=2x^2+3x+2$; calculate the function value at x=1.1

$$f(x+\Delta x)=f(x)+f'(x)\Delta x+\frac{f''(x)(\Delta x)^2}{2}+\frac{f'''(x)(\Delta x)^3}{6}+.........$$

$$f(1.1)=f(1+0.1)=f(1)+f'(1)\times 0.1+\frac{f''(1)(0.1)^2}{2}+\frac{f'''(1)(0.1)^3}{6}+.........$$

$$f(1)=2x^2+3x+2=2\times 1^2+3\times 1+2=7$$

$$f'(1)=4\times 1+3=7$$

$$f''(1)=4$$

$f'''(1) = 0$

Substitute in Eq. (1):

i. Two terms:

$$f(1.1) = f(1+0.1) = 7 + 7\times 0.1 = 7 + 0.7 = 7.7$$

ii. Three Terms:

$$f(1.1) = f(1+0.1) = 7 + 7\times 0.1 + \frac{4(0.1)^2}{2} = 7 + 0.7 + 0.02 = 7.72$$

iii. Four Terms: Same as with three terms as the third derivative is zero=7.72

The exact value of $f(1.1)$ **is:**

$$f(1) = 2x^2 + 3x + 2 = 2\times(1.1)^2 + 3\times 1.1 + 2 = 7.72$$

Thus, the result using 3 terms of Taylor series is identical to the exact one. This is not always the case as the number of terms of Taylor series we use does matter. In our case, we got exact value because we used three terms. Actually, 3 terms correspond to the second order polynomial. That is, look at Taylor series from a different angle: It represents a polynomial. How? Let $\Delta x = (x - x_0)$, $x = x_0 + \Delta x$; then Taylor Series becomes (we take two terms first):

$$f(x_0 + \Delta x) = f(x_0) + f'(x_0)\Delta x = f(x_0 + \Delta x) = f(x_0) + f'(x_0)(x - x_0)$$

$$= f(x_0) + f'(x_0)x - f'(x_0)x_0 = \left[f(x_0) - f'(x_0)x_0\right] + f'(x_0)x$$

Let: $a = \left[f(x_0) - f'(x_0)x_0\right]$; $b = f'(x_0)$; **Note:** any function of x_0 is a constant. So, we get:

$$f(x_0+\Delta x) = a + bx \text{;}$$

We get a linear polynomial as **a** is a constant and **b** is the slope. The same can be done with three or more terms and we get polynomials of varying degrees.

For three terms:

$f(x_0+\Delta x) = a + bx + cx^2$; here **c** is a collection of constants multiplying x^2 just like the **b** constant is a constant term multiplying **x,** the rest of the constant terms are absorbed by the coefficients **a & b** which becomes for the three terms as:

$$f(x_0+\Delta x) = f(x_0) + f'(x_0)\Delta x + \frac{f''(x_0)(\Delta x)^2}{2} = f(x_0) + f'(x_0)(x-x_0) + 0.5 f''(x_0)(x-x_0)^2$$

$$= f(x_0) + f'(x_0)x - f'(x_0)x_0 + 0.5 f''(x_0)\left[x^2 - 2x_0x + x_0^2\right]$$

$$= f(x_0) + f'(x_0)x - f'(x_0)x_0 + 0.5f''(x_0)x^2 - x_0 f''(x_0)x + 0.5f''(x_0)x_0^2$$

$$= \left(f(x_0) - f'(x_0)x_0 + 0.5f''(x_0)x_0^2\right) + \left(f'(x_0) - x_0 f''(x_0)\right)x + \left(0.5f''(x_0)\right)x^2$$

$$a = \left(f(x_0) - f'(x_0)x_0 + 0.5f''(x_0)x_0^2\right)$$

$$b = \left(f'(x_0) - x_0 f''(x_0)\right)$$

$$c = \left(0.5f''(x_0)\right)$$

$$f(x_0 + \Delta x) = a + bx + cx^2$$

So, the result should be exact for a first order polynomial when using two terms of Taylor Series and for a second order polynomial when using three terms of Taylor Series.

B. Approximation of the Derivatives Using Taylor Series:

$$f(x+\Delta x) = f(x) + f'(x)\Delta x + \frac{f''(x)(\Delta x)^2}{2} + \frac{f'''(x)(\Delta x)^3}{6} + ...$$

(b.1) <u>First Derivative</u>: Take two terms of Taylor Series:

$$f(x \pm \Delta x) = f(x) \pm f'(x)\Delta x.$$

i. Forward (FWD) Difference

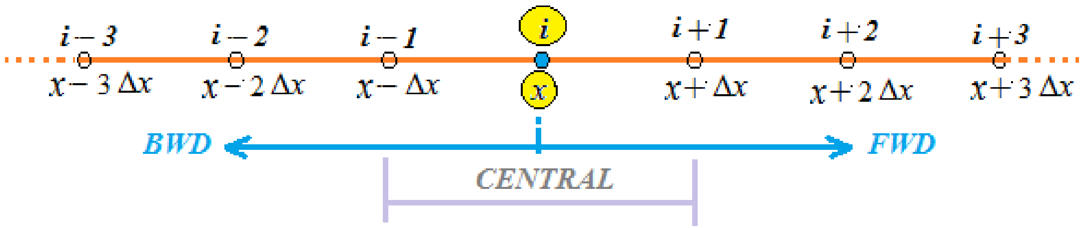
Use two terms: $f(x+\Delta x) = f(x) + f'(x)\Delta x.$

Solve for $f'(x)$

$$f'(x) = \frac{f(x+\Delta x) - f(x)}{\Delta x} + Error$$

FWD Difference

The error is due to the fact that we truncated the series to two terms only. This error is called <u>TRUNCATION ERROR</u>, $\boldsymbol{E_T}$.



ii. Backward (BWD) Difference

Use two terms: $f(x-\Delta x) = f(x) - f'(x)\Delta x.$

Solve for $f'(x)$

$$f'(x) = \frac{f(x) - f(x-\Delta x)}{\Delta x} + E_T$$

BWD Difference

iii. CENTRAL Difference: Take two terms of $f(x+\Delta x)$ & $f(x-\Delta x)$

$$f(x+\Delta x) = f(x) + f'(x)\Delta x$$

$$f(x-\Delta x) = f(x) - f'(x)\Delta x$$

Subtract the second expression from the first

$$f'(x) = \frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta \mathrm{x}} + E_T$$ **CENTRAL Difference**

Example: Find the derivative of $f(x) = 2x^2 + 3x + 2$ @ x=1

- ✓ Exact: $f'(x) = 4x + 3$

  $$f'(1) = 4 + 3 = 7$$

- ✓ Numerical: Using FWD Difference (Δx =0.1, 0.01, 0.001 & 10^{-6})

$$f'(x) \cong \frac{f(x+\Delta x) - f(x)}{\Delta \mathrm{x}} \cong \frac{f(1+0.1) - f(1)}{0.1} = \mathbf{7.2;}$$

$$\cong \frac{f(1+0.01) - f(1)}{0.01} = 7.02$$

$$\cong \frac{f(1+0.001) - f(1)}{0.001} = 7.002$$

$$\cong \frac{f(1+10^{-6}) - f(1)}{10^{-6}} = 7.0000007$$

$$E_T = Error = C(\Delta x)^1$$

$$f'(x) = \frac{f(x) - f(x - \Delta x)}{\Delta \mathrm{x}} + E_{truncation}$$ **BWD**

Using Central Difference:

$$f'(x) = \frac{f(x + \Delta x) - f(x - \Delta x)}{2\Delta \mathrm{x}} + E_T$$

$$f(x) = 2x^2 + 3x + 2$$

$$f'(x) = \frac{f(x + \Delta x) - f(x - \Delta x)}{2\Delta \mathrm{x}} = \frac{f(1 + 0.1) - f(1 - 0.1)}{0.2} = \mathbf{7.0}$$

Clearly, the **<u>CENTRAL Difference</u>** is more accurate than the FWD or BWD difference formula.

$$E_T = C(\Delta x)^2$$

Derivation of the truncation error: FWD Difference

$$f'(x)=\frac{f(x+\Delta x)-f(x)}{\Delta \mathrm{x}}+E_T$$

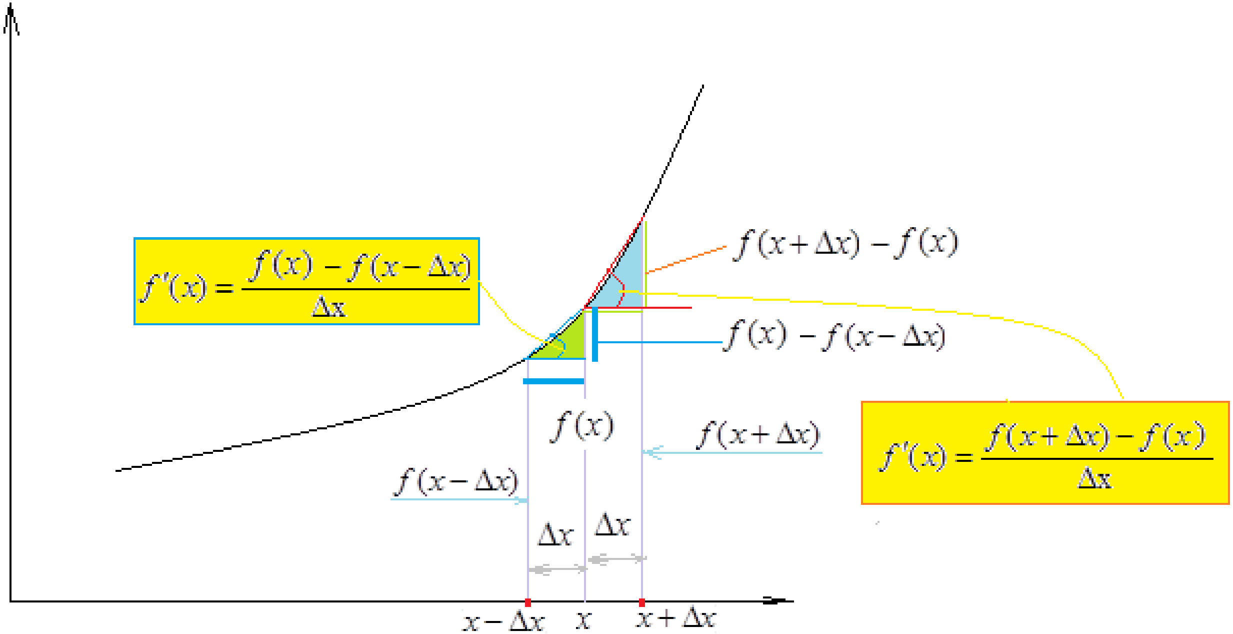
$$E_T=f'(x)-\frac{f(x+\Delta x)}{\Delta x}+\frac{f(x)}{\Delta \mathrm{x}}, \quad \frac{-f(x+\Delta x)}{\Delta x}=-\frac{f(x)}{\Delta x}-\frac{f'(x)\Delta x}{\Delta x}-\frac{f''(x)(\Delta x)^2}{2\Delta x}$$

$$E_T=f'(x)-\frac{f(x)}{\Delta x}-\frac{f'(x)\Delta x}{\Delta x}-\frac{f''(x)(\Delta x)^2}{2\Delta x}+\frac{f(x)}{\Delta \mathrm{x}}$$

$$E_T=\cancel{f'(x)}-\cancel{\frac{f(x)}{\Delta x}}-\frac{\cancel{f'(x)}\cancel{\Delta x}}{\cancel{\Delta x}}-\frac{f''(x)(\Delta x)^2}{2\Delta x}+\cancel{\frac{f(x)}{\Delta \mathrm{x}}}$$

$$E_T=-\frac{f''(x)(\Delta x)}{2}=\left(-\frac{f''(x)}{2}\right)\Delta x=\left(-\frac{f''(x^*)}{2}\right)\Delta x=C\Delta x$$

a. Approximation of derivatives: Using Graphical Approach



Second Derivative:

i. Taylor Series (three terms)

$$f(x+\Delta x) = f(x) + f'(x)\Delta x + \frac{f''(x)(\Delta x)^2}{2}$$

$$f(x-\Delta x) = f(x) - f'(x)\Delta x + \frac{f''(x)(\Delta x)^2}{2}$$

Sum the two equations:

$$f(x+\Delta x) + f(x-\Delta x) = 2f(x) + f''(x)(\Delta x)^2$$

$$f''(x) = \frac{f(x+\Delta x) - 2f(x) + f(x-\Delta x)}{(\Delta x)^2} + E_T$$

Example: $f(x) = 2x^3 + 3x^2 + 2x$; $f'(x) = 6x^2 + 6x + 2$

$f''(x) = 12x + 6$; $f''(1) = 12 + 6 = 18$ <----- Exact

$$f''(1) = \frac{f(1+0.1) - 2f(1) + f(1-0.1)}{(0.1)^2} = 18.0$$

$$f''(1) = \frac{f(1+10^{-5}) - 2f(1) + f(1-10^{-5})}{(10^{-5})^2} = 18.0$$

Truncation Error:

$$f''(x) = \frac{f(x+\Delta x) - 2f(x) + f(x-\Delta x)}{(\Delta x)^2} + E_T$$

$$E_T = f''(x) - \frac{f(x+\Delta x)}{(\Delta x)^2} + 2\frac{f(x)}{(\Delta x)^2} - \frac{f(x-\Delta x)}{(\Delta x)^2}$$

$$\frac{f(x+\Delta x)}{(\Delta x)^2} = \frac{f(x)}{(\Delta x)^2} + \frac{f'(x)\Delta x}{(\Delta x)^2} + \frac{f''(x)(\Delta x)^2}{2(\Delta x)^2} + \frac{f'''(x)(\Delta x)^3}{6(\Delta x)^2} + \frac{f^{(iv)}(x)(\Delta x)^4}{24(\Delta x)^2} \ldots\ldots\ldots$$

$$\frac{f(x-\Delta x)}{(\Delta x)^2} = \frac{f(x)}{(\Delta x)^2} - \frac{f'(x)\Delta x}{(\Delta x)^2} + \frac{f''(x)(\Delta x)^2}{2(\Delta x)^2} - \frac{f'''(x)(\Delta x)^3}{6(\Delta x)^2} + \frac{f^{(iv)}(x)(\Delta x)^4}{24(\Delta x)^2}$$

$$E_T = f''(x) - \frac{f(x+\Delta x)}{(\Delta x)^2} + 2\frac{f(x)}{(\Delta x)^2} - \frac{f(x-\Delta x)}{(\Delta x)^2} = \frac{-f^{(iv)}(x)(\Delta x)^2}{12} =$$

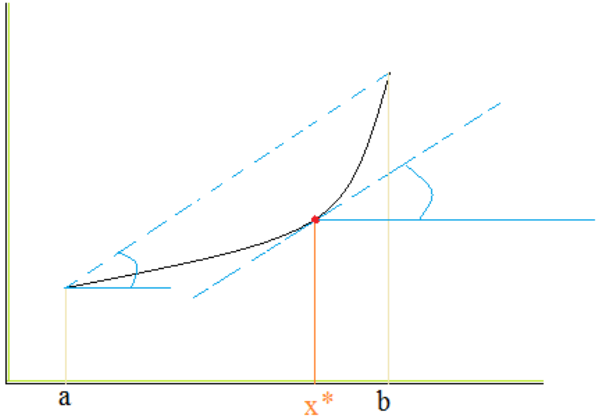
$$\frac{-f^{(iv)}(x^*)}{12}(\Delta x)^2$$

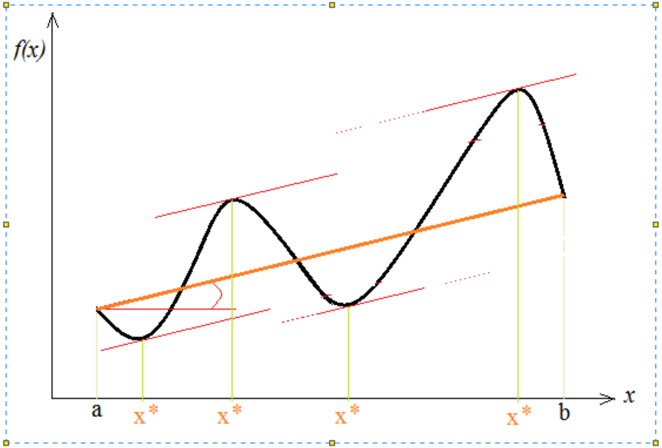
$$E_T = \frac{-f^{(iv)}(x^*)}{12}(\Delta x)^2 = C(\Delta x)^2$$

Leads that:

$$f''(x) = \frac{f(x+\Delta x)}{(\Delta x)^2} - 2\frac{f(x)}{(\Delta x)^2} + \frac{f(x-\Delta x)}{(\Delta x)^2}$$

2. Mean Value Theorem for Derivatives:





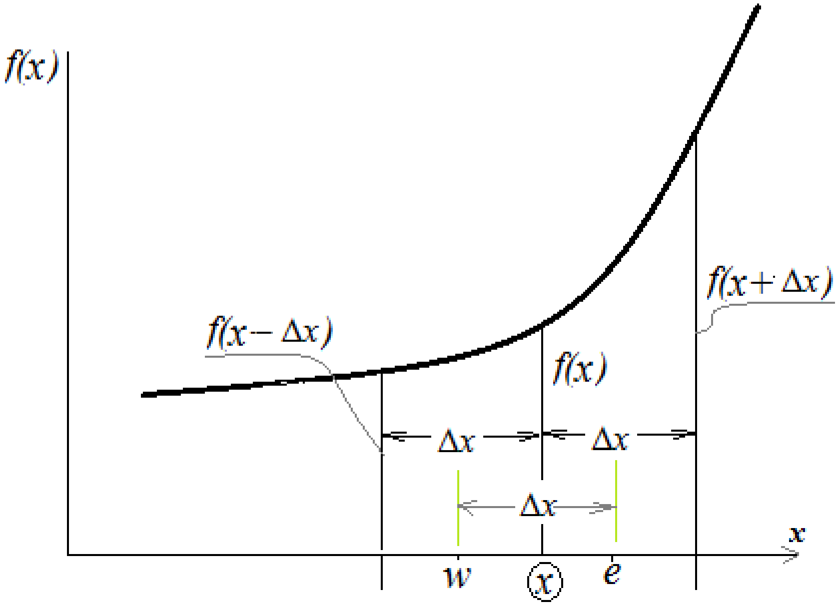
$$f(x) = 2x^6 + 3x^5 + 2x^2$$

$$f''(x) = 60x^4 + 60x^3 + 4$$

$$f''(1) = 60x^4 + 60x^3 + 4 = 124$$

$$f''(1) = \frac{f(1+0.1) - 2f(1) + f(1-0.1)}{(0.1)^2} = 124.9$$

ii. Graphical



$$f''(x) = \frac{d}{dx}\left(\frac{df}{dx}\right) = \frac{d}{dx}(\phi) = \frac{\phi_e - \phi_w}{\Delta x} = \frac{\left(\frac{df}{dx}\right)_e - \left(\frac{df}{dx}\right)_w}{\Delta x} =$$

$$= \frac{\left(\frac{f(x+\Delta x) - f(x)}{\Delta x}\right) - \left(\frac{f(x) - f(x-\Delta x)}{\Delta x}\right)}{\Delta x}$$

$$f''(x) \cong \frac{f(x+\Delta x) - 2f(x) + f(x-\Delta x)}{(\Delta x)^2}$$

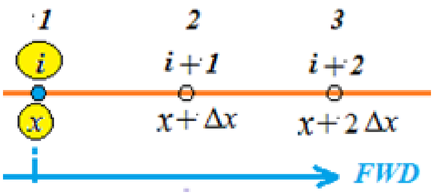
iii. The Method of Undetermined Coefficients

First Derivative: The derivative is assumed to have the following form. The number of points used is **n.**

$$f'(x) = \sum_{i=1}^{n} a_i f(x_i) = a_1 f(x_1) + a_2 f(x_2) + \ldots . a_n f(x_n)$$

For the first derivative using 2 points FWD (i and i+1):

$$f'(x) = a_1 f(x_1) + a_2 f(x_2)$$



Here, we have two unknowns (constants a_1 & a_2). We need 2 equations. We demand that the derivative is exact for *f*(x)=constant, *f*(x)=linear function, *f*(x) = quadratic and so on. We have 2 unknowns and thus we take the first two conditions, i.e., f(x)=constant & f(x)=linear function. The best constant is the unity, and the best line is x. So,

$$f(x)=1: \quad f'(x)=0=a_1\times 1+a_2\times 1 \quad ====> \quad a_1+a_2=0 \quad ......(1)$$

$$f(x)=x: \quad f'(x)=1=a_1\times x_1+a_2\times x_2 \quad ====> \quad a_1x_1+a_2x_2=1 \quad ......(2)$$

Solve Eqs. (1) and (2) for $a_1 \,\&\, a_2 \quad ====> \quad a_1=-a_2$

$$-a_2x_1+a_2x_2=(x_2-x_1)a_2=(\Delta x)a_2=1 ====> a_2=\frac{1}{\Delta x}$$

$$a_1=\frac{-1}{\Delta x}$$

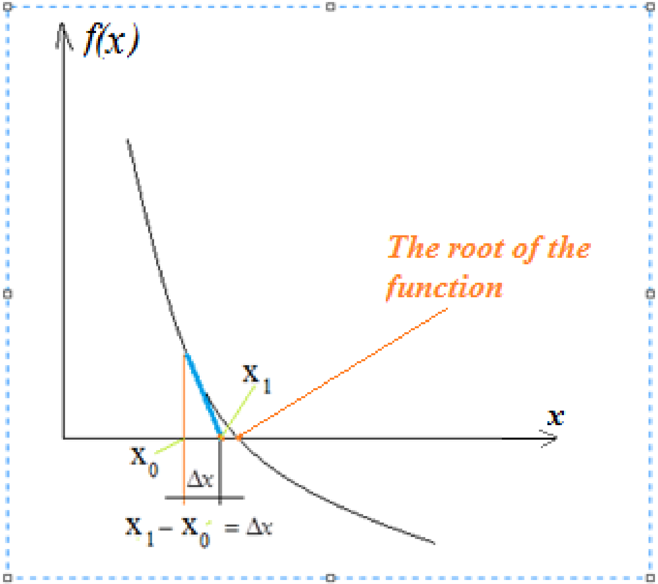
$$f'(x)=\frac{-1}{\Delta x}f(x_1)+\frac{1}{\Delta x}f(x_2)=\frac{f(x_2)-f(x_1)}{\Delta x} \quad \text{or}$$

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

FWD

C. Numerical method (Newton-Raphson Method)

Note the graph below. The tangent line is represented by: $f(x+\Delta x)=f(x)+f'(x)\Delta x$



The function interests the x-axis at $x+\Delta x$ at which the function is zero. That is,

$$\overbrace{f(x+\Delta x)}^{0} = f(x) + f'(x)\Delta x$$

$$\Delta x = \frac{f(x)}{f'(x)} \quad \textbf{..................(1);}$$

$$\Delta x = x_1 - x_0 = x_{i+1} - x_i$$

Eq. (1) Becomes:

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)} <\!=\!=\!=\!= \quad Newton - RaphsonMethod$$