SECTION 1: ROUNDOFF AND TRUNCATION ERRORS

ESC 440 – Computational Methods for Engineers

Introduction and Course Overview

Mathematical Models

- As engineers, we are interested in
  - Designing and analyzing physical systems
  - Analyzing data
- We can represent these systems or data with ***mathematical models***
  - An ***equation*** or ***system of equations*** that describe the system or behavior
    - Relates ***inputs*** to ***outputs***
- Mathematical models used for ***analysis*** and ***simulation***
  - May be done ***analytically*** – by hand
  - More often performed ***numerically*** – on a computer

Numerical Analysis

- In practice, most engineering problems are solved, and analyses are performed ***numerically***
  - Using computers

- Often, we use simulators
  - Electronic circuits
  - Electromagnetic fields
  - Thermal/fluid systems
  - Structural analysis

- Sometimes, we use existing packages, libraries, toolboxes, functions, etc. E.g.,
  - NumPy, SciPy in Python
  - MATLAB

- Other times, we must write our own code

Engineering Analyses

- Many of the types of analyses we perform as engineers are those you have learned about in previous classes
  - Solution of systems of equations
  - Integration/differentiation
  - Solution of differential equations
  - Optimization
  - Curve fitting, etc.

- You have learned to perform these operations analytically
  - By hand
  - Solutions are ***exact***

- In this course, you will learn to solve the same types of problems numerically
  - Using a computer
  - Solutions are ***estimates***

Numerical Analysis

- Numerical analysis yields an approximate solution
  - An ***estimate*** of the actual solution
- The solution is not exact
  - It includes ***error***
- In this first section of the course, we will learn about ***numerical error***
  - Where does it come from?
  - What causes it to increase? Decrease?
  - How do we approximate it?

Course Overview

1. Roundoff & Truncation Error
2. Root Finding & Optimization
3. Systems of Equations
4. Curve Fitting
5. Integration
6. Ordinary Differential Equations
7. Fourier Analysis

Definitions of Error

True Error

- ***Absolute error*** – the difference between an approximation and the true value

$$\boxed{E_t = (approx.value) - \ (true\ value) = \hat{x} - x}$$

- ***Relative error*** – the true error as a percentage of the true value

$$\boxed{\varepsilon_t = \frac{\hat{x} - x}{x} \cdot 100\%}$$

- Both definitions ***require knowledge of the true value!***
  - If we had that, why would we be approximating?

Approximating the Error

- Since we don’t know the true value, we can only approximate the error
- Often, approximations are made ***iteratively***
  - Approximate the error as the change in the approximate value from one iteration to the next

$$\boxed{\hat{E} = \hat{x}_{i+1} - \hat{x}_i}$$

Relative Approximate Error

- We don’t know the true value, so we can’t calculate the true error – approximate the error
- ***Relative approximate error*** – an approximation of the error relative to the approximation itself

$$\boxed{\varepsilon_a = \frac{approx.\,error}{approximation} \cdot 100\% = \frac{\hat{E}}{\hat{x}} \cdot 100\%}$$

Stopping Criterion

- For iterative approximations, continue to iterate until the relative approximate error magnitude is less than a specified ***stopping criterion***

$$\boxed{|\varepsilon_a| < \varepsilon_s}$$

- For accuracy to ***at least n significant figures*** set the stopping criterion to

$$\boxed{\varepsilon_s = (0.5 \times 10^{2-n})\%}$$

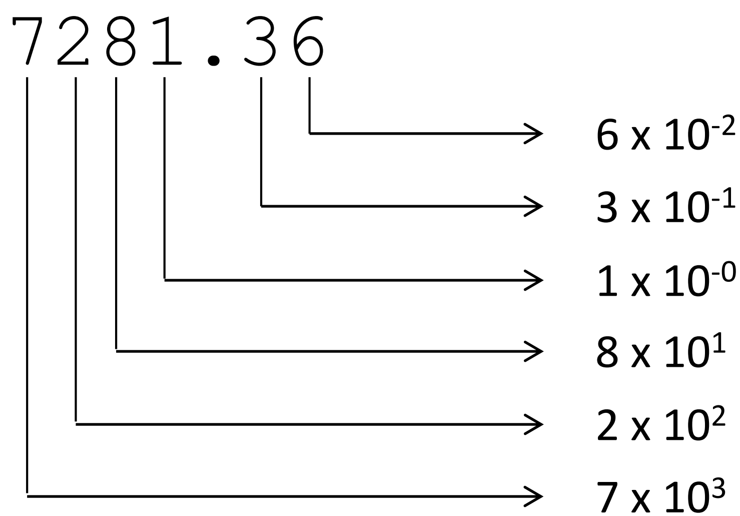
Roundoff Error

Roundoff Errors

- ***Roundoff errors*** occur due to the way in which computers represent numerical values
- Computer representation of numerical values is limited in terms of:
  - ***Magnitude*** – there are upper and lower bounds on the magnitude of numbers that can be represented
  - ***Precision*** – not all numbers can be represented exactly
- Certain types of mathematical manipulations are more susceptible to roundoff error than others

Number Systems – Decimal

- We are accustomed to the ***decimal*** number system
  - A ***base-10*** number system
  - Ten digits: 0, 1, 2, 3, 4, 5, 6, 7, 8, 9
  - Each digit represents an integer power of 10



Binary Number System

- Computers represent numbers in ***binary*** format
  - A ***base-2*** number system
  - Two digits: 0, 1
    - Easy to store binary values in computer hardware – an on or off switch – a high or low voltage
  - One digit is a ***bit*** – eight bits is a ***byte***
  - Each bit represents an integer power of 2

10110101

$1 \times 2^0 = 1$

$0 \times 2^1 = 0$

$1 \times 2^2 = 4$

$0 \times 2^3 = 0$

$1 \times 2^4 = 16$

$1 \times 2^5 = 32$

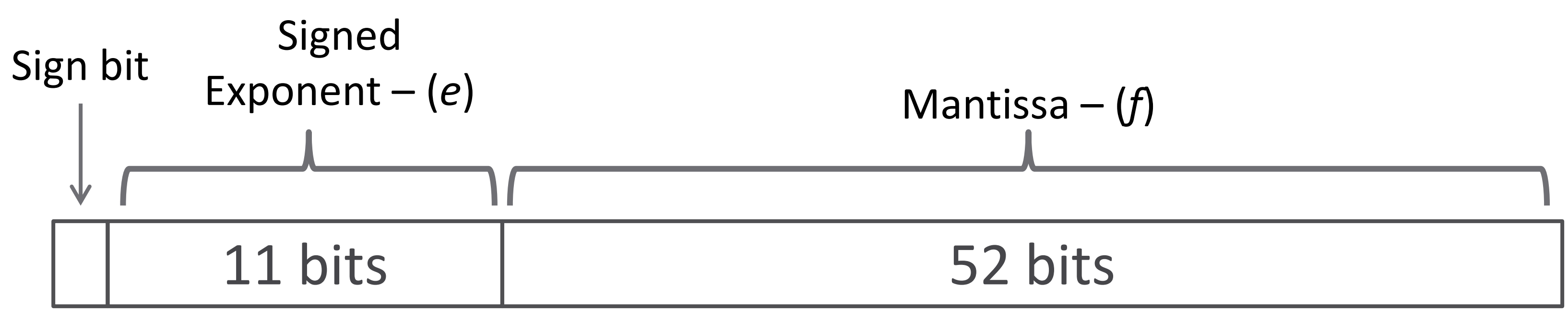
$0 \times 2^6 = 0$

$1 \times 2^7 = 128$

$= (181)_{10}$

IEEE Double-Precision Format

- Floating point numbers in Python are represented as 64-bit double-precision floating point values – `float64`
  - 64-bit binary word



$$\pm\left(1+\sum_{i=1}^{52} f_i \cdot 2^{-i}\right)\times 2^{e}$$

IEEE Double-Precision Format

- ***Mantissa***
  - Only the ***fractional portion*** of the mantissa stored
  - Bit to the left of the binary point assumed to be `1`
    - ***Normalized numbers***
    - Really a 53-bit value
- ***Exponent***
  - 11-bit signed integer value: -1022 … 1023
  - Two special cases:
    - e = 0x000 (i.e. ***all zeros***): zero if $f = 0$, ***subnormal #'s*** if $f \neq 0$
    - e = 0x7FF (i.e. ***all ones***): ∞ if $f = 0$, NaN if $f \neq 0$

Normalized numbers

- Leading zeros are removed
  - Most significant digit (must be a 1 in binary) moved to the left of the binary point
  - 53rd bit of the mantissa (always 1) needn't be stored
- Maximum mantissa

$$1.111\ldots\ldots11$$

f_0
Not stored

f_1

f_2

f_{51}

f_{52}

Subnormal Numbers

- If $f_0 = 1$, always, then the smallest number that could be represented is: $2^{-1022} \approx \mathbf{2.225 \times 10^{-308}}$
- If we allow for $f_0 = 0$, then the most significant bit is somewhere to the right of the binary point
  - Leading zeros – not normalized … ***subnormal***
  - Allows for smaller numbers, filling in the hole around zero
- Subnormal numbers represented by setting the exponent to zero
- Smallest subnormal number:

$$2^{-1022-52} = 2^{-1074} \approx \mathbf{5 \times 10^{-324}}$$

Doubles – Range

- **Maximum value:**

$$max = \left(1 + \sum_{i=1}^{52} 2^{-i}\right) \times 2^{1023} \approx \mathbf{1.798 \times 10^{308}}$$

- **Minimum normal value:**

$$min_{norm} = 2^{-1022} \approx \mathbf{2.225 \times 10^{-308}}$$

- **Minimum subnormal value:**

$$min_{sub} = 2^{-1022-52} = 2^{-1074} \approx \mathbf{5 \times 10^{-324}}$$

- **Precision – *machine epsilon***

$$\boldsymbol{\varepsilon = 2^{-52} \approx 2.22 \times 10^{-16}}$$

Roundoff Error – Mathematical Operations

Certain types of mathematical operations are more susceptible to roundoff errors:

- ***Subtractive cancellation*** – subtracting of two nearly-equal numbers results in a loss of significant digits
- ***Large computations*** – even if the roundoff error from a single operation is small, the cumulative error from many operations may be significant
- ***Adding large and small numbers*** – as in an infinite series
- ***Inner products*** – (i.e., dot product) very common operation – solution of linear systems of equations

Truncation Error

Truncation Errors

- Errors that result from ***the use of an approximation*** in place of an exact mathematical procedure
  - E.g., numerical integration, or the approximation derivatives with finite-difference approximations

- To understand how truncation errors arise, and to gain an understanding of their magnitudes, we'll make use of the ***Taylor Series***

Taylor Series

- ***Taylor's Theorem*** – any smooth (i.e., continuously differentiable) function can be approximated as a polynomial
- ***Taylor Series***

$$f(x_{i+1}) = \sum_{n=0}^{\infty} \frac{f^{(n)}(x_i)}{n!}(x_{i+1} - x_i)^n$$

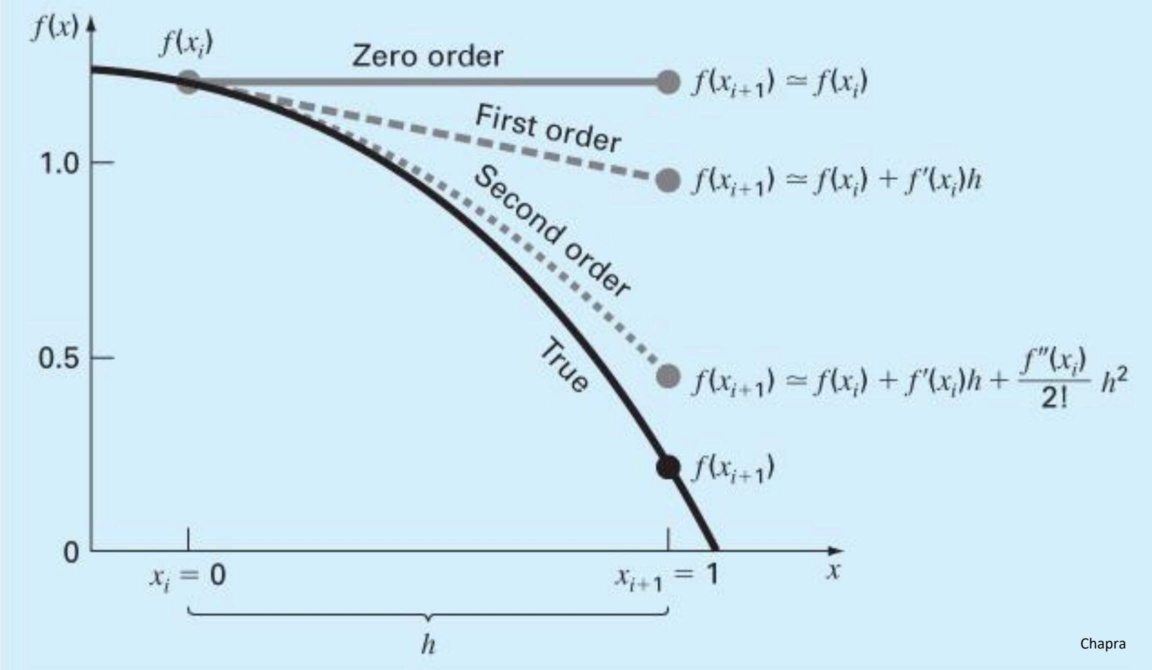
- This infinite series is an ***equality***
  - An ***exact*** representation of any smooth function as a polynomial
  - An ***infinite-order polynomial*** – impractical

Taylor Series Approximation

- Can approximate a function as a polynomial by ***truncating*** the Taylor series after a finite number of terms

$$f(x_{i+1}) \approx f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \cdots + \frac{f^{(n)}(x_i)}{n!}h^n$$

where $h = x_{i+1} - x_i$ is the ***step size***



Taylor Series Truncation Error

- Can account for error by lumping the $n+1$ and higher-order terms into a single term, R_n

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

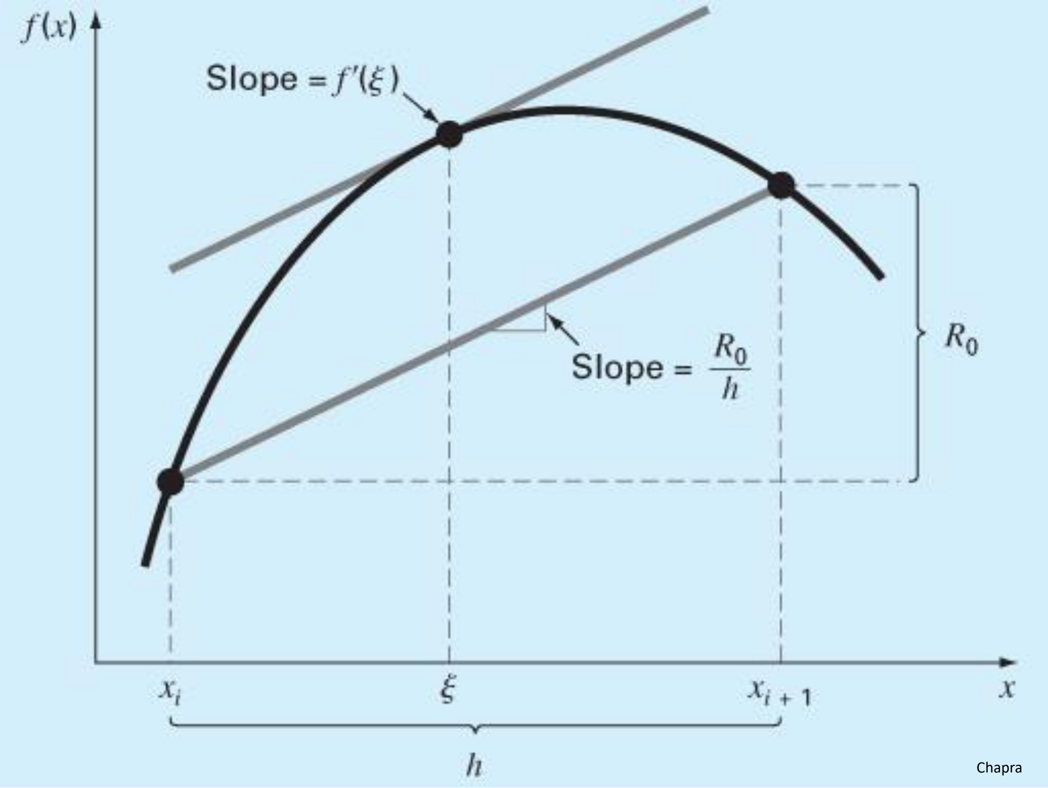
- R_n is the error associated with truncating after n terms

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

- ξ is some (***unknown***) value of x between x_i and x_{i+1}

Derivative Mean-Value Theorem

- If $f(x)$ and $f'(x)$ are continuous on $[x_i, x_{i+1}]$, then there is a point on this interval, ξ, where $f'(\xi)$ is the slope of the line joining $f(x_i)$ and $f(x_{i+1})$



Truncation Error – Dependence on Step Size

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

- We don't know ξ, so we don't know R_n
  - We do know it's proportional to h^{n+1}, where h is the ***step size***
  - Error is ***on the order of*** h^{n+1}

$$R_n = O(h^{n+1})$$

- If $n = 1$ (first-order approx.), ***halving*** the step size will ***quarter*** the error

Truncation Errors in Practice

- Discretizing equations
- Finite-difference approximations

Discretization of Equations

- As engineers, many of the mathematical expressions we are interested in are differential equations
  - We know how to evaluate derivatives analytically
  - Need an approximation for the derivative operation in order to solve numerically
- ***Discretization*** – conversion of a continuous function, e.g., differentiation, to a discrete approximation for numerical evaluation

Finite Difference Approximations

- Recall the definition of a derivative

$$f'(x_i) = \lim_{h \to 0} \frac{f(x_{i+1}) - f(x_i)}{h}$$

- Remove the limit to approximate this numerically

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

- This is the ***forward difference approximation***
  - Uses value at x_i and forward one step at x_{i+1} to approximate the derivative at x_i

Discretizing Equations – Example

- A free-falling object can be modeled as

$$\frac{dv}{dt} = g - \frac{c_d}{m} v^2$$

where v is velocity, m is mass, g is gravitational acceleration, and c_d is a lumped drag coefficient

- This is a non-linear ordinary differential equation (ODE), which can be solved analytically to yield

$$v(t) = \sqrt{\frac{mg}{c_d}} \tanh\left(\sqrt{\frac{g c_d}{m}} \cdot t\right)$$

Discretizing Equations – Example

- To solve numerically instead, approximate the derivative operation with a finite difference

$$\frac{v(t_{i+1}) - v(t_i)}{t_{i+1} - t_i} \cong g - \frac{c_d}{m} v(t_i)^2$$

- Solving for $v(t_{i+1})$ and using h to denote the time step yields

$$v(t_{i+1}) \cong v(t_i) + \left[g - \frac{c_d}{m} v(t_i)^2\right] h$$

- We've transformed the ***differential equation*** to a ***difference equation***
  - An ***algebraic*** equation
  - Can be solved iteratively – using a loop

Discretizing Equations – Example

$$v(t_{i+1}) \cong v(t_i) + \left[g - \frac{c_d}{m} v(t_i)^2\right] h$$

- The term in the square brackets is the original diff. eq., i.e., it is $v'(t)$
- The difference equation is a ***first-order Taylor series approximation***

$$v(t_{i+1}) = v(t_i) + v'(t_i)\, h + R_1$$

- Where we know that the error is on the order of the step size squared

$$R_1 = O(h^2)$$

- ***Taylor series provides a relation between the step size and the accuracy of the numerical solution to the diff. eqn.***

Finite Difference Methods

- The preceding example showed
  - One method – forward difference – for numerically approximating a derivative
  - Transformation of a differential equation to a difference equation
  - How Taylor series can provide an understanding of the error associated with an approximation
- Now we'll take a closer look at three ***finite difference methods*** and how Taylor series can help us understand the error associated with each

Forward Difference

- Can also derive the forward difference approximation from the Taylor Series

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

- Solving for $f'(x_i)$

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

- We've already seen that

$$R_1 = O(h^2)$$

- So, the error term is

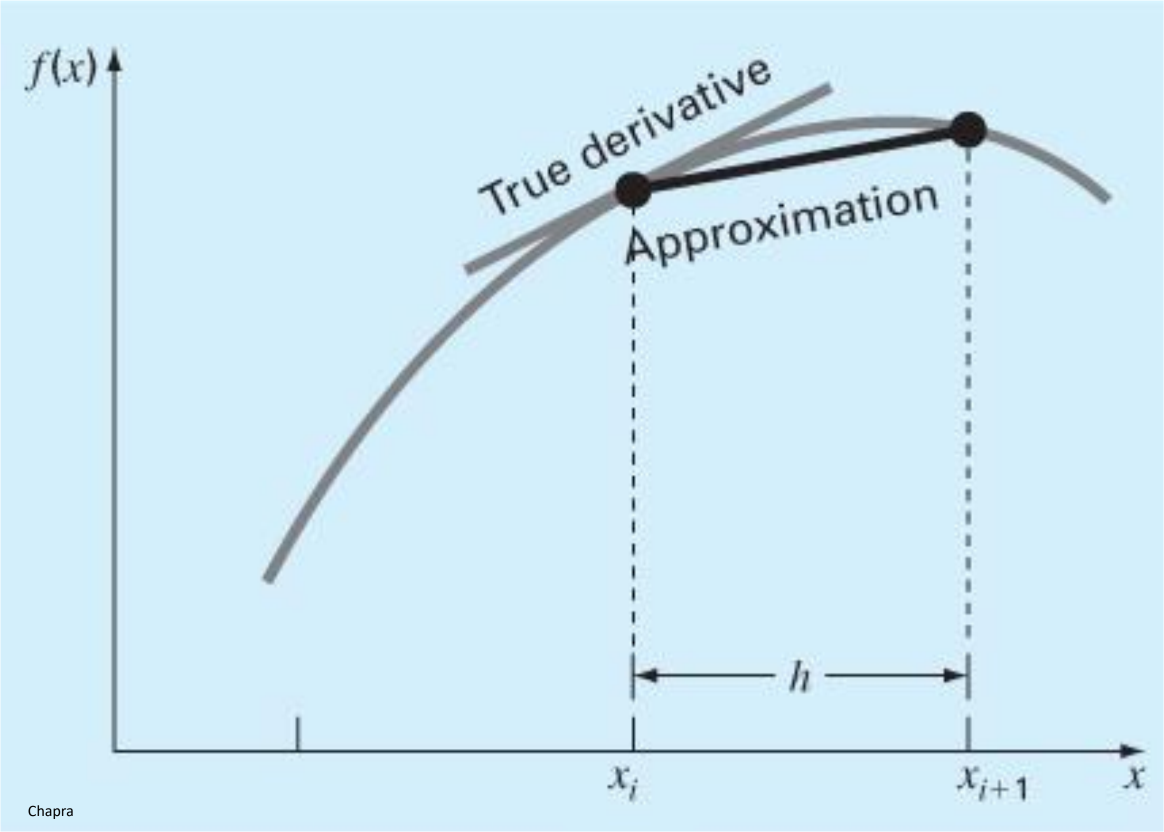
$$\frac{R_1}{h} = O(h)$$

- The forward difference, including error, is

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

- ***Error of the forward difference approximation is on the order of the step size***

Forward Difference



- Value of the function, $f(x)$, at x_i and forward one step at x_{i+1} used to approximate the derivative at x_i

Backward Difference

- ***Backward difference*** uses value of $f(x)$ at x_i and ***one step backward*** at x_{i-1} to approximate the derivative at x_i

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

- This can also be developed by expanding the Taylor series backward

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

- Then solving for $f'(x_i)$

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

- Again the error is on the order of the step size

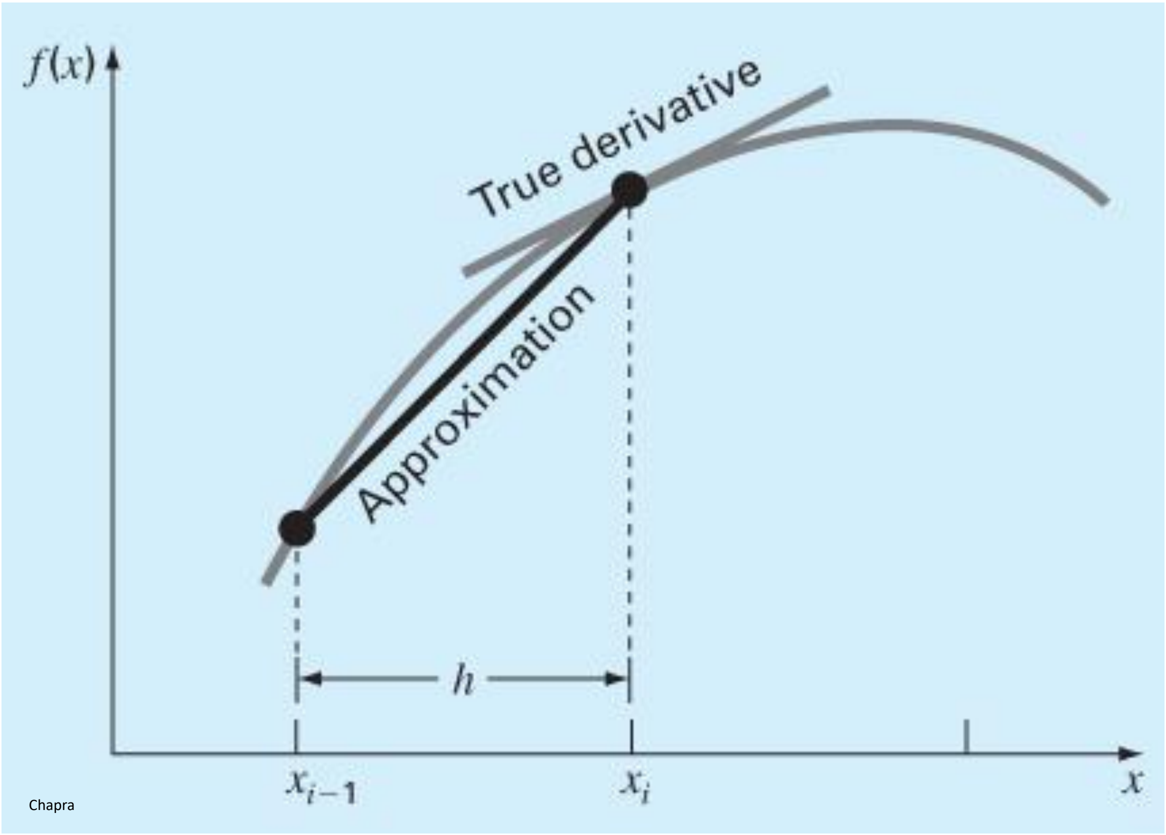
$$\frac{R_1}{h} = O(h)$$

- The backward difference expression, including error, becomes

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

- ***Error of the backward difference approximation is on the order of the step size***

Backward Difference



- Now use the value of $f(x)$ at x_i and backward one step at x_{i-1} to approximate the derivative at x_i
- Again, error is

$$R = O(h)$$

Central Difference

- ***Central difference*** uses value of $f(x)$ ***one step backward*** at x_{i-1} and ones step ahead at x_{i+1} to approximate the derivative at x_i

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

- This can also be developed by subtracting the backward Taylor series from the forward series
- Second-order derivative terms cancel, leaving

$$f(x_{i+1}) = f(x_{i-1}) + 2f'(x_i)h + R_2$$

- Now, the remainder term is

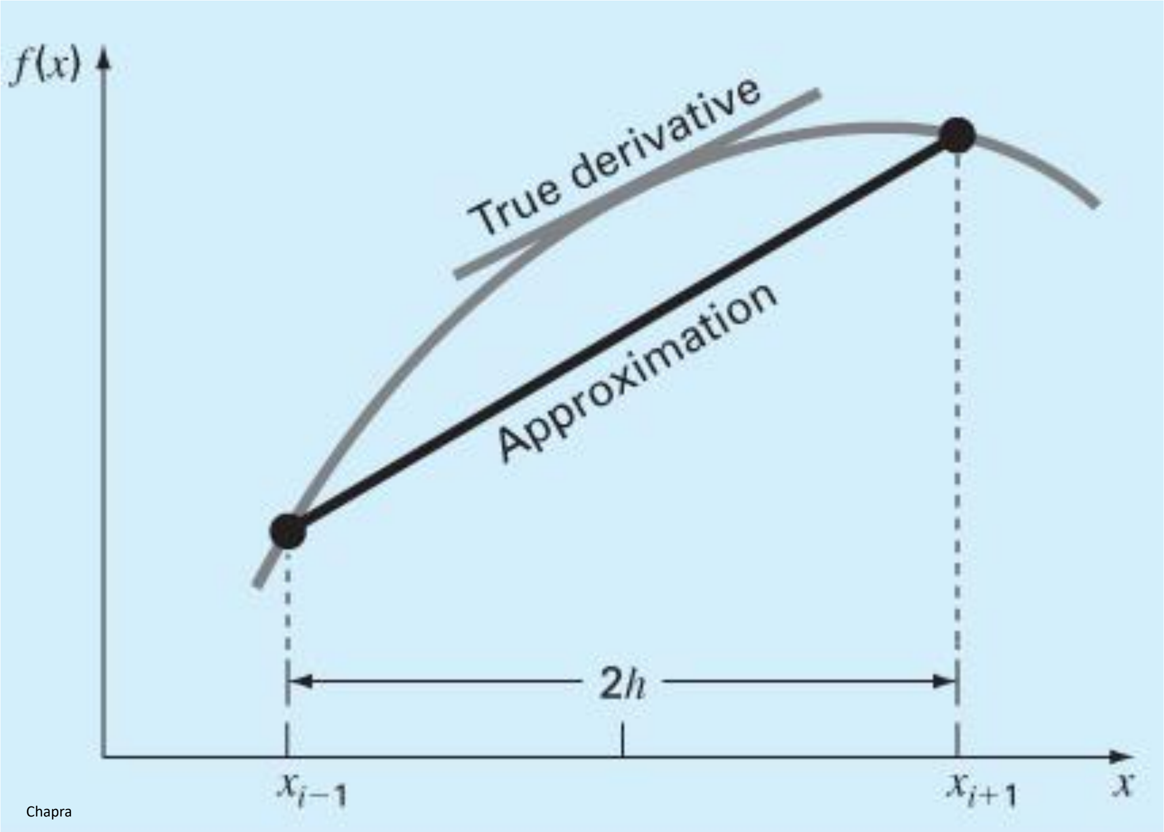
$$R_2 = O(h^3)$$

- The central difference expression, including error, becomes

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

- ***Error of the central difference approximation is on the order of the step size <u>squared</u>***
- Central difference method is more accurate than forward or backward
  - Uses more information

Central Difference



- Now use the value of $f(x)$ backward one step at x_{i-1} and forward one step at x_{i+1} to approximate the derivative at x_i
- ***Reduced error:***

$$R = O(h^2)$$

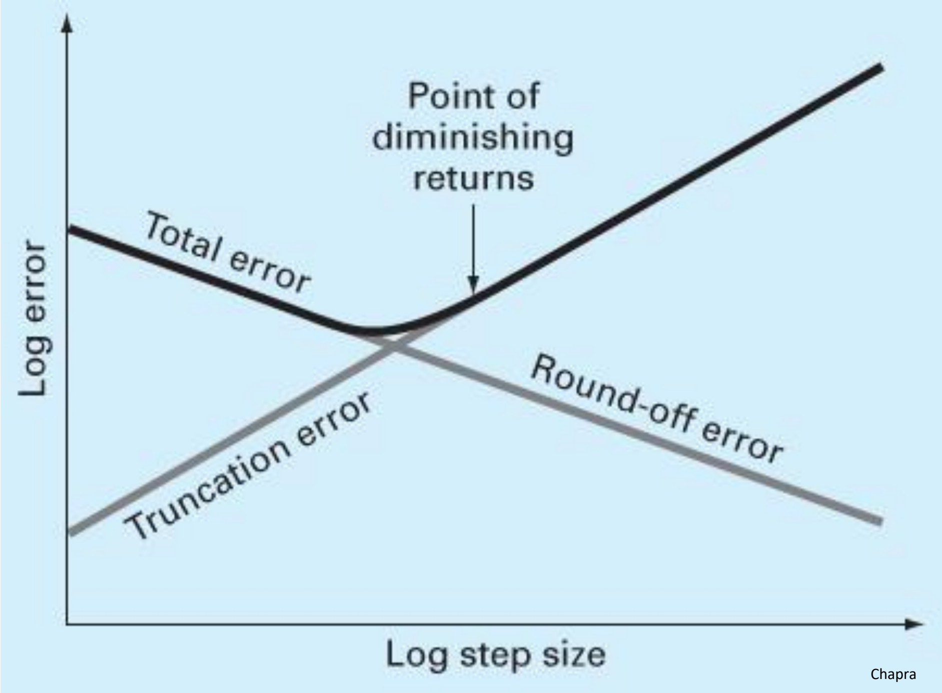
Total Numerical Error

Total Numerical Error

- Total numerical error is the ***sum of roundoff and truncation error***
  - ***Roundoff error*** is largely out of your control, and, with double precision arithmetic, it is not typically an issue
  - ***Truncation error*** can be a significant problem, but can be reduced by decreasing step size
- Reducing step size reduces truncation error, but may also result in subtractive cancellation, thereby increasing roundoff error
- Choose step size to minimize total error
  - Or, more typically, to reduce truncation error to an acceptable level

Total Numerical Error

- Reducing step size reduces truncation error, but may also result in subtractive cancellation, thereby increasing roundoff error
- Could choose step size to minimize total error
- But, more typically, reduce step size just enough to reduce truncation error to an acceptable level



Central Difference Error Analysis

- First derivative of a function in terms of the central difference approximation is

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

- The last term on the right is the truncation error
- There is also roundoff error associated with each value

$$f(x_{i-1}) = \tilde{f}\,(x_{i-1}) - e_{i-1}$$
$$f(x_{i+1}) = \tilde{f}\,(x_{i+1}) - e_{i+1}$$

were $\tilde{f}(x_i)$ represents a rounded value, and e_i is the corresponding roundoff error

Central Difference Error Analysis

- Substituting the expressions for the rounded values into the expression for the true derivative yields

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

- Giving a total error of

Roundoff error

Truncation error

$$err = \frac{e_{i+1} - e_{i-1}}{2h} - \frac{\mathrm{f}^{(3)}(\xi)}{6} h^2$$

- ***Truncation error increases with step size***
- ***Roundoff error decreases with step size***