Truncation Errors & Taylor Series

Ch. 4

Lecture Objectives

- To understand the basic utility of the Taylor series in numerical methods
- To understand the *Derivative Mean Value Theorem* and it's application to error analysis
- To understand the *Propagation of Error*

Truncation Errors & Taylor Series

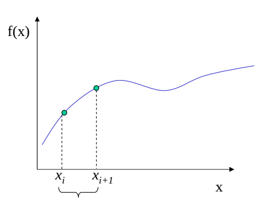
Taylor Series – provides a way to predict a value of a function at one point in terms of the function value and derivatives at another point.

* Any smooth function can be approximated by a polynomial

1. "Zeroth-Order" Approximation

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

   – Close if *h* is small
   – Exact if *f(x)=constant*

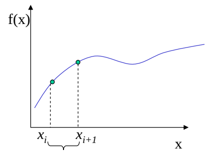


Truncation Errors & Taylor Series

2. 1^{st} - Order Approximation

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

↑ slope ↑ spacing



– Is an equation for a straight line (ie., y = mx + b) and is exact if *f(x)* is linear

Truncation Errors & Taylor Series

3. 2^{nd} - Order Approximation

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

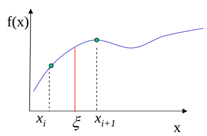
4. In general, if $h = (x_{i+1} - x_i)$

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

where $R_n = \dfrac{f^{n+1}(\xi)h^{n+1}}{(n+1)!}$

R_n is exact if f^{n+1} is evaluated at ξ

$$x_i < \xi < x_{i+1}$$



Example – 3^{rd} Order Polynomial

$$f(x) = x^3 - 3x^2 + 4x + 1$$

Estimate $f(x_{i+1} = 1)$ using information at $f(x_i = 0)$.
* Use h=1

Example – 3rd Order Polynomial

$$f(x) = x^3 - 3x^2 + 4x + 1$$

Estimate $f(x_{i+1} = 1)$ using information at $f(x_i = 0)$.
* Use h=1

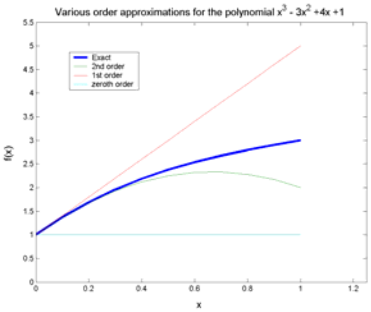
Exact: $f(1) = 1 - 3 + 4 + 1 = 3$

Approximate:
$$f'(x) = 3x^2 - 6x + 4$$
$$f''(x) = 6x - 6$$
$$f'''(x) = 6$$
$$f^{iv}(x) = 0$$

$$f(1) = f(0) + f'(0)h + \frac{f''(0)h^2}{2!} + \frac{f'''(0)h^3}{3!}$$

$$f(1) = 1 + 4(1) + \frac{(-6)1^2}{2} + \frac{(6)1^3}{6} = 1 + 4 - 3 + 1 = 3$$

Example – 3rd Order Polynomial



In general, the *N*th order TS expansion of a polynomial of order *N* is exact.

Truncation Error

In General, we do not have an infinite number of terms. Hence, our remainder term $R_n > 0$

$$R_n = \frac{f^{n+1}(\xi)h^{n+1}}{(n+1)!}$$

"Error Order" is expressed as $R_n = O(h^{n+1})$

- Truncation error is of order *h* to the n+1
- Truncation Error is proportional to *h* to *n*+1
- Allows comparison of truncation errors

For example, let's approximate f(x) with p(x)

$$p(x) = f(a) + f'(a)h + \frac{f''(a)h^2}{2!} + \frac{f'''(a)h^3}{3!} + R_3$$
$$R_3 = O(h^4)$$

Is read as, the error incurred using the third order Taylor series expansion *p(x)* to apprximate *f(x)* is of order *h* to the 4th.

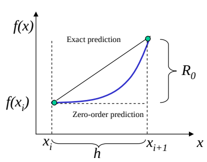
Truncation Error

What does this mean?

$R_n = O(h)$ Cut h in half → ½ error

$R_n = O(h^2)$ Cut h in half → 1/4 error

Understanding ξ
Derivative Mean Value Theorem



Zero Order Approximation

$$f(x_{i+1}) \approx f(x_i)$$

$$R_0 = f'(a)h + \frac{f''(a)h^2}{2!} + \cdots$$

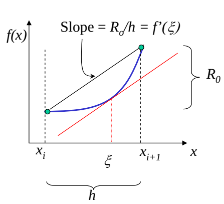
$$f(x_{i+1}) = f(x_i) + R_0$$

$$R_0 = f'(\xi)h$$

$$x_i < \xi < x_{i+1}$$

Derivative Mean Value Theorem: if a function f(x) and its 1st derivative are continuous over $x_i < x < x_{i+1}$ then there exists at least one point on the function that has a slope (I.e. derivative) parallel to the line connecting $f(x_i)$ and $f(x_{i+1})$

Understanding ξ
Derivative Mean Value Theorem



Taylor Series & Truncation Estimates (Finite Difference Approximations)

1. Forward Finite Difference Method – 1st derivative

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

Solve for *f'(x)*

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

The truncation error may be written:

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

the error is of "order h"

Taylor Series & Truncation Estimates (Finite Difference Approximations)

2. Backward Finite Difference Method – 1st derivative:
Subtract Backward expansion from Forward exp

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

Solve for *f'(x)*

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

Taylor Series & Truncation Estimates (Finite Difference Approximations)

3. Central Finite Difference Method – 1st derivative

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

$$-\left[f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{f''(x_i)h^2}{2!} - \frac{f'''(x_i)h^3}{3!} + ... \right]$$

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

Solve for *f'(x)*

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

Finite Difference Approximations – Higher Order derivatives

4. Forward Finite Difference Method – 2nd derivative

$$f(x_{i+2}) = f(x_i) + f'(x_i)2h + \frac{f''(x_i)4h^2}{2!} + \frac{f'''(x_i)8h^3}{3!} + \ldots$$

$$-\left[2f(x_{i+1}) = 2f(x_i) + 2f'(x_i)h + \frac{2f''(x_i)h^2}{2!} + \frac{2f'''(x_i)h^3}{3!} + \ldots\right]$$

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

Solve for *f'(x)*

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

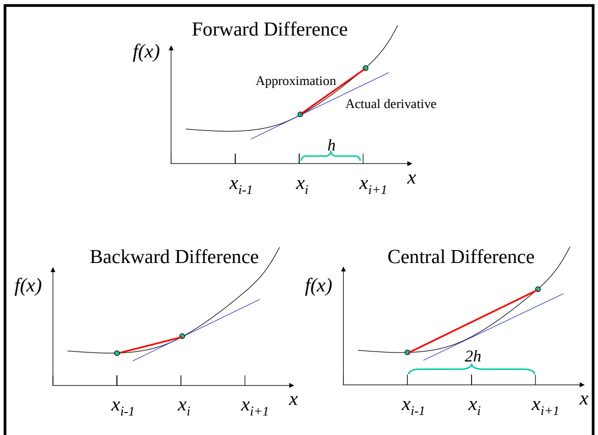
Finite Difference Approximations – Higher Order derivatives

5. Backward Finite Difference Method – 2nd derivative

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

5. Central Finite Difference Method – 2nd derivative

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



<u>Error Propagation</u>- How do errors in individual variables propagate through calculations?

Consider a true value x and an approximate value $\tilde{x}$ (for a 4 digit computer):

$$x = 0.123456\times10^{1}$$
$$\tilde{x} = 0.1234\times10^{1}$$

How much error is introduced in *f(x)* by $\tilde{x}$ approximation?

$$\Delta f(\tilde{x}) = \left|f(x) - f(\tilde{x})\right|$$

Difficult to estimate since x is unknown.
We can write a TS expansion for f(x) about $\tilde{x}$

$$f(x) = f(\tilde{x}) + f'(\tilde{x})(x-\tilde{x}) + \frac{f''(\tilde{x})(x-\tilde{x})^2}{2!} + \ldots$$

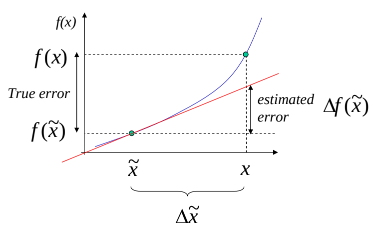
Truncate at 1st derivative:

$$\Delta f(\tilde{x}) = \left|f(x) - f(\tilde{x})\right| = \left|f'(\tilde{x})\right|\left|x-\tilde{x}\right| = \left|f'(\tilde{x})\right|\Delta\tilde{x}$$

Estimate of Error in *f*

Estimate of Error in *x*

Graphical Interpretation of Error Estimate



Example: Given $f(x) = e^{-2x} + 3x$

Estimate the error $\Delta f(\tilde{x})$ for $\tilde{x} = 1$ with $\Delta\tilde{x} = 0.01$

<u>Error Propagation</u>- Functions of more than one variable

Apply Taylor Series to functions of multiple variables, I.e., *f(x,y,z)*

$$f(x_{i+1}, y_{i+1}, z_{i+1}) = f(x_i, y_i, z_i) + \left.\frac{\partial f}{\partial x}\right|_i (x_{i+1} - x_i) + \left.\frac{\partial f}{\partial y}\right|_i (y_{i+1} - y_i) + \left.\frac{\partial f}{\partial z}\right|_i (z_{i+1} - z_i) + H.O.T.$$

Neglecting 2nd order and higher terms, the error in *f* is:

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Neglecting 2nd order and higher terms, the error in *f* is:

$$\Delta f(\tilde{x}, \tilde{y}, \tilde{z}) = \left|\frac{\partial f}{\partial x}\right| \Delta\tilde{x} + \left|\frac{\partial f}{\partial y}\right| \Delta\tilde{y} + \left|\frac{\partial f}{\partial z}\right| \Delta\tilde{z}$$

Where $\Delta\tilde{x}\ \Delta\tilde{y}\ \Delta\tilde{z}$ are estimates of the error in *x*, *y* and *z*

In general, 1st order approximation of the error in *f* is:

$$\Delta f(\tilde{x}_1, \tilde{x}_2, \tilde{x}_3, \ldots, \tilde{x}_n) = \left|\frac{\partial f}{\partial x_1}\right| \Delta\tilde{x}_1 + \left|\frac{\partial f}{\partial x_2}\right| \Delta\tilde{x}_2 + \left|\frac{\partial f}{\partial x_3}\right| \Delta\tilde{x}_3 + \ldots + \left|\frac{\partial f}{\partial x_n}\right| \Delta\tilde{x}_n$$

Error Propagation- Reynolds Number Example

$$\mathrm{Re} = \frac{UD}{\nu}$$

Where: V = average fluid velocity (m/s)
D = pipe diameter (m)
ν = kinematic viscosity (m^2/s) water

Estimate the error in Re for the Given data:

$\tilde{U} = 0.5$ $\Delta\tilde{U} = 0.01$ m/s
$\tilde{D} = 0.1$ $\Delta\tilde{D} = 0.001$ m
$\tilde{\nu} = 1.0\times10^{-6}$ $\Delta\tilde{\nu} = 0.005\times10^{-6}$ m^2/s

$$\mathrm{Re} = \frac{UD}{\nu} = \frac{(.5)(.1)}{1\times10^{-6}} = 50{,}000$$

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$$\Delta\mathrm{Re}(\tilde{U}, \tilde{D}, \tilde{\nu}) = \left|\frac{\partial \mathrm{Re}}{\partial U}\right| \Delta\tilde{U} + \left|\frac{\partial \mathrm{Re}}{\partial D}\right| \Delta\tilde{D} + \left|\frac{\partial \mathrm{Re}}{\partial \nu}\right| \Delta\tilde{\nu}$$

$$\Delta\mathrm{Re}(\tilde{U}, \tilde{D}, \tilde{\nu}) = \left|\frac{D}{\nu}\right| \Delta\tilde{U} + \left|\frac{U}{\nu}\right| \Delta\tilde{D} + \left|\frac{-UD}{\nu^2}\right| \Delta\tilde{\nu}$$

$$\Delta\mathrm{Re}(\tilde{U}, \tilde{D}, \tilde{\nu}) = \left|\frac{.1}{1\times10^{-6}}\right| .01 + \left|\frac{.5}{1\times10^{-6}}\right| .001 + \left|\frac{(.5)(.1)}{(1\times10^{-6})^2}\right| (0.005\times10^{-6})$$

$$\Delta\mathrm{Re}(\tilde{U}, \tilde{D}, \tilde{\nu}) = 1000 + 500 + 250$$

$$\boxed{\begin{array}{l}\mathrm{Re} = 50{,}000 \pm 1750 \\ \mathrm{Re} = 50{,}000 \pm 3.5\%\end{array}}$$

Total Numerical Error

Total Error = Round-Off Error + Truncation Error

- Truncation Error: can be decreased by decreasing h or increasing the number of terms retained in the expansion
- R.O. Error: is increased by increasing the number of computations or do to effects such as subtractive cancellation, adding large and small numbers, smearing, etc (can be minimized with extended precision)

- Decreasing h leads to an increase in the total number of calculations → increase in R.O. Error.
- There is a point of diminishing returns with decreasing h
- Typically RO do not dominate since computers carry enough significant digits, but be careful!

Control of Numerical Error

avoid significance loss {

1. Avoid Subtracting Nearly Equal Numbers (use Extended Precision).
2. When Adding or Subtracting numbers sort them & begin adding the smallest numbers first.

}

3. Estimate accuracy by checking against a known solution … or by substituting the result back into the original Equation to see if it is satisfied.
4. Try a different algorithm.

Other Sources of Error

1. **Blunders**
   - Incorrect data entry
   - Improper programming
   - Departures from a prescribed procedure
2. **Formulation Error**
   - Incorrect Mathematical model
   - Not accounting for all important physical phenomena
3. **Experimental Data Uncertainty**
   - Measured uncertainty
   - Property data is imprecise
   - Can be reduced through uncertainty analysis