CSC 427
Computational Science and Numerical Analysis (3 Units) - C

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Course Outline

Numerical Data representation on computer, Computer as a crunching tool, Floating Point number, representation and arithmetic: Error, Stability, Convergence. Theory of computational solution to problem: numerical algorithm formulation and design, numeric software systems. Introduction to use of Matlab and Maple in numerical computation and engineering applications. Emphasis is on the use of software to solve real problems. Iterative solution of non-linear systems (Newton's method) Numerical solution of linear systems. Numerical computation of Eigenvalues eigenvectors. Curve fitting; Function approximation. Numerical differentiation and integration (Simpson's rule, etc). Explicit and Implicit methods. Differential equations (Euler's Method, etc). Linear Algebra: Finite Differences. High performance computation.

CSC 427: Numerical Methods

Topic 1:

Introduction to Numerical Methods and Taylor Series

Lectures 1-4:

Lecture 1
Introduction to Numerical Methods

- What are **NUMERICAL METHODS**?
- Why do we need them?
- Topics covered in CSC 427.

Numerical Methods

Numerical Methods:

Algorithms that are used to obtain numerical solutions of a mathematical problem.

Why do we need them?

1. No analytical solution exists,
2. An analytical solution is difficult to obtain or not practical.

What do we need?

Basic Needs in the Numerical Methods:

- Practical:

  Can be computed in a reasonable amount of time.

- Accurate:
  - Good approximate to the true value,
  - Information about the approximation error (Bounds, error order,…).

Outlines of the Course

- Taylor Theorem
- Number Representation
- Solution of nonlinear Equations
- Interpolation
- Numerical Differentiation
- Numerical Integration

- Solution of linear Equations
- Least Squares curve fitting
- Solution of ordinary differential equations
- Solution of Partial differential equations

Solution of Nonlinear Equations

- Some simple equations can be solved analytically:

$$x^2 + 4x + 3 = 0$$

$$\text{Analytic solution } roots = \frac{-4 \pm \sqrt{4^2 - 4(1)(3)}}{2(1)}$$

$$x = -1 \; and \;\; x = -3$$

- Many other equations have no analytical solution:

$$\left.\begin{aligned} x^9 - 2x^2 + 5 = 0 \\ x = e^{-x} \end{aligned}\right\} \text{No analytic solution}$$

Methods for Solving Nonlinear Equations

- **Bisection Method**
- **Newton-Raphson Method**
- **Secant Method**

Solution of Systems of Linear Equations

$$x_1 + x_2 = 3$$

$$x_1 + 2x_2 = 5$$

We can solve it as:

$$x_1 = 3 - x_2, \qquad 3 - x_2 + 2x_2 = 5$$

$$\Rightarrow x_2 = 2,\ x_1 = 3 - 2 = 1$$

What to do if we have

1000 equations in 1000 unknowns.

Cramer's Rule is Not Practical

Cramer's Rule can be used to solve the system:

$$x_1 = \frac{\begin{vmatrix} 3 & 1 \\ 5 & 2 \end{vmatrix}}{\begin{vmatrix} 1 & 1 \\ 1 & 2 \end{vmatrix}} = 1, \qquad x_2 = \frac{\begin{vmatrix} 1 & 3 \\ 1 & 5 \end{vmatrix}}{\begin{vmatrix} 1 & 1 \\ 1 & 2 \end{vmatrix}} = 2$$

But Cramer's Rule is not practical for large problems.

To solve N equations with N unknowns, we need $(N+1)(N-1)N!$ multiplications.

To solve a 30 by 30 system, 2.3×10^{35} multiplications are needed.

A super computer needs more than 10^{20} years to compute this.

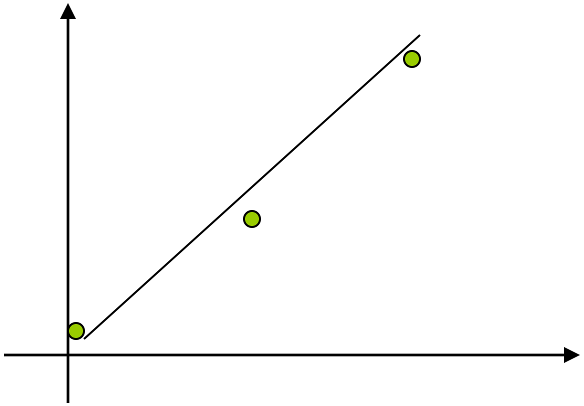
Methods for Solving Systems of Linear Equations

- **Naive Gaussian Elimination**
- **Gaussian Elimination with Scaled Partial Pivoting**
- **Algorithm for Tri-diagonal Equations**

Curve Fitting

- Given a set of data:

x	0	1	2
y	0.5	10.3	21.3

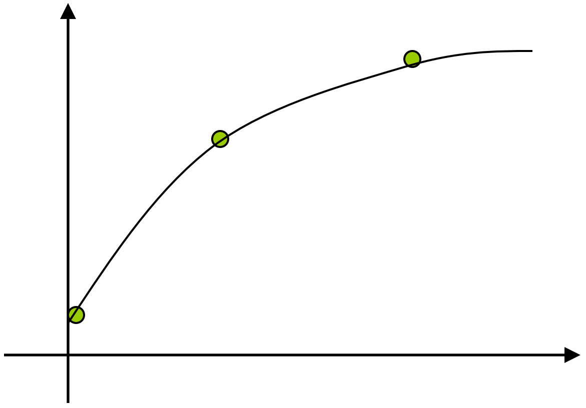


- Select a curve that best fits the data. One choice is to find the curve so that the sum of the square of the error is minimized.

Interpolation

- Given a set of data:

x_i	0	1	2
y_i	0.5	10.3	15.3



- Find a polynomial *P(x)* whose graph passes through all tabulated points.

$$y_i = P(x_i) \quad if\ x_i \text{ is in the table}$$

Methods for Curve Fitting

- **Least Squares**
  - **Linear Regression**
  - **Nonlinear Least Squares Problems**

- **Interpolation**
  - **Newton Polynomial Interpolation**
  - **Lagrange Interpolation**

Integration

- Some functions can be integrated analytically:

$$\int_1^3 x\,dx = \frac{1}{2}x^2\Big|_1^3 = \frac{9}{2} - \frac{1}{2} = 4$$

But many functions have no analytical solutions:

$$\int_0^a e^{-x^2}\,dx = ?$$

Methods for Numerical Integration

- **Upper and Lower Sums**
- **Trapezoid Method**
- **Romberg Method**
- **Gauss Quadrature**

Solution of Ordinary Differential Equations

A solution to the differential equation :

$$\ddot{x}(t) + 3\dot{x}(t) + 3x(t) = 0$$

$$\dot{x}(0) = 1; x(0) = 0$$

is a function *x(t)* that satisfies the equations.

* Analytical solutions are available for special cases only.

Solution of Partial Differential Equations

Partial Differential Equations are more difficult to solve than ordinary differential equations:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial t^2} + 2 = 0$$

$$u(0,t) = u(1,t) = 0,\ u(x,0) = \sin(\pi x)$$

Summary

- **Numerical Methods:** Algorithms that are used to obtain numerical solution of a mathematical problem.
- **We need them when** No analytical solution exists or it is difficult to obtain it.

Topics Covered in the Course

- Solution of Nonlinear Equations
- Solution of Linear Equations
- Curve Fitting
  - Least Squares
  - Interpolation
- Numerical Integration
- Numerical Differentiation
- Solution of Ordinary Differential Equations
- Solution of Partial Differential Equations

Lecture 2
Number Representation and Accuracy

- Number Representation
- Normalized Floating Point Representation
- Significant Digits
- Accuracy and Precision
- Rounding and Chopping

Representing Real Numbers

- You are familiar with the decimal system:

$$312.45 = 3\times10^2 + 1\times10^1 + 2\times10^0 + 4\times10^{-1} + 5\times10^{-2}$$

- Decimal System: Base = 10 , Digits (0,1,…,9)

- Standard Representations:

$$\underbrace{\pm}_{\text{sign}} \quad \underbrace{3\ 1\ 2}_{\text{integral part}} \quad . \quad \underbrace{4\ 5}_{\text{fraction part}}$$

Normalized Floating Point Representation

- Normalized Floating Point Representation:

$$\underset{\text{sign}}{\pm} \quad \underbrace{0.\,d_1\ d_2\ d_3\ d_4}_{\text{mantissa}} \times 10^{\overset{\text{exponent}}{n}}$$

$$d_1 \neq 0, \qquad n : \text{integer}$$

- No integral part,
- Advantage: Efficient in representing very small or very large numbers.

Calculator Example

- Suppose you want to compute:

  3.578 * 2.139

  using a calculator with two-digit fractions

3.57	*	2.13	=	7.60

True answer: 7.653342

Binary System

- Binary System: Base = 2, Digits {0,1}

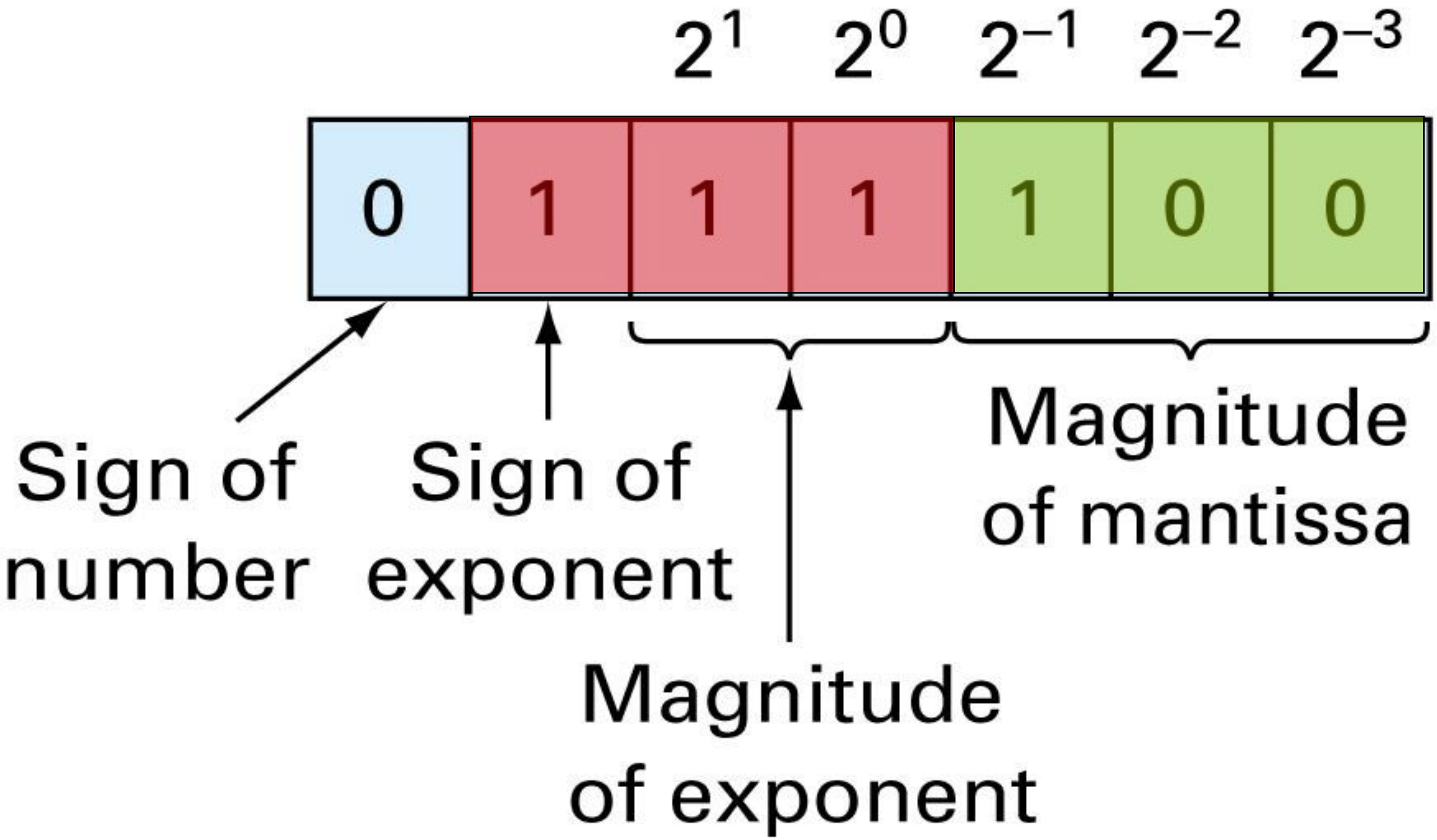
$$\underset{\text{sign}}{\pm} \quad \underbrace{0.1\, b_2\, b_3\, b_4}_{\text{mantissa}} \times 2^{n}$$

exponent

$$b_1 \neq 0 \quad \Rightarrow b_1 = 1$$

$$(0.101)_2 = (1 \times 2^{-1} + 0 \times 2^{-2} + 1 \times 2^{-3})_{10} = (0.625)_{10}$$

7-Bit Representation
(sign: 1 bit, mantissa: 3bits, exponent: 3 bits)



Fact

- Numbers that have a finite expansion in one numbering system may have an infinite expansion in another numbering system:

$$(0.1)_{10} = (0.0001100110011 00\ldots)_2$$

- You can never represent 0.1 exactly in any computer.

Representation

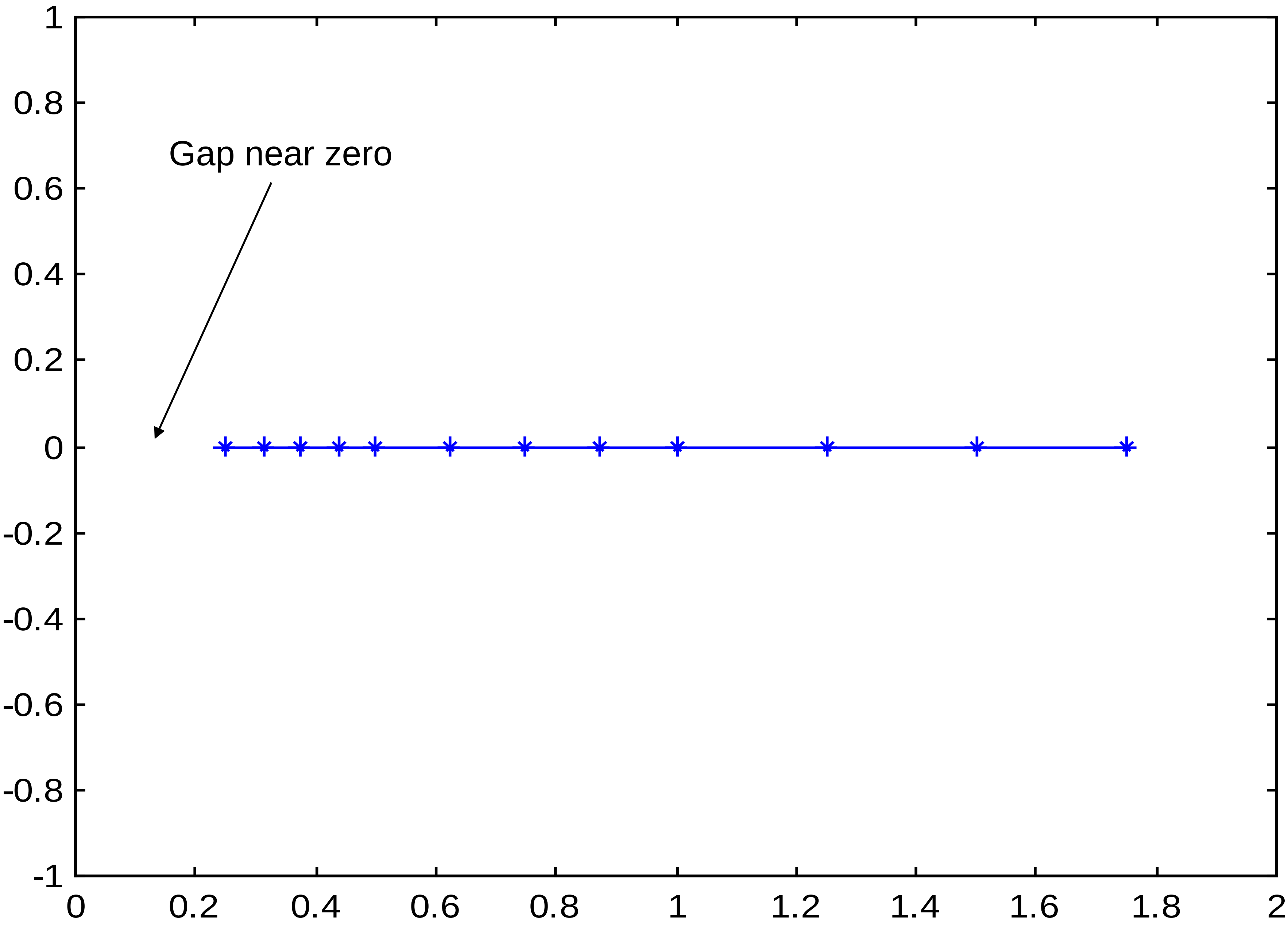
Hypothetical Machine (real computers use ≥ 23 bit mantissa)

Mantissa: 3 bits   Exponent: 2 bits   Sign: 1 bit

Possible positive machine numbers:

.25   .3125   .375   .4375   .5   .625   .75   .875

1   1.25   1.5   1.75


Gap near zero
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-1
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2

Remarks

- Numbers that can be exactly represented are called machine numbers.
- Difference between machine numbers is not uniform
- Sum of machine numbers is not necessarily a machine number:

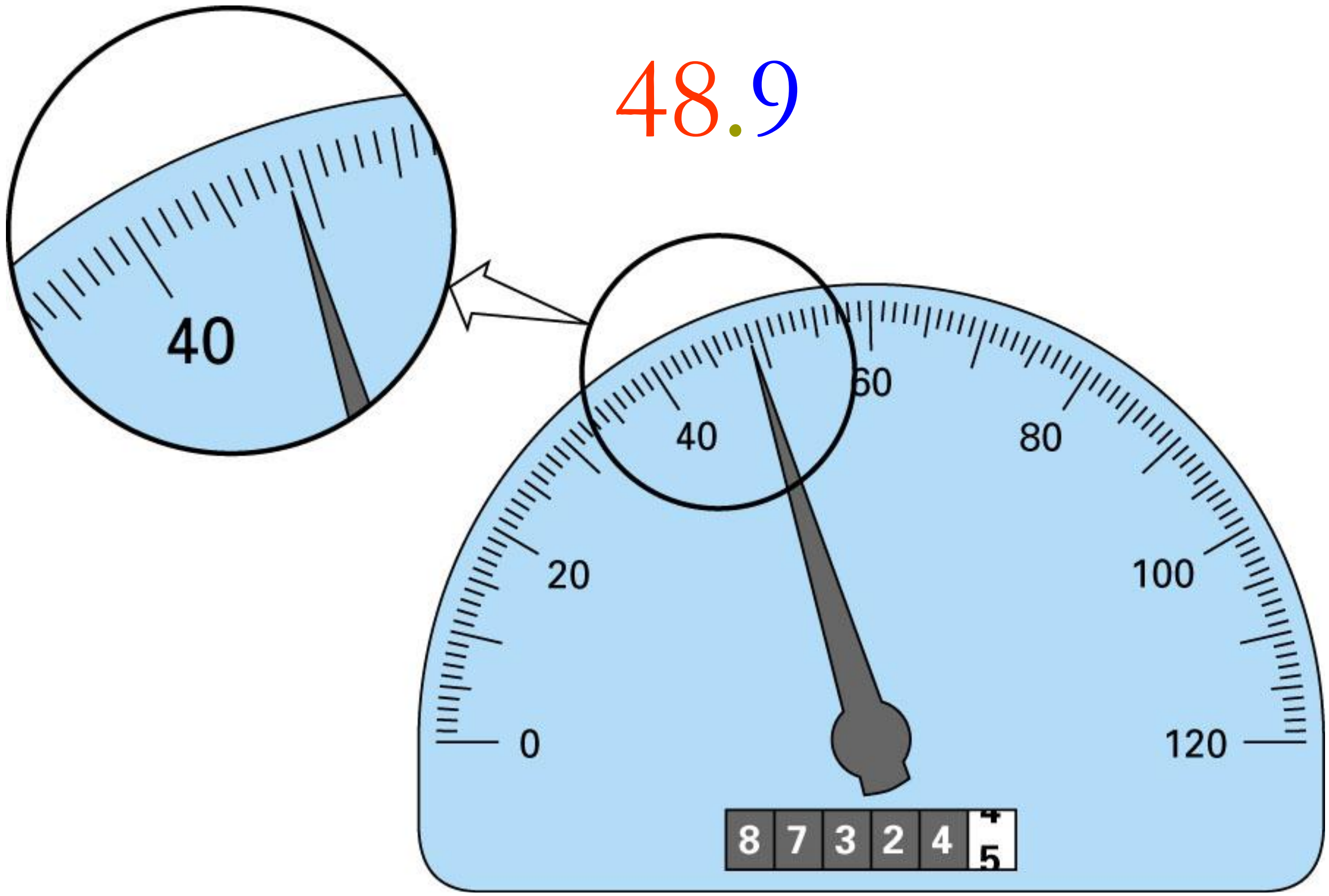
  0.25 + .3125 = 0.5625 (not a machine number)

Significant Digits

- Significant digits are those digits that can be used with confidence.

Significant Digits - Example

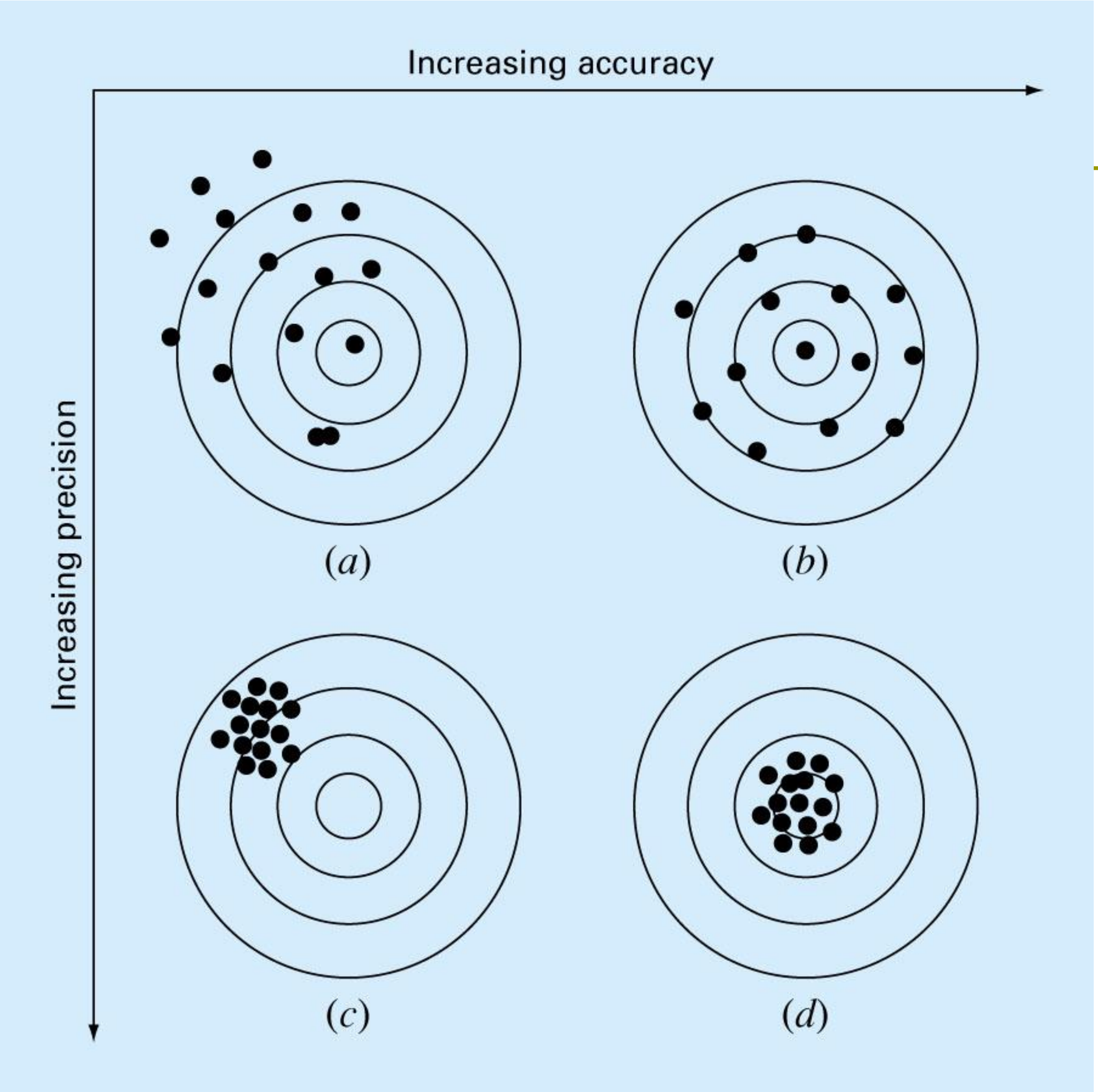
48.9



Accuracy and Precision

- Accuracy is related to the closeness to the true value.

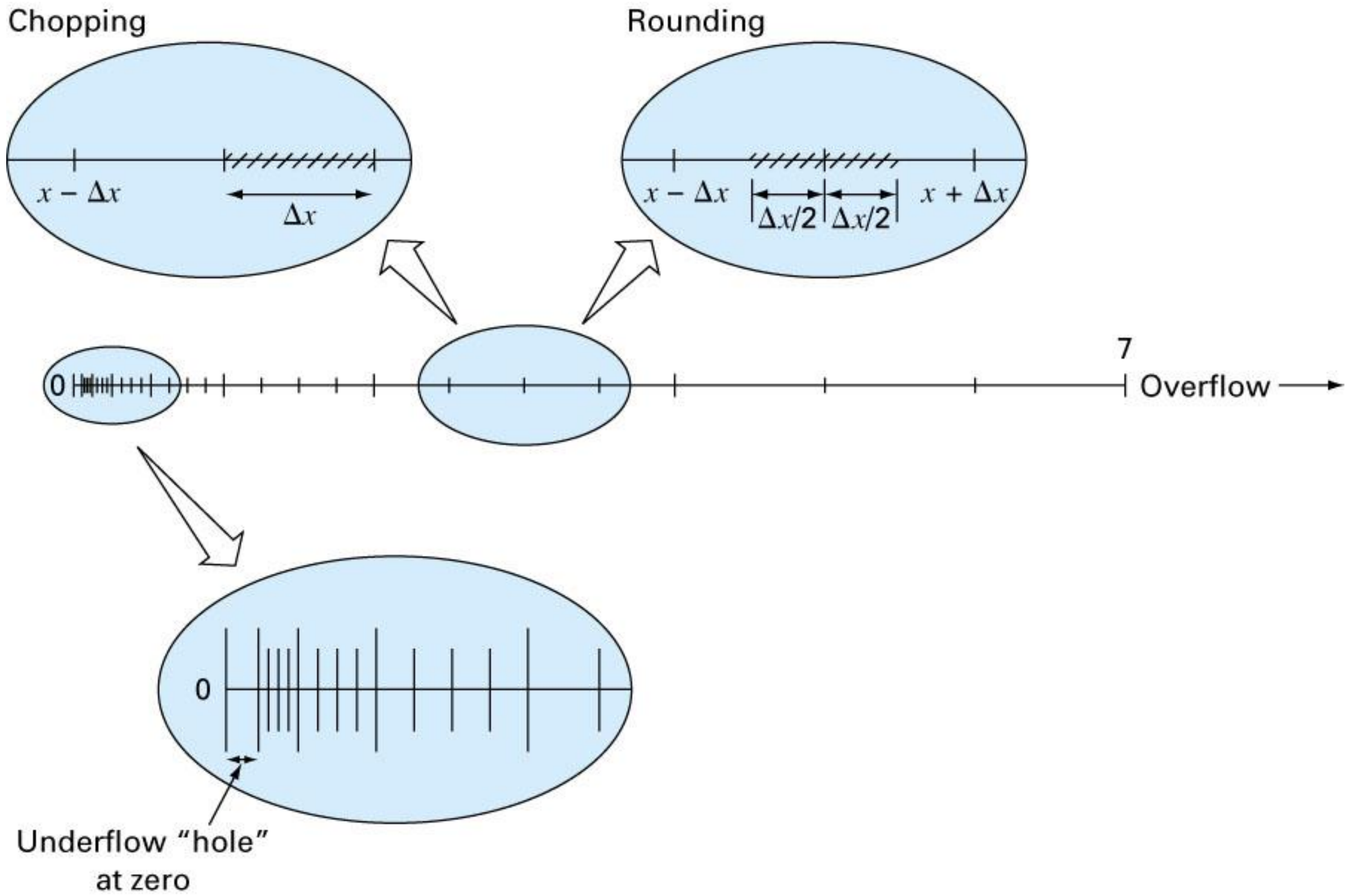
- Precision is related to the closeness to other estimated values.


Increasing accuracy
Increasing precision
(a)
(b)
(c)
(d)

Rounding and Chopping

- Rounding: Replace the number by the nearest machine number.
- Chopping: Throw all extra digits.

Rounding and Chopping - Example



Error Definitions – True Error

Can be computed if the true value is known:

Absolute True Error

$$E_t = \left| \text{true value} - \text{approximation} \right|$$

Absolute Percent Relative Error

$$\varepsilon_t = \left| \frac{\text{true value} - \text{approximation}}{\text{true value}} \right| * 100$$

Error Definitions – Estimated Error

When the true value is not known:

Estimated Absolute Error

$$E_a = \left| \text{current estimate} - \text{previous estimate} \right|$$

Estimated Absolute Percent Relative Error

$$\varepsilon_a = \left| \frac{\text{current estimate} - \text{previous estimate}}{\text{current estimate}} \right| * 100$$

Notation

We say that the estimate is correct to *n* decimal digits if:

$$|\,\text{Error}\,| \leq 10^{-n}$$

We say that the estimate is correct to *n* decimal digits **rounded** if:

$$|\,\text{Error}\,| \leq \frac{1}{2} \times 10^{-n}$$

Summary

- Number Representation

  Numbers that have a finite expansion in one numbering system may have an infinite expansion in another numbering system.

- Normalized Floating Point Representation
  - Efficient in representing very small or very large numbers,
  - Difference between machine numbers is not uniform,
  - Representation error depends on the number of bits used in the mantissa.

Lectures 3-4
Taylor Theorem

- Motivation
- Taylor Theorem
- Examples

Reading assignment: Chapter 4

Motivation

- We can easily compute expressions like:

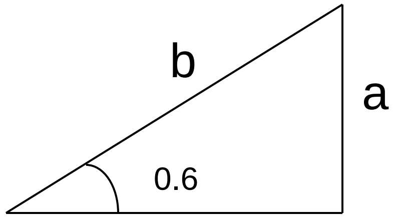
$$\frac{3\times 10^{2}}{2(x+4)}$$

But, How do you compute $\sqrt{4.1}$, $\sin(0.6)$?

We can use the definition to compute

$\sin(0.6)$?

is this a practical way?



Taylor Series

The Taylor series expansion of $f(x)$ about x_0:

$$f(x_0)+f^{'}(x_0)(x-x_0)+\frac{f^{(2)}(x_0)}{2!}(x-x_0)^2+\frac{f^{(3)}(x_0)}{3!}(x-x_0)^3+\ldots$$

or

$$\textit{Taylor Series}=\sum_{k=0}^{\infty}\frac{1}{k!}f^{(k)}(x_0)\,(x-x_0)^k$$

If the series converge, we can write:

$$f(x)=\sum_{k=0}^{\infty}\frac{1}{k!}f^{(k)}(x_0)\,(x-x_0)^k$$

Taylor Series – Example 1

Obtain Taylor series expansion of $f(x) = e^x$ about $x = 0$:

$$f(x) = e^x \qquad f(0) = 1$$

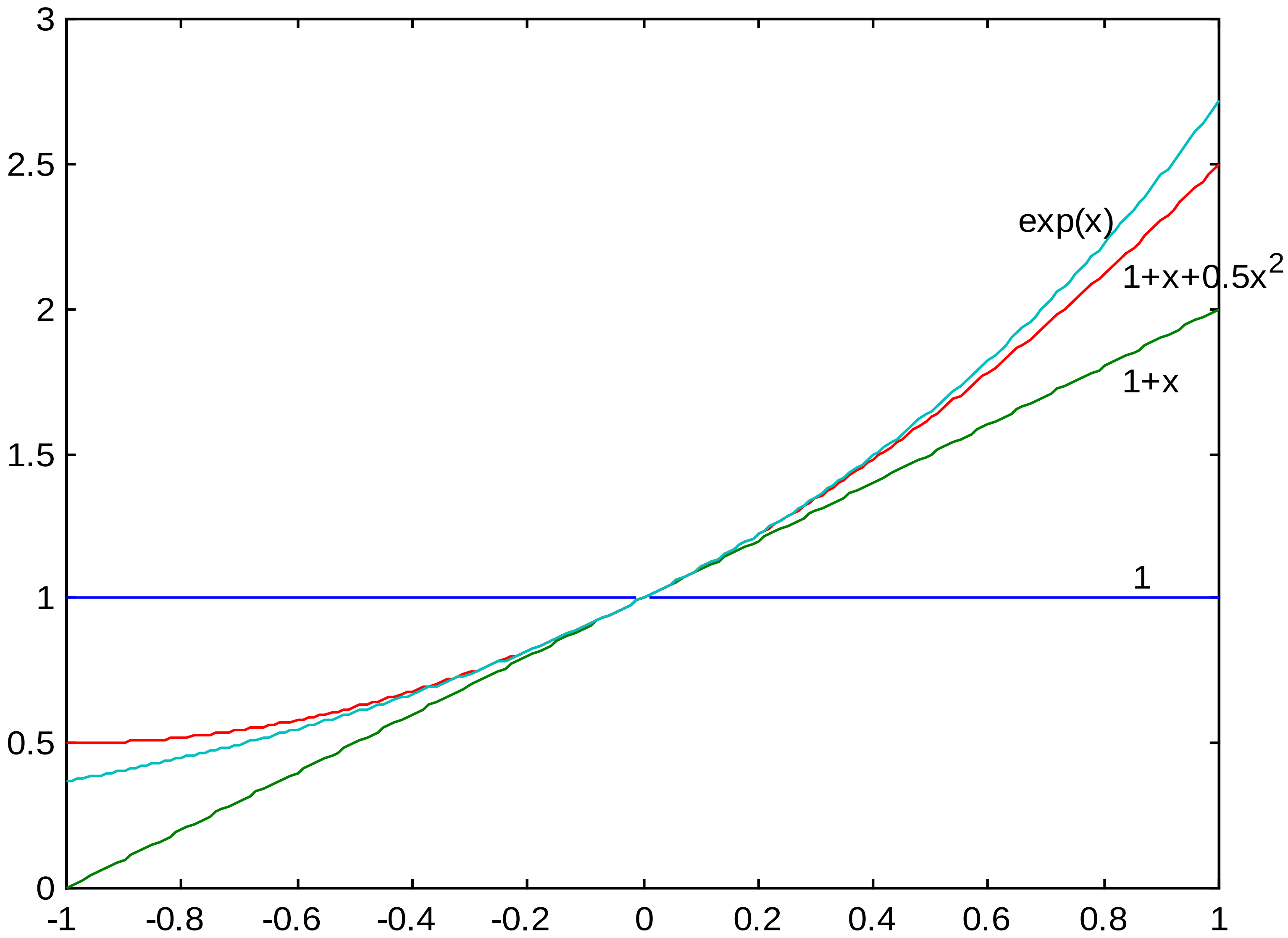
$$f'(x) = e^x \qquad f'(0) = 1$$

$$f^{(2)}(x) = e^x \qquad f^{(2)}(0) = 1$$

$$f^{(k)}(x) = e^x \qquad f^{(k)}(0) = 1 \quad for\, k \geq 1$$

$$e^x = \sum_{k=0}^{\infty} \frac{1}{k!} f^{(k)}(x_0)\,(x - x_0)^k = \sum_{k=0}^{\infty} \frac{x^k}{k!}$$

The series converges for $|x| < \infty$.



exp(x)
1+x+0.5x2
1+x
1
3
2.5
2
1.5
1
0.5
0
-1
-0.8
-0.6
-0.4
-0.2
0
0.2
0.4
0.6
0.8
1

Taylor Series – Example 2

Obtain Taylor series expansion of $f(x) = \sin(x)$ about $x = 0$:

$$f(x) = \sin(x) \qquad f(0) = 0$$

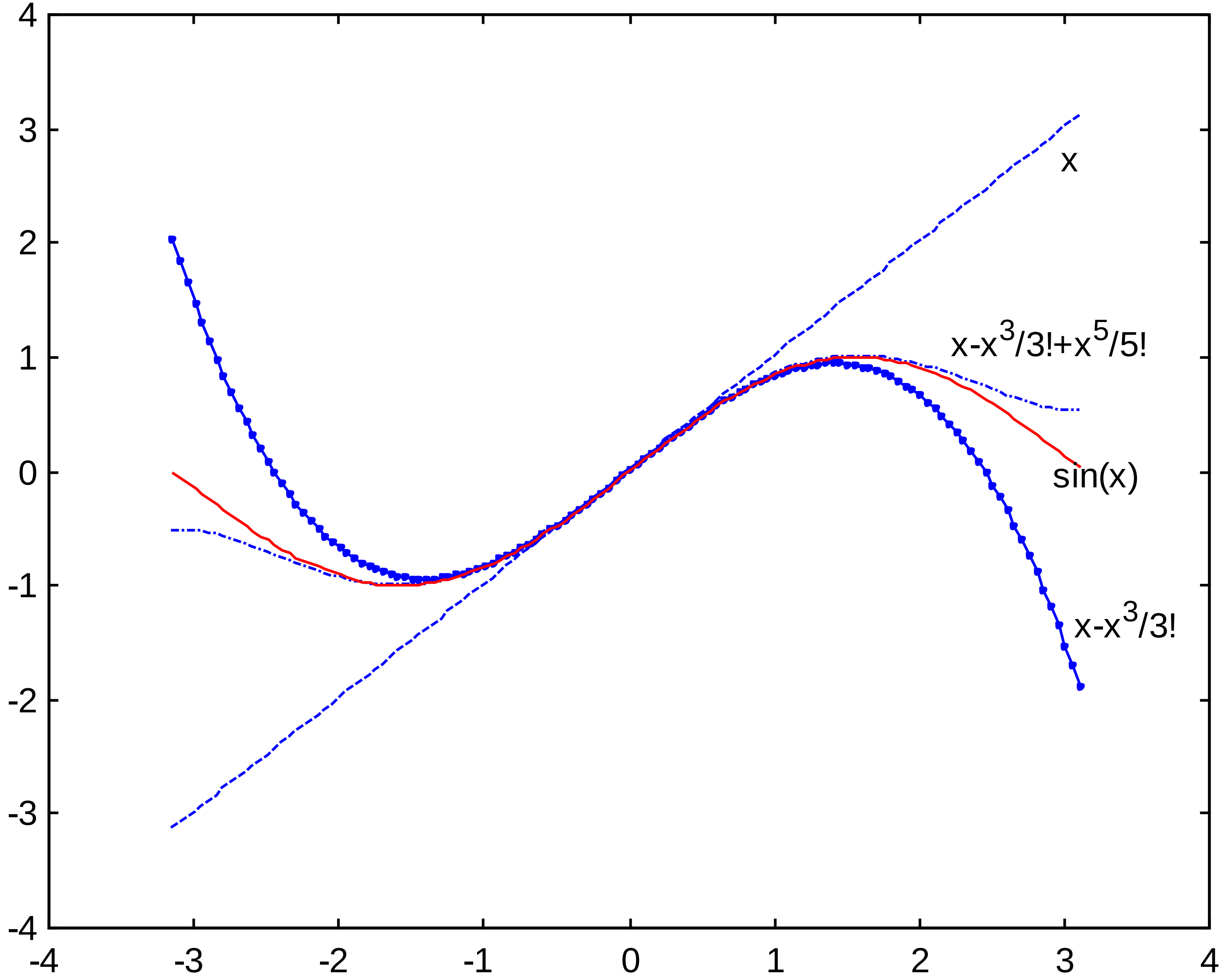
$$f'(x) = \cos(x) \qquad f'(0) = 1$$

$$f^{(2)}(x) = -\sin(x) \qquad f^{(2)}(0) = 0$$

$$f^{(3)}(x) = -\cos(x) \qquad f^{(3)}(0) = -1$$

$$\sin(x) = \sum_{k=0}^{\infty} \frac{f^{(k)}(x_0)}{k!} (x - x_0)^k = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \ldots.$$

The series converges for $|x| < \infty$.


x
x-x3/3!+x5/5!
sin(x)
x-x3/3!
4
3
2
1
0
-1
-2
-3
-4
-4
-3
-2
-1
0
1
2
3
4

Convergence of Taylor Series

(Observations, Example 1)

- The Taylor series converges fast (few terms are needed) when ***x*** is near the point of expansion. If $|x-c|$ is large then more terms are needed to get a good approximation.

Taylor Series – Example 3

Obtain Taylor series expansion of $f(x) = \dfrac{1}{1-x}$ about $x = 0$:

$$f(x) = \frac{1}{1-x} \qquad\qquad f(0) = 1$$

$$f'(x) = \frac{1}{(1-x)^2} \qquad\qquad f'(0) = 1$$

$$f^{(2)}(x) = \frac{2}{(1-x)^3} \qquad\qquad f^{(2)}(0) = 2$$

$$f^{(3)}(x) = \frac{6}{(1-x)^4} \qquad\qquad f^{(3)}(0) = 6$$

Taylor Series Expansion of : $\dfrac{1}{1-\mathrm{x}} = 1 + \mathrm{x} + \mathrm{x}^2 + \mathrm{x}^3 + \ldots.$

Example 3 – Remarks

- Can we apply Taylor series for $x>1$??

- How many terms are needed to get a good approximation???

These questions will be answered using Taylor's Theorem.

Taylor's Theorem

If a function f(x) possesses continuous derivatives of orders $1, 2, \ldots, (n+1)$ in a closed interval $[a, b]$, then for any $c \in [a, b]$:

(n+1) terms Truncated Taylor Series

$$f(x) = \sum_{k=0}^{n} \frac{f^{(k)}(c)}{k!}(x-c)^k + E_{n+1}$$

Remainder

where:

$$E_{n+1} = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x-c)^{n+1} \quad \textit{and } \xi \text{ is between } c \text{ and } x.$$

Taylor's Theorem

We can apply Taylor's theorem for:

$f(x) = \dfrac{1}{1-x}$ with the point of expansion $c = 0$ if $|x| < 1$.

If $[a, b]$ includes $x = 1$, then the function and its derivatives are not defined.

$\Rightarrow$ Taylor Theorem is not applicable.

Error Term

To get an idea about the approximation error, we can derive an upper bound on:

$$E_{n+1} = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x-c)^{n+1}$$

for all *values of* ξ between c and x.

Error Term – Example 4

How large is the error if we replaced $f(x)=e^x$ by the first 4 terms (n = 3) of its Taylor series expansion about $x=0$ $when$ $x=0.2$?

$$f^{(k)}(x)=e^x \qquad f^{(k)}(\xi) \le e^{0.2} \quad for\, k \ge 1$$

$$E_{n+1}=\frac{f^{(n+1)}(\xi)}{(n+1)!}(x-c)^{n+1}$$

$$\left|E_{n+1}\right| \le \frac{e^{0.2}}{(n+1)!}(0.2)^{n+1} \Rightarrow \left|E_4\right| \le 8.14268E-05$$

Alternative form of Taylor's Theorem

$Let\ f(x)$ have continuous derivatives of orders $1, 2, ..., (\mathrm{n}+1)$ on an interval $[a,b]$, and $x \in [a,b]$ and $x+h \in [a,b]$, then:

$$f(x+h) = \sum_{k=0}^{n} \frac{f^{(k)}(x)}{k!} h^k + E_{n+1}$$

$$E_{n+1} = \frac{f^{(n+1)}(\xi)}{(n+1)!} h^{n+1} \quad where\ \xi \text{ is between } x \text{ and } x+h$$

Taylor's Theorem – Alternative forms

$$f(x) = \sum_{k=0}^{n} \frac{f^{(k)}(c)}{k!}(x-c)^k + \frac{f^{(n+1)}(\xi)}{(n+1)!}(x-c)^{n+1}$$

$where\ \xi$ is between c and x.

$$x \to x+h, \quad c \to x$$

$$f(x+h) = \sum_{k=0}^{n} \frac{f^{(k)}(x)}{k!}h^k + \frac{f^{(n+1)}(\xi)}{(n+1)!}h^{n+1}$$

$where\ \xi$ is between x and $x+h$.

Mean Value Theorem

If f(x) is a continuous function on a closed interval [a, b]
and its derivative is defined on the open interval (a, b)
then there exists $\xi \in [a, b]$

$$\frac{df(\xi)}{dx} = \frac{f(b) - f(a)}{(b\text{-}a)}$$

Proof : Use Taylor's Theorem for $n = 0, x = a, \ x + h = b$

$$f(b) = f(a) + \frac{df(\xi)}{dx} \ (b\text{-}a)$$

Alternating Series Theorem

Consider the alternating series:

$$S = a_1 - a_2 + a_3 - a_4 + \cdots$$

$$\text{If } \boxed{\begin{cases} a_1 \ge a_2 \ge a_3 \ge a_4 \ge \cdots \\ \quad and \\ \lim\limits_{n\to\infty} a_n = 0 \end{cases}} \quad \text{then} \quad \boxed{\begin{cases} \text{The series converges} \\ \qquad and \\ \quad \left| S - S_n \right| \le a_{n+1} \end{cases}}$$

S_n : Partial sum (sum of the first n terms)

a_{n+1} : First omitted term

Alternating Series – Example 5

$\sin(1)$ can be computed using: $\quad sin(1) = 1 - \frac{1}{3!} + \frac{1}{5!} - \frac{1}{7!} + \cdots$

This is a convergent alternating series since:

$$a_1 \geq a_2 \geq a_3 \geq a_4 \geq \cdots \;\; and \;\; \lim_{n\to\infty} a_n = 0$$

Then:

$$\left| sin(1) - \left(1 - \frac{1}{3!}\right) \right| \leq \frac{1}{5!}$$

$$\left| sin(1) - \left(1 - \frac{1}{3!} + \frac{1}{5!}\right) \right| \leq \frac{1}{7!}$$

Example 6

Obtain the Taylor series expansion

of $f(x) = e^{2x+1}$ about $c = 0.5$ (the center of expansion)

How large can the error be when $(n+1)$ terms are used

to approximate e^{2x+1} with $x = 1$?

Example 6 – Taylor Series

Obtain Taylor series expansion of $f(x) = e^{2x+1}$, $c = 0.5$

$$f(x) = e^{2x+1} \qquad f(0.5) = e^{2}$$

$$f'(x) = 2e^{2x+1} \qquad f'(0.5) = 2e^{2}$$

$$f^{(2)}(x) = 4e^{2x+1} \qquad f^{(2)}(0.5) = 4e^{2}$$

$$f^{(k)}(x) = 2^{k}\ e^{2x+1} \qquad f^{(k)}(0.5) = 2^{k} e^{2}$$

$$e^{2x+1} = \sum_{k=0}^{\infty} \frac{f^{(k)}(0.5)}{k!}\,(x-0.5)^{k}$$

$$= e^{2} + 2e^{2}(x-0.5) + 4e^{2}\frac{(x-0.5)^{2}}{2!} + \ldots + 2^{k} e^{2}\frac{(x-0.5)^{k}}{k!} + \ldots$$

Example 6 – Error Term

$$f^{(k)}(x) = 2^k \; e^{2x+1}$$

$$Error = \frac{f^{(n+1)}(\xi)}{(n+1)!}\,(x-0.5)^{n+1}$$

$$\left|Error\right| = \left|2^{n+1} e^{2\xi+1} \quad \frac{(1-0.5)^{n+1}}{(n+1)!}\right|$$

$$\left|Error\right| \le 2^{n+1} \frac{(0.5)^{n+1}}{(n+1)!} \max_{\xi\in[0.5,1]} \left|e^{2\xi+1}\right|$$

$$\left|Error\right| \le \frac{e^3}{(n+1)!}$$

Remark

- In this course, all angles are assumed to be in radian unless you are told otherwise.

Maclaurin Series

- Find Maclaurin series expansion of *cos (x)*.

- Maclaurin series is a special case of Taylor series with the center of expansion $c = 0$.

Maclaurin Series – Example 7

Obtain Maclaurin series expansion of : $f(x) = \cos(x)$

$$f(x) = \cos(x) \qquad f(0) = 1$$

$$f'(x) = -\sin(x) \qquad f'(0) = 0$$

$$f^{(2)}(x) = -\cos(x) \qquad f^{(2)}(0) = -1$$

$$f^{(3)}(x) = \sin(x) \qquad f^{(3)}(0) = 0$$

$$\cos(x) = \sum_{k=0}^{\infty} \frac{f^{(k)}(0)}{k!} (x)^k = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \ldots.$$

The series converges for $|x| < \infty$.