SE301: Numerical Methods

Topic 1:

Introduction to Numerical methods and Taylor Series

Lectures 1-4:

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(Term 071)

Lecture 1

Introduction to Numerical Methods

- What are **NUMERICAL METHODS**?
- Why do we need them?
- Topics covered in SE301.

Reading Assignment: pages 3-10 of text book

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

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

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

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

- Many other equations have no analytical solution

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

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 in 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.

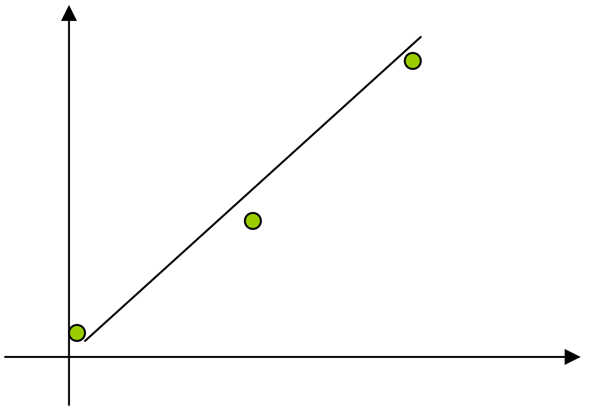
Methods for solving Systems of Linear Equations

- **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

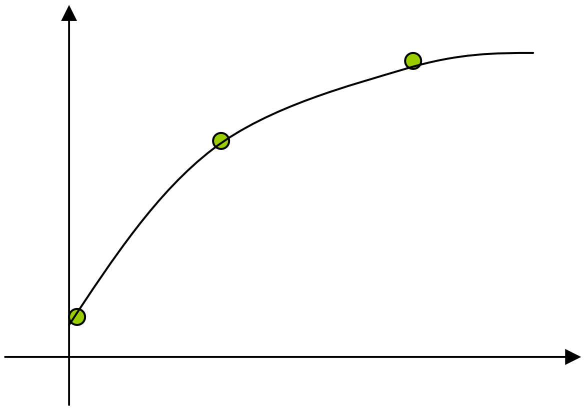


- Select a curve that best fit the data. One choice is find the curve so that the sum of the square of the error is minimized.

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 exist or it is difficult to obtain.

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 accurcy

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

- Reading assignment: Chapter 3

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

$$\pm \quad 3 \ 1 \ 2 \quad . \quad 4 \ 5$$

sign integral part fraction part

Normalized Floating Point Representation

- Normalized Floating Point Representation

$$\pm \quad \underline{0.\, d_1\ d_2\ d_3\ d_4} \times 10^n$$

sign mantissa exponent

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

- 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}

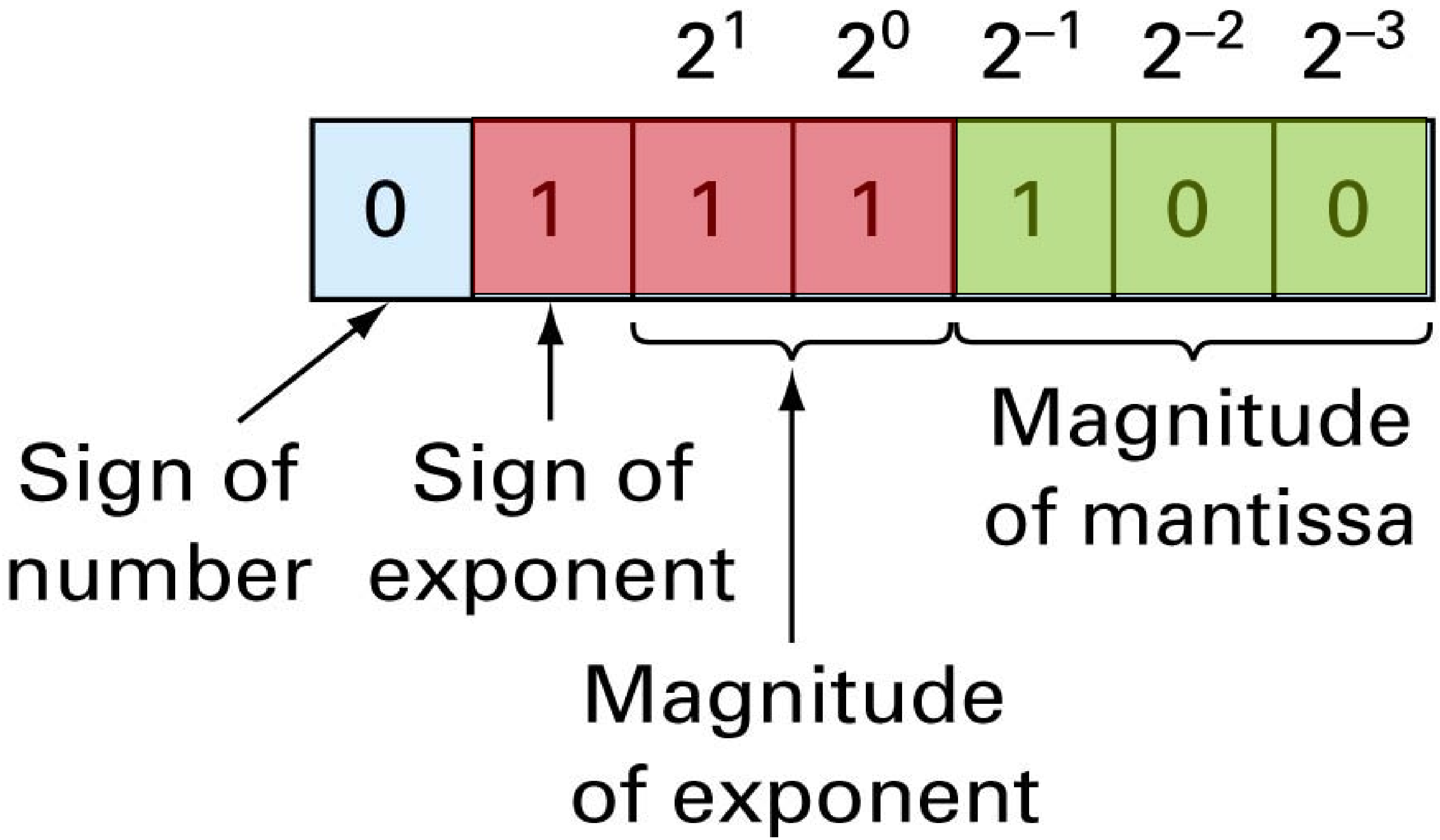
$$\underset{\text{sign}}{\pm} \quad \underbrace{0.1\ b_2\ b_3\ b_4}_{\text{mantissa}} \times 2^{n} \leftarrow \text{exponent}$$

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

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

7-Bit Representation

(sign: 1 bit, Mantissa 3bits,exponent 3 bits)



Fact

- Number that have finite expansion in one numbering system may have an infinite expansion in another numbering system

$$(0.1)_{10} = (0.000110011001100...)_2$$

- You can never represent 0.1 exactly in any computer

Representation

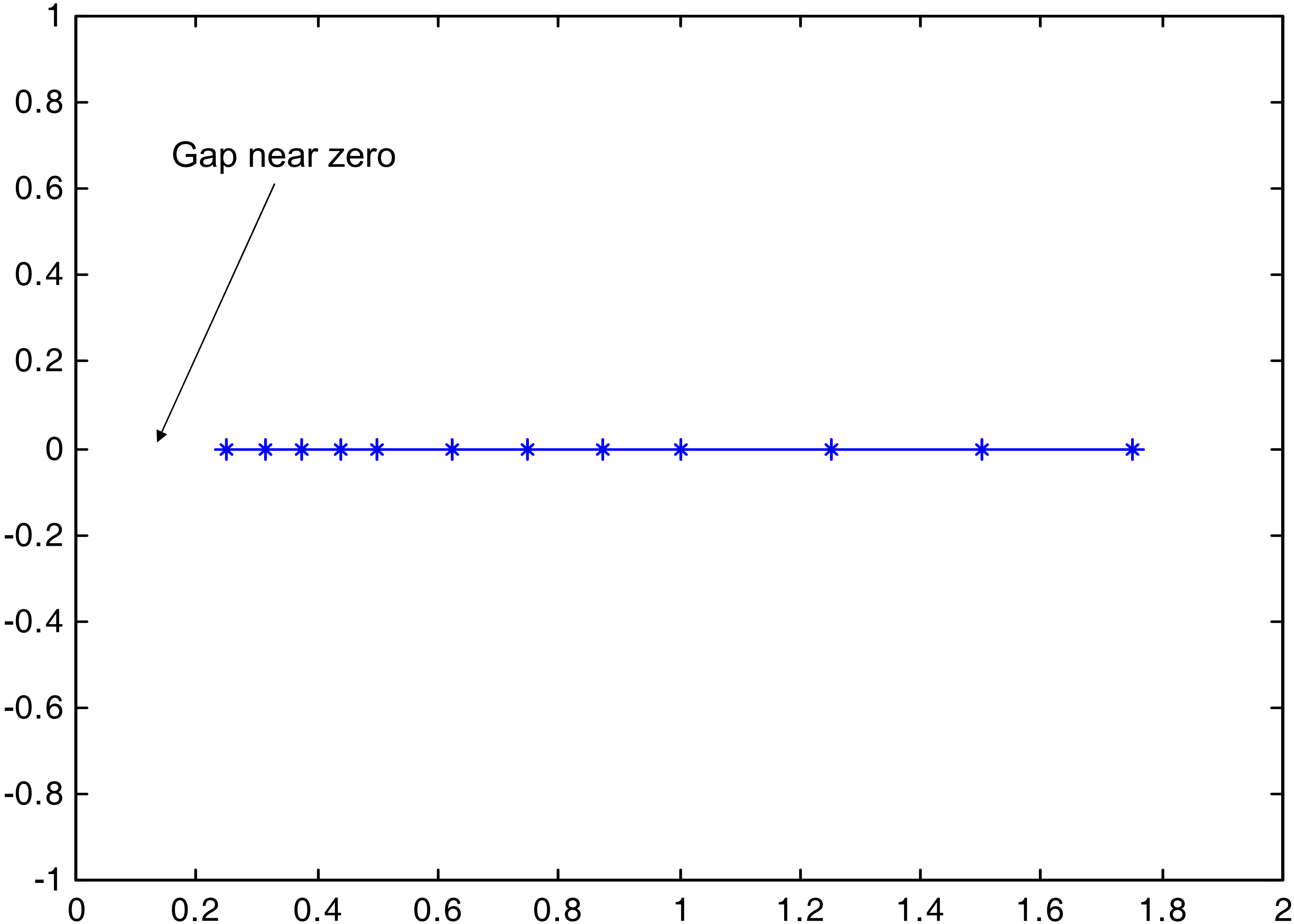
Hypothetical Machine (real computers use $\geq$ 23 bit mantissa)

Mantissa 2 bits   exponent 2 bit   sign 1 bit

Possible 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.

Accuracy and Precision

- Accuracy is related to closeness to the true value
- Precision is related to the closeness to other estimated values

Rounding and Chopping

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

Error Definitions

True Error

can be computed if the true value is known

Absolute True Error

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

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

$$E_a = |\text{current estimate} - \text{prevoius estimate}|$$

Estimated Absolute Percent Relative Error

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

Notation

We say the estimate is correct to n decimal digits if

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

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

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

Summary

- Number Representation

  Number that have 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

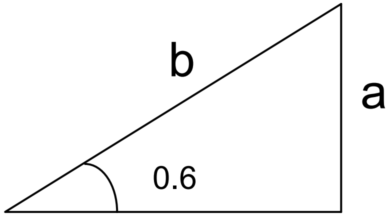
$$\frac{3\times 10^{2}}{2(x+4)}$$

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

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

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 $x = 0$

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

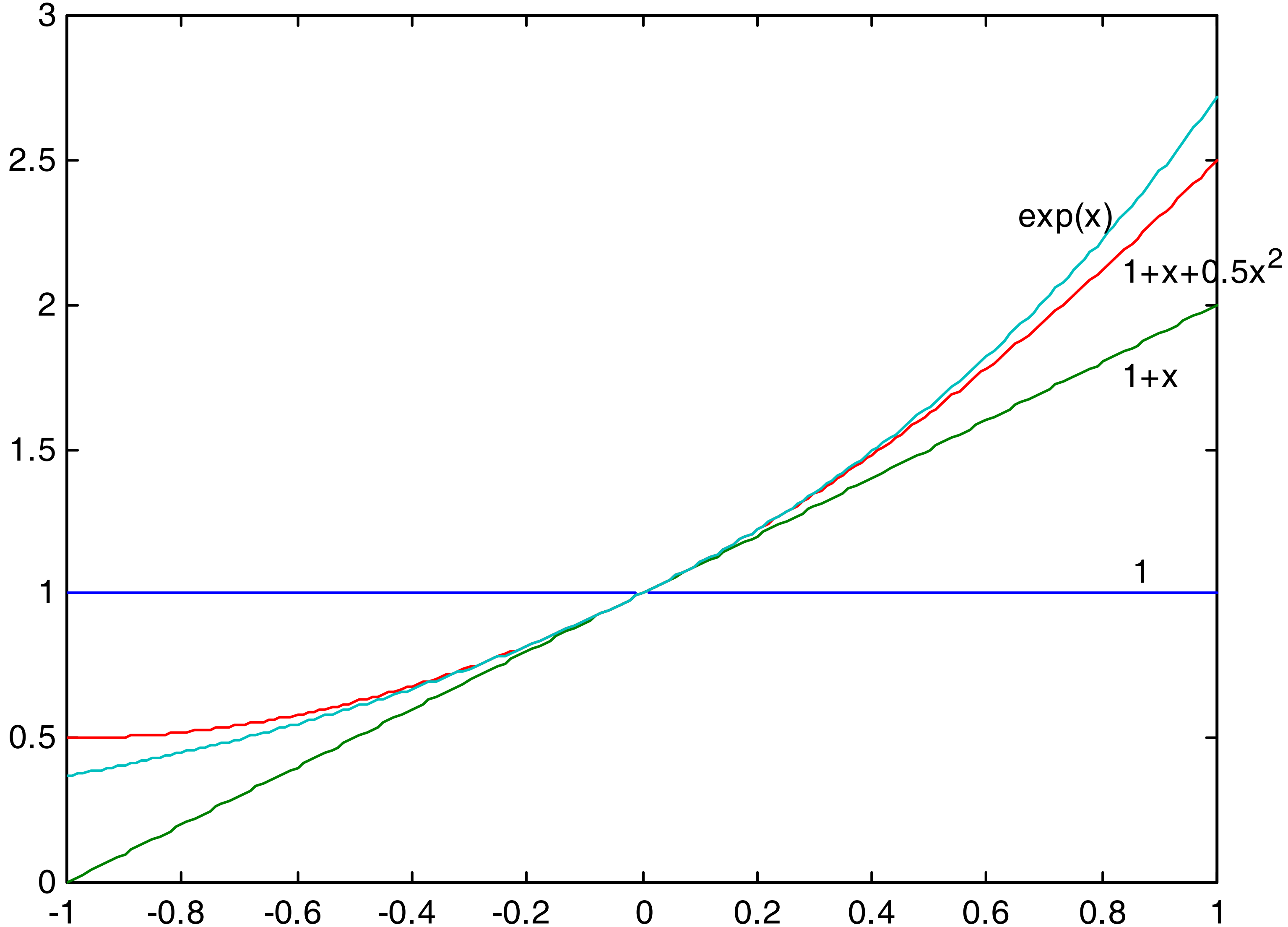
$$f'(x) = e^x \qquad f'(0) = 1$$

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

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

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

The series converges for $|\mathrm{x}| < \infty$


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
exp(x)
1+x+0.5x2
1+x
1

Taylor Series
Example 2

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

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

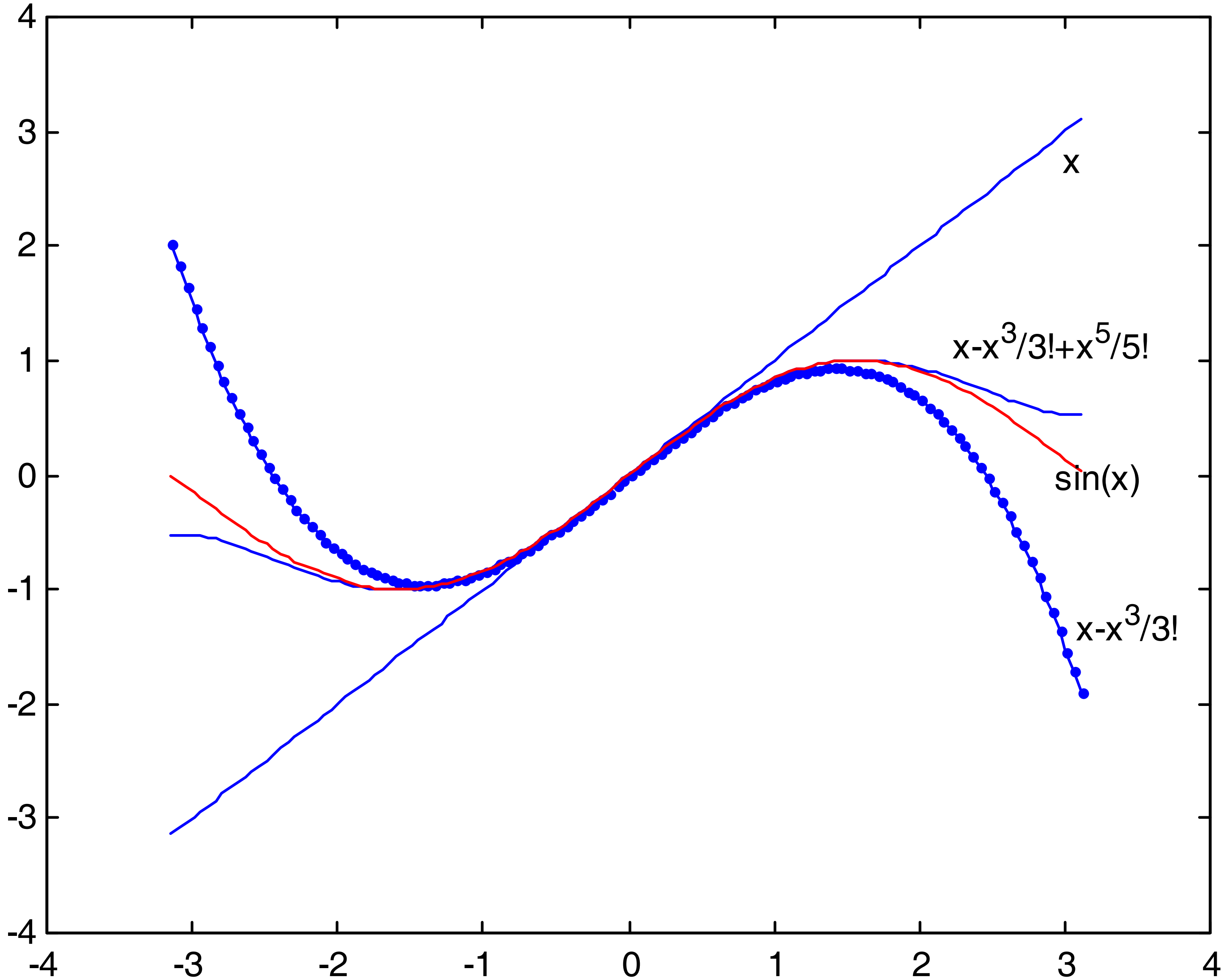
$$f'(x) = \cos(x) \qquad f'(0) = 1$$

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

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

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

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 good approximation.

Taylor Series
Example 3

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

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

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

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

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

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

Example 3
remarks

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

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

These questions will be answered using Taylor Theorem

Taylor Theorem

If a function f(x) posses continuous derivatives

of orders 1,2,...,(n + 1) in a closed interval [a, b]

then for any $c \in [a, b]$

(n+1) terms Truncated Taylor Series

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

Reminder

where

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

Taylor Theorem

We can apply Taylor thorem for

$$f(x) = \frac{1}{1-x} \quad \text{with point of expansion} \quad c = 0 \;\; \text{if} \;\; |x| < 1$$

$if\ [a,b]\ includes\ x = 1$ 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 x and c.

Error Term for 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* $x = 0.2$?

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

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

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

Alternative form of Taylor Theorem

$Let\ f(x)$ have continuous derivatives of orders 1,2,...(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 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 ξ is between x and c

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

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

where ξ 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 exist $\xi \in [a,b]$

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

Proof : Use Taylor Theorem 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

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

$$If \begin{cases} a_1 \geq a_2 \geq a_3 \geq a_4 \geq \cdots \\ \quad and \\ \lim_{n\to\infty} a_n = 0 \end{cases} \quad then \begin{cases} \text{The series converges} \\ and \\ |S - S_n| \leq a_{n+1} \end{cases}$$

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 $\sin(1) = 1 - \frac{1}{3!} + \frac{1}{5!} - \frac{1}{7!} + \cdots$

This is a convergent alternating series since

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

Then

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

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

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

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

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

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

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

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

$$|Error| \le 2^{n+1} \frac{(x-0.5)^{n+1}}{(n+1)!} e^{3}$$

Remark

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

Maclurine series

Find Maclurine series expansion of cos (x)

Maclurine series is a special case of Taylor series with the center of expansion $c = 0$

Taylor Series
Example 7

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

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

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

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

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

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

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

Homework problems

- Check the course webCT for the Homework Assignment