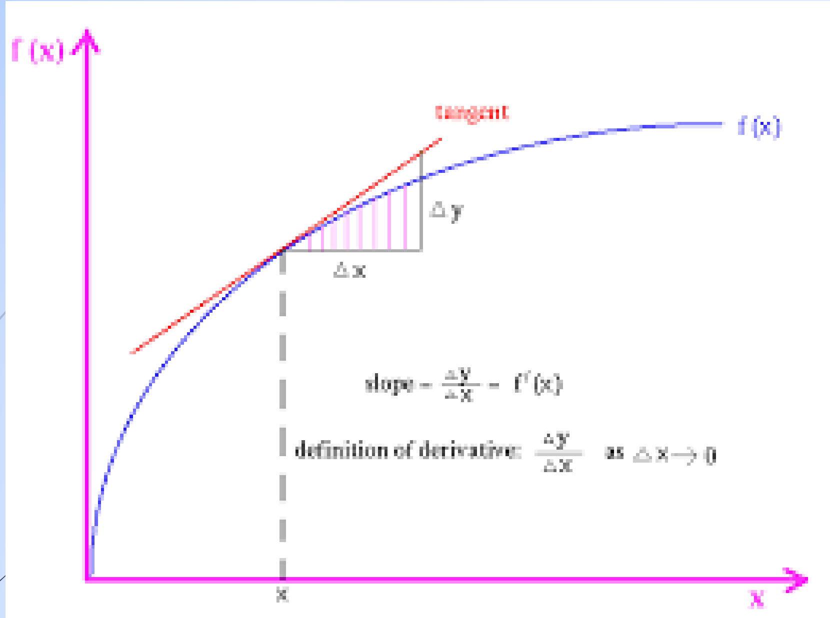

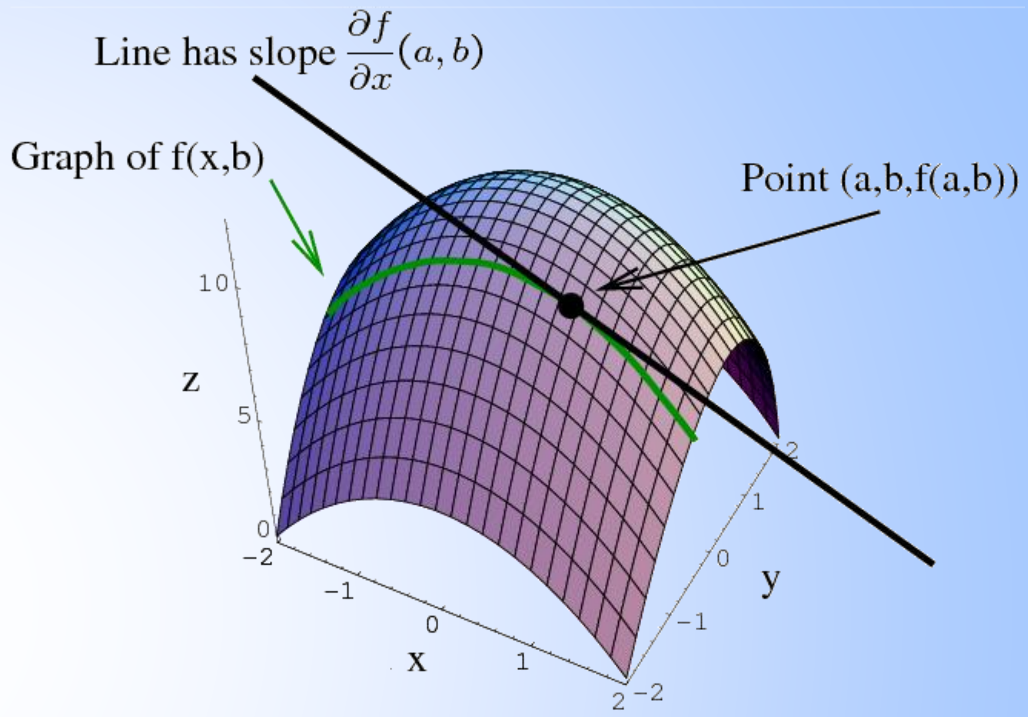

- Hadi Bordbar
- School of Engineering, Aalto University, Finland.

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ENG-A1003 - Numerical Methods in Engineering

Week #5: Numerical Differentiation

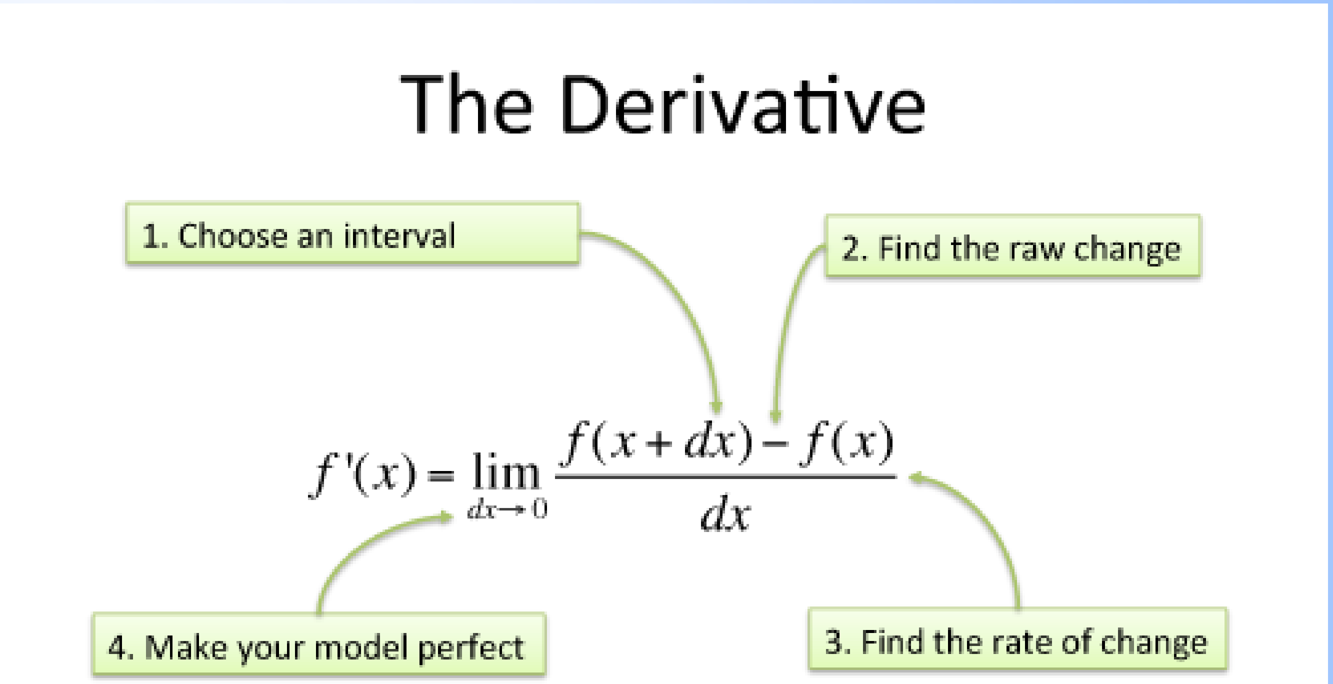
What is the problem?

1. We are **given a function** and we need to calculate its **derivative (s)?**

2. *What is the derivative?* in very simple words it is **change of a function in respect of change of one of its variables**.

3. *What the given function means?* We either have **a formula or algorithm** to calculate the function or we are **<u>given with a set of data</u>.**

It is more challenging and relevant to numerical methods



Concept of Finite Differencing

Analytical Differentiation Indefinite Differentiation with Matlab

- Symbolic Math Toolbox™ provides functions for solving, plotting, and manipulating symbolic math equations.
- More info: https://www.mathworks.com/products/symbolic.html

- **How to use it for differentiation of indefinite functions**

- Start with *sysm* … to declare the symbolic variables: for example

  syms x y z …

- Write the function whose derivative is required either in a line
  - using the function handle such as:

    Func=@(x) x^2+3x-1
  - *Or as simple as we write a mathematical equation*

    Func= x^2+3x-1

  Or in a separate in file function.

- Use *diff(Func)*

Example 1: in class exercise(10 minutes)

1. Write an script to find derivative of

$$f1 = x^2 + 1$$
$$f2 = x^6 \sin^2(x^2) \; + \cos(x)\tan(x)$$

2. Use commands *fplot* and *hold on* to plot the functions and their derivatives in same curves.

Simple syntax: fplot(func,'-')

Example 2: Apply the same method to find the partial derivatives of multivariable functions

Example: find the $df/dx, df/dy, df/dz$ of $f = x^2y + xyz - z^3 + 1$

```
% Partial Derivatives with Symbolic Math Toolbox
clear;
clc;
close all
syms x  y  z
f1=x^2*y+x*y*z-z^3+1;
df_dx=diff(f1,x)
df_dy=diff(f1,y)
df_dz=diff(f1,z)
```

Week 5: Assignment 1 (Submission deadline Feb. 11th)

1. Obtain the Jacobian matrix of the given system of equations by using the Symbolic Math Toolbox

$$\begin{cases} x^2yz + y^2z - 3z^4 = 0 \\ x - \dfrac{1}{y} + z^3x = 0 \\ yx + yz + xz = 0 \end{cases}$$

Finite Difference Approximations (FDA); History and Background

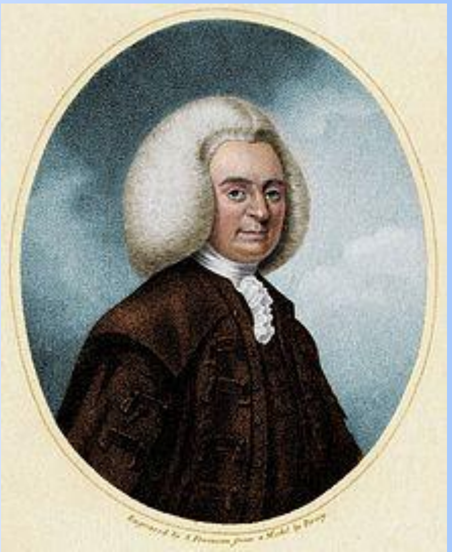
- A Taylor series is a series expansion of a function about a point. A one-dimensional Taylor series is an expansion of a real function $f(x)$ about a point $x = a$ is given by

$$f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(a)}{n!}(x-a)^n = f(a) + f'(a)(x-a) + \frac{f^{(2)}(a)}{2!}(x-a)^2 + \dots,$$

- If $(a = 0)$, then it's called Maclaurin series as

$$f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!}x^n = f(0) + f'(0)x + \frac{f^{(2)}(0)}{2!}x^2 + \dots,$$

Brook Taylor (1685-1731)



Colin Maclaurin (1698–1746)

Taylor's theorem states that any function satisfying certain conditions can be expressed as a Taylor series.

Finite Difference Approximations (FDA)

- FDA of derivative of function $f(x)$ is based on **forward and backward Taylor series expansions**

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f^{(4)}(x) + \cdots \qquad \text{(a)}$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!}f''(x) - \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f^{(4)}(x) - \cdots \qquad \text{(b)}$$

$$f(x+2h) = f(x) + 2hf'(x) + \frac{(2h)^2}{2!}f''(x) + \frac{(2h)^3}{3!}f'''(x) + \frac{(2h)^4}{4!}f^{(4)}(x) + \cdots \qquad \text{(c)}$$

$$f(x-2h) = f(x) - 2hf'(x) + \frac{(2h)^2}{2!}f''(x) - \frac{(2h)^3}{3!}f'''(x) + \frac{(2h)^4}{4!}f^{(4)}(x) - \cdots \qquad \text{(d)}$$

Sum of FDAs

- We can also derive the sum of FDAs as followings

$$f(x+h)+f(x-h)=2f(x)+h^2f''(x)+\frac{h^4}{12}f^{(4)}(x)+\cdots \tag{e}$$

$$f(x+h)-f(x-h)=2hf'(x)+\frac{h^3}{3}f'''(x)+\ldots \tag{f}$$

$$f(x+2h)+f(x-2h)=2f(x)+4h^2f''(x)+\frac{4h^4}{3}f^{(4)}(x)+\cdots \tag{g}$$

$$f(x+2h)-f(x-2h)=4hf'(x)+\frac{8h^3}{3}f'''(x)+\cdots \tag{h}$$

First Central Difference Approximations

- We can solve $Eq.(f)$ for $f'(x)$

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{6} f'''(x) - \cdots$$

- It can be transformed to

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} + \mathcal{O}(h^2)$$

- which is called the ***<u>first central difference approximation</u>*** for $f'(x)$. The term $O(h^2)$ represents a truncation error which behaves as h^2.

Second Central Difference Approximations

- For $f''(x)$ from $Eq.(e)$, we can write

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + \frac{h^2}{12} f^{(4)}(x) + \cdots$$

- It can be transformed to

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + \mathcal{O}(h^2)$$

- which is called the ***central difference approximation*** for the second order derivative of $f(x)$. The term $O(h^2)$ represents a truncation error which behaves as h^2.

Higher Order Central Difference Approximation

- In the same way for the higher order derivatives we can derive

$$f'''(x) = \frac{f(x+2h) - 2f(x+h) + 2f(x-h) - f(x-2h)}{2h^3} + \mathcal{O}(h^2)$$

$$f^{(4)}(x) = \frac{f(x+2h) - 4f(x+h) + 6f(x) - 4f(x-h) + f(x-2h)}{h^4} + \mathcal{O}(h^2)$$

Summary of Central Difference Approximation

	$f(x-2h)$	$f(x-h)$	$f(x)$	$f(x+h)$	$f(x+2h)$
$2hf'(x)$		-1	0	1	
$h^2 f''(x)$		1	-2	1	
$2h^3 f'''(x)$	-1	2	0	-2	1
$h^4 f^{(4)}(x)$	1	-4	6	-4	1

Summary of CDA: Coefficients of central finite difference approximations of $O(h^2)$

Example 3: In Class Exercise (10 minutes):

- Write a code to calculate the values of $f(x) = 5x^3 + 2x^2 - 4x + 2$ for $0 \leq x \leq 2$ with a suitable step size of ∇x, given by the user.
- Plot the curve.
- Save the output data in an array.
- Use the values stored in the array to calculate first and second derivate of $f(x)$ by central difference approximates. Check it at $x = 0.5$.
- compare it with the exact analytical value.
- Do the calculations for ∇x=0.5, 0.4, 0.25, 0.1, 0.01 and see how change of step size affect the accuracy of numerical differentiation.

A sample script will be given in mycourses.

Non-central Finite Difference Approximation

- Central finite difference approximations **are not always usable**.
- For instance, a function is given at the n discrete points $x_1, x_2, \ldots, x_n$. Since central differences use values of the function on both sides of x, we can not obtain the derivatives at x_1 and x_n by central FDAs.
- We need finite difference expressions with evaluations of the function **on one side of x only**. These kind of approximations **are called forward and backward finite difference approximations**.

Non-central Finite Difference Approximation

- Deriving $f\ (x)$ from Eq. (a), we can have:

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{h}{2}f''(x) - \frac{h^2}{6}f'''(x) - \frac{h^3}{4!}f^{(4)}(x) - \cdots$$

- If we keep the first term on the right hand we will reach the first order forward finite difference approximation as:

$$f'(x) = \frac{f(x+h) - f(x)}{h} + \mathcal{O}(h)$$

Note that the truncation error is of order of $O(h)$

- In the same way for the first order backward finite difference approximation, we can write:

$$f'(x) = \frac{f(x) - f(x-h)}{h} + \mathcal{O}(h)$$

Non-central Finite Difference Approximation

- In the same manner, we can derive the **higher order derivatives** from forward or backward finite difference approximation. For instance, Eqs. (a) and (c) yield to

$$f''(x) = \frac{f(x+2h) - 2f(x+h) + f(x)}{h^2} + \mathcal{O}(h)$$

- As seen in all these three equations, the truncation errors are from the order of $O(h)$ which is not as good as $O(h^2)$. Hence, there is a need for higher accuracy forward and backward finite difference approximation

Higher Order Forward and Backward Finite Difference Approximations

- To derive the higher order non central finite difference approximation, we need to keep more terms in Taylor series expansions. For instance, we can start from equations (a) and (c) as:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(x) + \cdots$$

$$f(x+2h) = f(x) + 2hf'(x) + 2h^2 f''(x) + \frac{4h^3}{3}f'''(x) + \frac{2h^4}{3}f^{(4)}(x) + \cdots$$

- We eliminate $f''(x)$ by multiplying the Eq.(a) by 4 and subtract it from Eq(c), then we would have

$$f(x+2h) - 4f(x+h) = -3f(x) - 2hf'(x) + \frac{h^4}{2}f^{(4)}(x) + \cdots$$

Higher Order Forward and Backward Finite Difference Approximations

- Therefore

$$f'(x) = \frac{-f(x+2h) + 4f(x+h) - 3f(x)}{2h} + \frac{h^2}{4} f^{(4)}(x) + \cdots$$

Or

$$f'(x) = \frac{-f(x+2h) + 4f(x+h) - 3f(x)}{2h} + \mathcal{O}(h^2)$$

This is the formula of the ***second order forward finite difference approximation***.

- We can derive the similar formulas for $f''(x)$ and $f'''(x)$ and higher derivatives as summarized in the next two tables

Coefficients of Forward Finite Difference Approximations of $O(h^2)$

	$f(x)$	$f(x+h)$	$f(x+2h)$	$f(x+3h)$	$f(x+4h)$	$f(x+5h)$
$2hf'(x)$	-3	4	-1			
$h^2 f''(x)$	2	-5	4	-1		
$2h^3 f'''(x)$	-5	18	-24	14	-3	
$h^4 f^{(4)}(x)$	3	-14	26	-24	11	-2

Coefficients of Backward Finite Difference Approximations of $O(h^2)$

	$f(x-5h)$	$f(x-4h)$	$f(x-3h)$	$f(x-2h)$	$f(x-h)$	$f(x)$
$2hf'(x)$				1	-4	3
$h^2 f''(x)$			-1	4	-5	2
$2h^3 f'''(x)$		3	-14	24	-18	5
$h^4 f^{(4)}(x)$	-2	11	-24	26	-14	3

Example 4:

Given the data

x	0.84	0.92	1.00	1.08	1.16
$f(x)$	0.431711	0.398519	0.367879	0.339596	0.313486

Calculate f' and f'' at $x = 0.84, 1.00,$ and 1.16. Calculate them manually and by a Matlab script using the finite difference approximations of $O(h^2)$.

Example 4: Solution

(1) X=0.84 is the first point→ there is no data before it→ we need forward FDA:

Table given in slides for forward FDA with $O(h^2)$:

	$f(x)$	$f(x+h)$	$f(x+2h)$	$f(x+3h)$	$f(x+4h)$	$f(x+5h)$
$2hf'(x)$	-3	4	-1			
$h^2 f''(x)$	2	-5	4	-1		
$2h^3 f'''(x)$	-5	18	-24	14	-3	
$h^4 f^{(4)}(x)$	3	-14	26	-24	11	-2

Hence: $f'(x) = \frac{1}{2h}(-3f(x) + 4f(x+h) - f(x+2h))$

For the given data is $h = 0.08 \rightarrow f'(0.84) = \frac{1}{2\times 0.08}(-3\times 0.431711 + 4\times 0.398519 - 0.367879) = -0.430850$

and

$$f''(x) = \frac{1}{h^2}(2f(x) - 5f(x+h) + 4f(x+2h) - f(x+3h))$$

$$f''(0.84) = \frac{1}{0.08^2}(2\times 0.431711 - 5\times 0.398519 + 4\times 0.367879 - 0.339596) = 0.429218$$

Example 4: Solution

(2) X=1.00, there are enough data on both sides of the point, therefore we can use the central finite difference approximation

Table given in slides for central FDA:

	$f(x-2h)$	$f(x-h)$	$f(x)$	$f(x+h)$	$f(x+2h)$
$2hf'(x)$		-1	0	1	
$h^2 f''(x)$		1	-2	1	
$2h^3 f'''(x)$	-1	2	0	-2	1
$h^4 f^{(4)}(x)$	1	-4	6	-4	1

Hence: $f^{'}(x) = \frac{1}{2h}(-f(x-h) + f(x+h))$

→ $f'(1.0) = \frac{1}{2\times 0.08}(-0.339596 + 0.398519) = -0.368269$

and $f^{'}{'}(x) = \frac{1}{h^2}(f(x-h) - 2f(x) + f(x+h))$

$$f''(1.0) = \frac{1}{0.08^2}(0.398519 - 2 \times 0.367879 + 0.339596) = 0.368281$$

Example 4: Solution

(3) **X=1.16,** there is no data on upward direction, therefore we need to apply the backward FDA. The table of backward FDA is given in the slides as:

	$f(x-5h)$	$f(x-4h)$	$f(x-3h)$	$f(x-2h)$	$f(x-h)$	$f(x)$
$2hf'(x)$				1	-4	3
$h^2 f''(x)$			-1	4	-5	2
$2h^3 f'''(x)$		3	-14	24	-18	5
$h^4 f^{(4)}(x)$	-2	11	-24	26	-14	3

Hence: $f'(x) = \frac{1}{2h}(f(x-2h) - 4f(x-h) + 3f(x))$

→ $f'(1.16) = \frac{1}{2\times 0.08}(0.367879 - 4\times 0.339596 + 3\times 0.313486) = -0.312794$

and

$$f''(x) = \frac{1}{h^2}(-f(x-3h) + 4f(x-2h) - 5f(x-h) + 2f(x))$$

$$f''(1.16) = \frac{1}{0.08^2}(-0.398519 + 4\times 0.367879 - 5\times 0.339596 + 2\times 0.313486) = 0.310781$$

Error Analysis in FDA

- **A major question:** What is the right value for h in FDA?
- **Observations:**
  - Using very small h→ the values of $\boldsymbol{f(x), f(x \pm h)}$, **and** $\boldsymbol{f(x \pm 2h)}$ **are very close**→ Higher precisions for numbers are needed→ round off error is getting important.
  - Using larger h→ The effect of **error due to skipping extra terms** in Taylor series expansion is getting more significant (truncation error).
- There is **no explicit solution** for this complex behavior to choose the right optimal h.
- **Recommendation:**
  - Use higher precision numbers→ decrease the round off error.
  - Use higher order formulation of FDA, at least $O(h^2)$→ less skipped terms→ less truncation error.
  - Use tricks for improvement such as Richardson extrapolation.

Example 5:

- Using two different precisions of 6 and 8 digits, centeral FDA calculates the following values for $f''(x)$ at $x = 1$ for $\boldsymbol{f(x) = e^{-x}}$. The exact solution is known from calculus as $e^{-1} =$ 0.367879441171442.

h	6-digit precision	8-digit precision
0.64	0.380 610	0.380 609 11
0.32	0.371 035	0.371 029 39
0.16	0.368 711	0.368 664 84
0.08	$\boxed{0.368\,281}$	0.368 076 56
0.04	0.368 75	0.367 831 25
0.02	0.37	$\boxed{0.3679}$
0.01	0.38	0.3679
0.005	0.40	0.3676
0.0025	0.48	0.3680
0.00125	1.28	0.3712

Above the optimal h, the error is mainly coming from truncation error, below it is mostly due to round off error.

Week 5: Assignment 2 (Submission Deadline is Feb. 18th)

- Write a Matlab function which takes a function $f(x)$ in the form x and y discrete points with at least 5 data points and calculates the $f'(x)$ and $f''(x)$ by FDA of $O(\boldsymbol{h}^2)$.
- The code should recognize which of FDA schemes, i.e. backward, central and forward, is suitable and should be used for each of the points.
- Test your function to calculate $f'(x)$ and $f''(x)$ for a set of x, y data given in a text file in mycourses. Practice Matlab commands for reading from files.

Introduction to the Concept of Probability and Statistical Methods Via A GAME

- Statistical methods: Solving a physical or mathematical problem by finding the probability of a conditional event. The desired conditions can be based on physics and our targeted design, etc. One of the most famous one is Monte Carlo method.

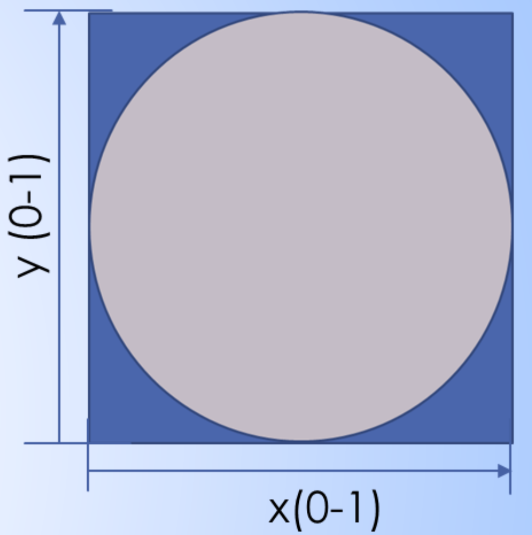
- They are based on generating random numbers usually between 0 and 1. There are specific algorithms (not subject of this course) for generating such numbers.

A Game; Play Dart with Matlab

- From geometry we know that area of a circle is simply $\frac{\pi D^2}{4}$.
- Here we want to solve this simple problem with a more complex way to learn the concept of probability and random number generators and statistical methods.

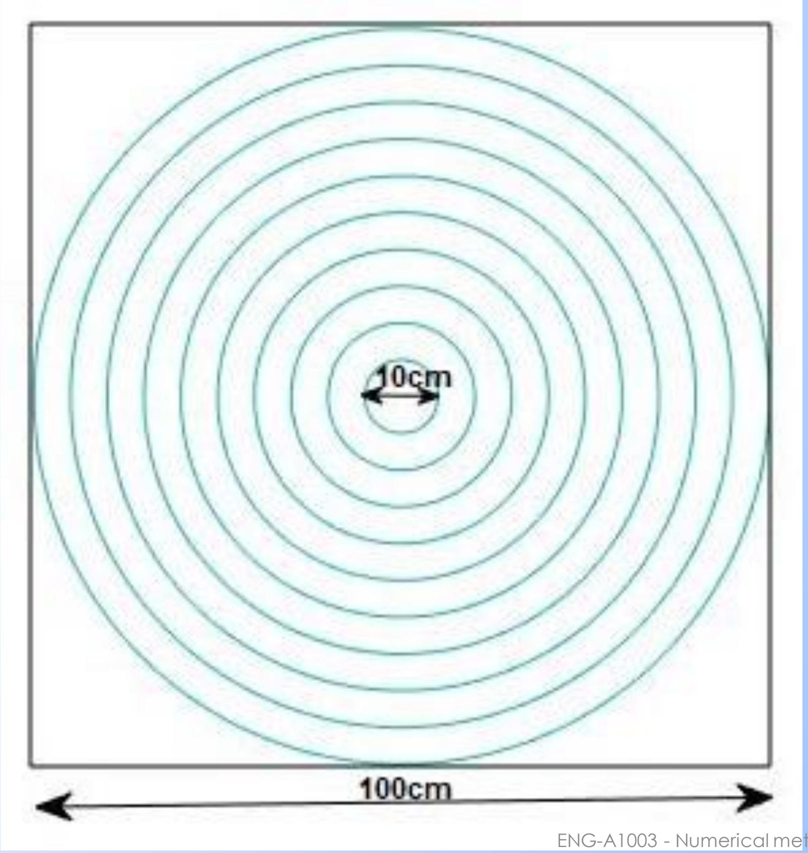
Example 6 (In Class Exercise): Calculation of Area of a Circle With the Matlab Command $rand()$

- Consider a square of $1 * 1$ unit of length, lets say $1m * 1m$.
- The coordinates of each point in this square is defined by (x,y) coordinates where x and y are between 0 and 1.
- Assume a circle with diameter 1m inscribed within the square.
- Use the command $rand(n)$ to calculate the area of the circle.
- Note that $rand(n)$ produce an square matrix of random numbers between 0 and 1. you can also use it to produce arrays of other sizes by defining the number of rows and columns and other dimensions if any, e.g. $rand(M,N,P,\dots)$ or $rand([M,N,P,\dots])$ returns $M-by-N-by-P-by-\dots$ array.
- Quality of random number generator affect on the accuracy (i.e. how the generated numbers are really random?)



Week 5, Assignment 3 (Submission Date: Feb. 18^{th})

- Consider a dart with 10 same centered circles whose diameters are evenly changing from 10 to 100 cm.
- Assume that the worst shot is not outside the square inscribing the largest circle.
- Write a Matlab script and find the probability of hitting each of the point from zero (outside the largest circle) to 10 the smallest circle in the middle.
- The exact solution for each of the points is the ratio of the area of that point to the area of the square. Check the accuracy of your numerical results with the exact solutions.
- Observe and report by suitable plot, how change the size of the random number set may affect the accuracy?
- Observe the change of computational time with the size of the random number set.
- Bonus point: discover and use suitable techniques which may improve the computational performance (higher accuracy with less computational time)?



Richardson Extrapolation -1

- It is a trick to quickly improve the accuracy of the FDA by reducing the truncation error.
- Based on FDA, the value of derivate is G is function of h. It can be written as

$$G = g(h) + E(h)$$

- $E(h)$ represents the error associated with truncation of extra terms in FDA, it therefore can be written as ch^p. Therefore with two different values of h, one can write

$$G = g(h_1) + ch_1^p$$
$$G = g(h_2) + ch_2^p$$

- Skipping the error of Eliminating c and solving for G, we can find the Richardson Extrapolation formula

$$G = \frac{(h_1/h_2)^p g(h_2) - g(h_1)}{(h_1/h_2)^p - 1}$$

Richardson Extrapolation-2

- If we work with the second order FDA, the term of error is of power two of h, i.e. $O(h^2)$. As a common practice h_2=$h_1/2$ is used. Hence using p=2 in Richardson formula, we can have:

$$G = \frac{2^p g(h_1/2) - g(h_1)}{2^p - 1}$$

$$\text{Exact Value} = \; 0.3678794411714 42.$$

Example 7

- Apply the Richardson extrapolation formula to the previous example and improve the calculation of 6 digits

We use $h_1 = 0.64$ and $h_2 = 0.32$. From the table, the g values obtained by the original central FDA for h_1 and h_2 are:

$$g(h_1) = 0.380610$$

$$\text{and } g(h_2 = \frac{h_1}{2}) = 0.371035$$

This results in

$$G = \frac{2^2 g(0.32) - g(0.64)}{2^2 - 1} = 0.367843$$

Checking the values of the table of example 5, we can see that this is as accurate as the best results of 8 digits calculations.

Therefore, we saw how Richardson extrapolation boost the FDA.

Derivation by interpolation

- It is simply based on this fact that any set of n pair of x, y data can be interpreted by a function fitted to the points.
- It is particularly useful for the data which are not evenly distributed. For evenly distributed data, the results of this method is identical to FDA.
- The most popular function for fitting to derive derivative is polynomial and cubic spline interpolant.
- Any n data can be fitted by a polynomial of order of n-1 .
- Use of higher order polynomial than 6th order may lead to non-sensible noises and therefore should be avoided.

Summary of Week 5

- Review the concept of derivatives and how it is defined for numerical functions, e.g. a set of discrete points.
- Differentiation of indefinite function with Matlab.
- Finite difference approximation (FDA) to find the derivatives of a numerical function.
- Different schemes of FDA; i.e. central, forward and backward FDA.
- Error analysis of FDA.
- Improvement techniques for FDA.
- Probability and statistical methods based on random number generation. How to use Matlab for such a problem.