ME - 310

NUMERICAL METHODS

Fall 2007

Group 02

Instructor: Prof. Dr. Eres Söylemez (Rm C205, email:eres@metu.edu.tr)

Class Hours and Room:

Monday	13:40 - 15:30	Rm: B101
Wendesday	12:40 - 13:30	Rm: B103

Course TextBook: "Numerical Methods for Engineers" by S.C. Chapra and R.P. Canale, 4th ed., McGraw Hill.

Web Page: http://www.me.metu.edu.tr/me310

Preriquisite: Calculus, Linear Algebra, Differentiation and integration, Differential Equations, Taylor and binomial expansion. Computer literacy and a programming language such as C, Pascal, VBA, Delphi, Fortran, etc.

- Grading
  - Homework and Lab assignments and attendance (25%)
  - 2 Midterms (2nd midterm using computer) (22% and 23%)
  - 1 Final (30%)
- Cheating!!!!

  Will be very severely punished.

  Please read

  "Academic Code of Ethics"

  *http://**www.me.metu.edu.tr/me310***

- Study regularly
- Do your homeworks on your own. If you have any questions, please ask (to your friends, to the assistants and to me)
- Attendance is compulsory. No excuse. %2^{n-2}

AIM of ME Education

- Solve mechanical engineering problems
  - Simplify and obtain
    - analytical solutions
    - Graphical solutions
    - Solutions using calculator
    - Solutions using computer at all levels
  - Solve complex (nonlinear, or multi parameter) problems using computer.

AIM of ME310

- Algorithmic Thinking

- Solution of complex engineering problems using numerical techniques.

  – Programming on a computer
  – Use new mathematical tools
  – Learn methods of Numerical Analysis
  – Analyze errors due to digital computation

Why learn Numerical Methods?

- Powerful problem solving
  - Large systems of equations
  - Solution of nonlinear equations
  - Complex geometry
  - Repetitative solutions by changing parameters (What if? Question)
- Efficient way of learning computer logic and programming
- Learn how math is utilized in engineering
- Introduction to the logic of package programs
- Solving problems that cannot be solved by the available package programs

Main Topics in ME310

- Roots of Equations
- System of equations (linear and nonlinear)
- Introduction to Optimization
- Curve fitting
- Differentiation
- Integration
- Solution of Ordinary Differential equations (Initial value problems)

Reading assignments are given for each week. Please look at *http://**www.me.metu.edu.tr/me310***

2+2 =?

Scientist	Engineer	Social Scientist
=4	$=4\pm\varepsilon$	= 2,4,8....

Approximations and Errors

Math vs Engineering

significant digits.

π=? =3.1415 (5 digit)

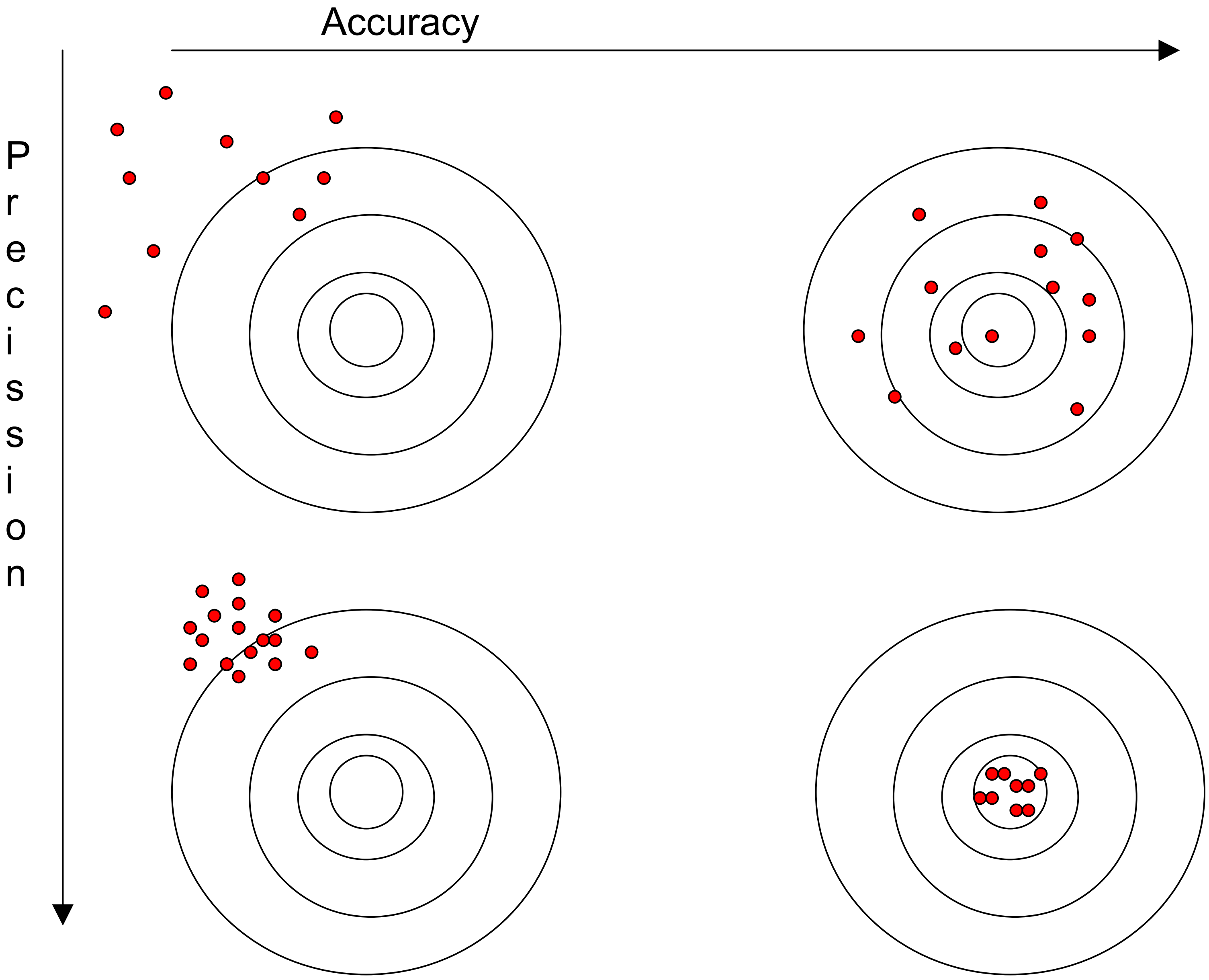
=3.1415926 (8 digit)

=3.14159265358979 (15 digit)

Accuracy and Precission

- Accuracy is the difference between the computed (or measured) value and the true value.
- Precission is the spread between the repeated calculations or measurements

Ex: Target Problem


Accuracy
Precision

Errors in Numerical Computation

- Truncation errors.

i.e.

$$\sin(x) = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \frac{x^9}{9!} .... = +\sum_{n=1}^{\infty} (-1)^n \frac{x^{2n+1}}{(2n+1)!}$$

We can use m terms. There will be some error

- Round-off errors

i.e. π =3.1415

True Value = Approximation + error

True Value= Approximate Value + E_{true}

Or: E_t= True Value- Approximation

Fractional Relative Error= $\%\varepsilon_t = \frac{E_{true}}{TrueValue}100$

Approximate Relative Error = $\%\varepsilon_a = \frac{PresentApprox. - PreviousApprox.}{PresentApprox} * 100$

Example

x= $\pi/4$ = 0.785398163397448 (45^0) sin($\pi/4$)=0.707106781186547

$$\sin(x) = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \frac{x^9}{9!}........ = +\sum_{n=1}^{\infty} (-1)^n \frac{x^{2n+1}}{(2n+1)!}$$

#Term	f(x)	$\%\varepsilon_t$	$\%\varepsilon_a$
1	0.785398163397448	11.072073453959200	-
2	0.704652651209168	0.347066389783707	11.458909868532200
3	0.707143045779360	0.005128587898981	0.352176915979992
4	0.707106469575178	0.000044068502476	0.005172658680970
5	0.707106782936867	0.000000247532581	0.000044316034947
6	0.707106781179619	0.000000000979769	0.000000248512350
7	0.707106781186568	0.000000000002889	0.000000000982658
8	0.707106781186547	0.000000000000000	0.000000000002889
9	0.707106781186547	0.000000000000000	0.000000000000000
10	0.707106781186547	0.000000000000000	0.000000000000000

Example

x= 1.553343034274950 (89^0)   sin(x)=0.999847695156391

Terms	f(x)	$\% \varepsilon_t$	$\% \varepsilon_a$
1	1.553343034274950	55.357965198088200	-
2	0.928672713486365	7.118582361575920	67.264851407498600
3	1.004035270448470	0.418821317723176	7.505967089028960
4	0.999705737159465	0.014197962111061	0.433080768477656
5	0.999850829115375	0.000313443637339	0.014511360263465
6	0.999847646490898	0.000004867290675	0.000318310943507
7	0.999847695717011	0.000000056070528	0.000004923361201
8	0.999847695151409	0.000000000498300	0.000000056568828
9	0.999847695156426	0.000000000003520	0.000000000501820
10	0.999847695156391	0.000000000000022	0.000000000003542

Can we estimate the truncation error?

Review of Calculus:

- Taylor's Theorem

If the function f(x) and its n+1 derivatives are continuous on an interval containing a and x, then the value of the funxtion at x is given by:

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

$$+\frac{f'''(a)}{3!}(x-a)^3 + \dots\dots\dots + \frac{f^n(a)}{n!}(x-a)^n + R_n$$

Where the remainder R_n is defined as

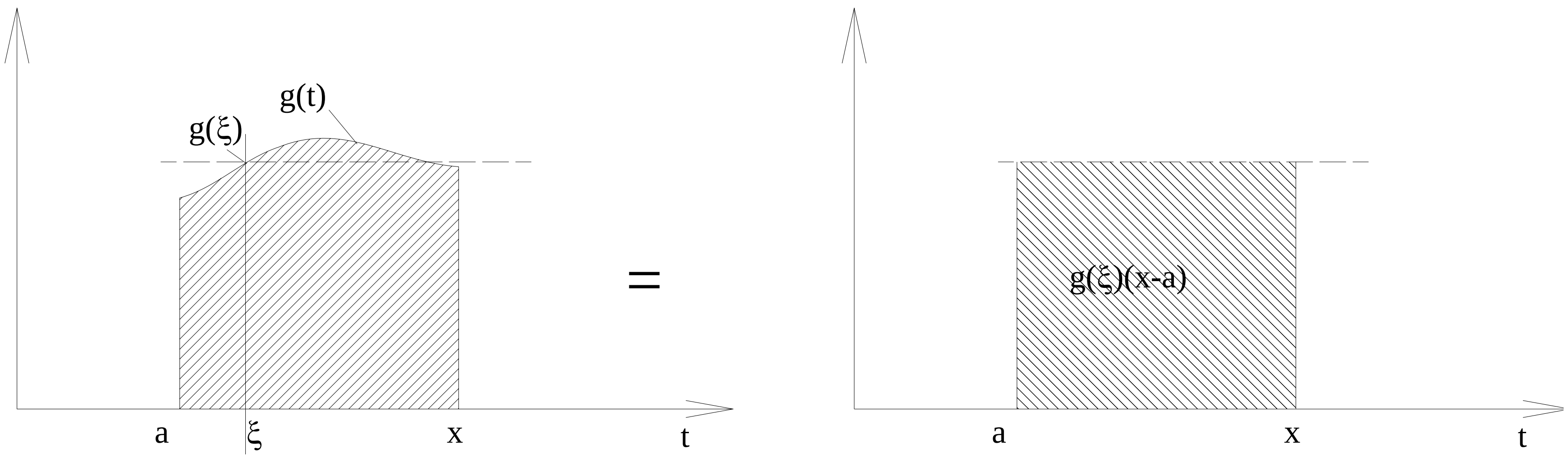
$$R_n = \int_a^x \frac{(x-t)^n}{n!} f^{n+1}(t)\,dt$$ "Integral form"

Hence, every continuous function can be approximated by a polynomial of order n

First Theorem of the mean

- If the function g is continuous and integrable in the interval containing a and x, then there exists a point ξ between a and x such that

$$\int_a^x g(t)dt = g(\xi)(x-a)$$



Second Theorem of the mean

- If the functions g and h are continuous and integrable on an interval containing a and x, and h does not change sign in the interval, then there exists a point ξ in between a and x such that:

$$\int_a^x g(t)h(t)dt = g(\xi)\int_a^x h(t)dt$$

Remainder, of the Taylor Series:

$$R_n = \int_a^x \frac{(x-t)^n}{n!} f^{n+1}(t)dt$$

Let $g = f^{n+1}(t)$ and $h(t) = \frac{(x-t)^n}{n!}$

Then according to the second theorem of the mean:

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

$a < \xi < x$

Let x= x_{i+1} and a=x_i

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

$$+ \frac{f'''(x_i)}{3!}(x_{i+1} - x_i)^3 + ... + \frac{f^{n}(x_i)}{n!}(x_{i+1} - x_i)^n + R_n$$

Where $R_n = \frac{f^{(n+1)}(\xi)}{(n+1)!}(x_{i+1} - x_i)^{n+1}$

İf we let : h=(x_{i+1} – x_i)

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

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

Example : f(x)=sin(x) expand in Taylor series about x_0=0

$$f(x_0) = \sin(0) = 0, \quad \left.\frac{\mathrm{df}}{\mathrm{dx}}\right|_{x_0} = \cos(0) = 1,$$

$$\left.\frac{\mathrm{d}^2\mathrm{f}}{\mathrm{dx}^2}\right|_{x_0} = -\sin(0) = 0, \quad \left.\frac{\mathrm{d}^3\mathrm{f}}{\mathrm{dx}^3}\right|_{x_0} = -\cos(0) = -1, \quad \left.\frac{\mathrm{d}^4\mathrm{f}}{\mathrm{dx}^4}\right|_{x_0} = \sin(0) = 0$$

$$\left.\frac{\mathrm{d}^n\mathrm{f}}{\mathrm{dx}^n}\right|_{x_0} = 0 \quad \text{if n is even,} \qquad \left.\frac{\mathrm{d}^n\mathrm{f}}{\mathrm{dx}^n}\right|_{x_0} = (-1)^{\frac{n+3}{2}} \quad \text{if n is odd}$$

$$(\mathrm{x}-\mathrm{x}_0)^n = x^n$$

$$\sin(x) = 0 + x + 0 - \frac{x^3}{3!} + 0 + \frac{x^5}{5!} + 0 - \frac{x^7}{7!} + 0 + \frac{x^9}{9!}$$

$$\sin(x) = 0 + x + 0 - \frac{x^3}{3!} + 0 + \frac{x^5}{5!} + 0 - \frac{x^7}{7!} + 0 + \frac{x^9}{9!}$$

<u>One term appoximation: (n=2)</u>

$$\sin(\frac{\pi}{4}) = +\frac{\pi}{4} = 0.785398163 \qquad R_n = \frac{f^{(n+1)}(\xi)}{(n+1)!}h^{n+1} = f'''(\xi)\frac{(\pi/4)^3}{3!} \qquad 0<\xi<\pi/4$$

$$f'''(\xi) = -\cos(\xi) \quad \text{and} \quad f'''(0) = -1; \;\; f'''(\pi/4) = -0.707106781$$

$$R_n = f'''(\xi)\frac{(\pi/4)^3}{3!} \;\; ; \quad -0.0807455122<R_n<-0.0570956992$$

<u>Two term appoximation: (n=4)</u>

$$\sin(\frac{\pi}{4}) = +\frac{\pi}{4} - \frac{(\pi/4)^3}{3!} = 0.704652651 \qquad R_n = f^{v}(\xi)\frac{(\pi/4)^5}{5!} \qquad 0<\xi<\pi/4$$

$$f^{v}(\xi) = \cos(\xi) \quad \text{and} \quad f^{v}(0) = 1; \;\; f^{v}(\pi/4) = 0.707106781$$

$$R_n = f^{v}(\xi)\frac{(\pi/4)^5}{5!} \;\; ; \quad 0.00176097489<R_n<0.00249039457$$

In both cases the true value is within the bounds.

Accumulation of errors (Due to Round off errors)

Small errors add up due to very large numbers of mathematical operations.

Division of a large number with a small number, or division of a small number with a large number may result in loss of significant digits.

$\tilde{x}$

Stability and Condition

(A guess on how the uncertainty is magnified)

If x is the input f(x) is the output

If $\tilde{x}$ is a value very close to x. i.e (x- $\tilde{x}$)is small,

Taking Taylor series expansion of f(x) about $\tilde{x}$ and keeping only the first two terms:

$$f(x) = f(\tilde{x}) + f'(\tilde{x})(x - \tilde{x})$$

Relative Error on x: $\varepsilon[x] = \dfrac{\tilde{x} - x}{\tilde{x}}$

Relative error on f(x): $\varepsilon[f(x)] = \dfrac{f(\tilde{x}) - f(x)}{f(\tilde{x})}$

Condition Number: $\dfrac{\varepsilon[f(x)]}{\varepsilon[x]} = \dfrac{\tilde{x} f'(\tilde{x})}{f(\tilde{x})}$

If the condition number is large, then the function is ill conditioned in the region of interest

Condition Number: $\frac{\varepsilon\left[f(x)\right]}{\varepsilon\left[x\right]}=\frac{\tilde{x}f'(\tilde{x})}{f(\tilde{x})}$ Is the ratio in the change of f(x) for a small change in x

$$f(x)=\frac{e^x-1}{x} \quad \text{for x=0.01}$$

$$\frac{\varepsilon\left[f(x)\right]}{\varepsilon\left[x\right]}=\frac{\tilde{x}f'(\tilde{x})}{f(\tilde{x})}$$

$$f(0.01)=\frac{e^{0.01}-1}{0.01}=1.0050167 \quad f'(0.01)=\frac{e^{0.01}}{0.01}-\frac{e^{0.01}-1}{0.01^2}=0.50334587$$

The Condition Number= $\frac{0.01*0.50334587}{1.0050167}$ =0.005 (well behaving at x=0.01)

$$f(x)=\frac{2.5}{1-x^2} \quad \text{for x=0.999000}$$

$$f(0.999)=\frac{2.5}{1-0.999^2}=1250.62531 \quad f'(0.999)=\frac{2x*2.5}{(1-x^2)^2}=\frac{5*0.999}{(1-0.999^2)^2}=1249999.686$$

The Condition Number= $\frac{0.999*1249999.686}{1250.62531}$ =999

(too large, function is ill conditioned at x=0.999)