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# Computational Science and Numerical Analysis

## introduction

What to learn:

- understand numerical tools for problem solving. Computation is about a method or framework for solving problem.
- how to translate mathematical problems to code.
- errors and convergence analysis

## Why do we need numerical computing?

**Ans** We need numerical computing because it give us a framework that accurately provide an approximation to a given problem.

## * Application area.

- Engineering
- physics
- chemistry
- image processing, animations, computer vision
- HIV research, financial mathematics etc.

## Numerical tools

computer speed is getting better by the release of different generations.

computer speed depend on flop - [ floating point operations a measure of computer performance useful in

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## Solution of Nonlinear Equations (Root finding problems)

- Analytical
- Graphical
- Numerical

- Definitions
- classification of methods
  - Analytical solutions
  - Graphical methods
  - Numerical methods
    - Bracketing methods
    - open Methods
- convergence Notations

**Root finding problems**

Many problems in Science and Engineering are expressed as: Given a continuous function $f(x)$, find the value $r$ such that $f(r) = 0$

These problem are called ~~root~~ root finding problems.

**Roots of Equations**

A number $r$ that satisfies an equation is called a root of the equation.

The equation: $x^4 - 3x^3 - 7x^2 + 15x = -18$

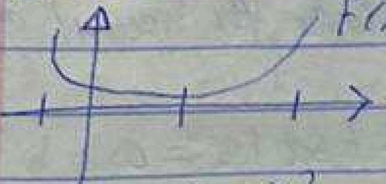
has four roots: $-2, 3, 3,$ and $-1$

i.e $x^4 - 3x^3 - 7x^2 + 15x + 18 = (x+2)(x-3)^2(x+1)$

The equation has two simple roots ($-1$ and $-2$) and a repeated roots ($3$) with ~~multiar~~ multiplicity $= 2$.

multiple zeros

$f(x) = (x-1)^2$



$f(x) = (x-1)^2 = x^2 - 2x + 1$

has double zeros (zeros with multiplicity = 2) at $x = 1$

Roots of equations & zeros of function

Given the equation:

$x^4 - 3x^3 - 7x^2 + 15x = -18$

Make all terms to one side of the equation:

$x^4 - 3x^3 - 7x^2 + 15x + 18 = 0$

Define $f(x)$ as:

$f(x) = x^4 - 3x^3 - 7x^2 + 15x + 18$

The zeros of $f(x)$ are the same as the roots of the equation $f(x) = 0$

(which are -2, 3, 3, and -1)

Solution methods

several ways to solve nonlinear equation are possible:

- Analytical solutions
  possible for special equations only
- Graphical solutions
  useful for providing initial guesses for other methods.
- Numerical solutions
  * open methods
  * bracketing methods

$0 \times -1$

$1x$

Note this

## Zeros of a function

let $f(x)$ be a real-valued function of a real variable. Any number $r$ ~~that~~ for which $f(r) = 0$ is called a zero of the function.

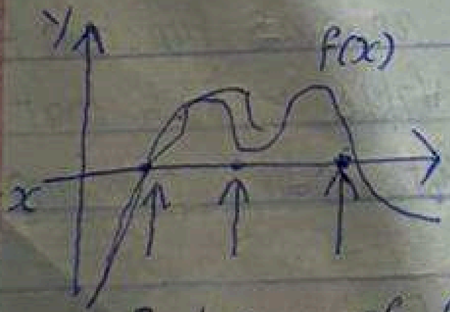
Examples:

2 and 3 are zeros of the function $f(x) = (x-2)(x-3)$ because when put into the function makes the function equal zero.

Note this

## Graphical interpretation of zeros

The real zeros of a function $f(x)$ are the values of $x$ at which the graph of the function crosses (or touches) the $x$-axis



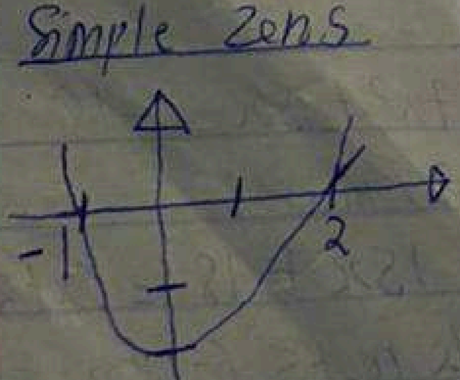

Real zeros of $f(x)$

$x = -1$

$x = 2$

## Simple zeros

$f(x) = (x+1)(x-2)$




$f(x) = (x+1)(x-2) = x^2 - x - 2$

has two simple zeros (one at $x = 2$ and one at $x = -1$)

Method to find a zero of a Non-linear function
1 Bisection 2. Secant
3. Newton

Analytical Methods

Analytical solutions are available for special equations only.

Analytical solution of: $ax^2+bx+c=0$

$$\text{Roots} = \frac{-b \pm \sqrt{b^2-4ac}}{2a}$$

No analytical solution is available for: $x-e^{-x}=0$

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Number Representation and Accuracy

whole number part

after d decimal point

fractional part

$$312.45 = 3\times10^2 + 1\times10^1 + 2\times10 + 4\times10^{-1} + 4\times10^{-2}$$
$$= 3\times100 + 1\times10 + 2\times1 + 4\times0.1 + 4\times0.01$$
$$= 300 + 10 + 2 + 0.4 + 0.04$$
$$= 312.44$$

Decimal system: Base = 10, (0, 1, ..., 9)

small numbers - negative

large numbers - positive

Standard Representations

| $\pm$ | 312 | . 45 |
|---|---|---|
| sign | integral part | fraction part |

- Normalized floating point representation:

$$\underset{\text{sign}}{\pm} \quad \underbrace{d.f_1 f_2 f_3 f_4}_{\text{mantissa}} \times 10^{\overset{\pm n}{\text{exponent}}}$$

$d \neq 0$ $\pm n$: Signed exponent

- Scientific Notation: Exactly one non-zero digit appears before decimal point.
- Advantage: Efficient in representing very small or large numbers.

Binary System

Base = 2, Digits {0, 1}

$$\underset{\text{sign}}{\pm} \quad \underbrace{1.f_1 f_2 f_3 f_4}_{\text{mantissa}} \times 2^{\overset{\pm n}{\text{exponent}}}$$

$(1.101)_2 = (1 + 1 \times 2^{-1} + 0 \times 2^{-2} + 1 \times 2^{-3})_{10} = (1.625)_{10}$

Fact

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

$(1.1)_{10} = (1.000110011001100\ldots)_2$

You can never represent 1.1 exactly in binary system.

IEEE 754 floating-point representation

- Single precision 32-bit representation
  8-bit exponent and 23-bit fraction
- Double precision 64-bit representation

11-bit exponent and 52-bit fraction

Significant digits

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

- Single-precision: 7 significant Digits
  $1.175494... \times 10^{-38}$ to $3.402823... \times 10^{38}$
- Double-Precision: 15 ~~Significant~~ significant digits
  $2.2250738... \times 10^{-308}$ to $1.7976931... \times 10^{308}$

Note: 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.

example: Suppose you want to compute:

$3.578 * 2.139$

using a calculator with two-digit fraction:

$3.57 * 2.13 = 7.60$

true answer: 7.653342

Accuracy and precision

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

Diagram

a. inaccurate and imprecise
b. accurate and imprecise
c. inaccurate and precise
d. accurate and precise


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

Rounding and chopping

<u>Rounding</u> - Replace the number by the nearest machine number.

<u>Chopping</u> - Throw all extra digits.

| | Chopping | Rounding |
|---|---|---|
| e.g to 3 S.D | 4.24/7 | 4.24/7 |
| | 4.24 | 4.25 |

<u>Error Definitions - true Error</u>

* can be computed if the true value is known:

Absolute true error

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

Absolute percent relative error

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

* When the true value is not known — estimated absolute true error

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

Estimated absolute percent relative error

$$\varepsilon_a = \left|\frac{\text{current estimate} - \text{Previous estimate}}{\text{current estimate}}\right| \times 100$$

1-5+4

- Validation of the Solution.

* ## Rolles theorem

Rolles theorem states that for any continous differentiable function that has two equal values at two distinct points, the function must have a point which satisfies the function where the first derivative is zero.

If $f(x)$ is continous in a interval $a <= x <= b$
If $f'(x)$ exist in the interval $a, x, b$
$f(a) = f(b) = 0$ then
There exist at least one value of $x$ say as $c$
Such that $f'(c) = 0$ $a < c < b$

e.g $f(x) = x^2 - 5x + 4$ and the interval is $[1,4]$

$$f'(x) = 2x - 5$$

$$f(1) = 1^2 - 5(1) + 4$$
$$= 0$$

$$f(4) = 4^2 - 5(4) + 4$$
$$= 0$$

$$f'(x) = 2x - 5$$
$$2x = 5$$
$$x = 5/2$$

$= 5/2$

$= 5/2$

Which are discrete in nature. The input data are numbers that may represent numerals, letters, or other special symbols.
Digital computers are more accurate than analog computers. Digital computers are widely used for many different applications and are often called general purpose computer.

* Characteristics of numerical computing

1. Accuracy - Every method of numerical computing introduces errors. They may be either due to using an appropriate in pace of an exact mathematical procedure or due to inexact representation and manipulation of numbers in the computer. These errors affect the accuracy of the result.
2. Efficiency - Another important is the ability of numerical methods to provide high level of efficiency
3. Numerical stability - Another problem is numerical instability.

* Process of numerical computing

- formulation of a mathematical method
- construction of an appropriate numerical method
- implementation of the method to obtain a solution

14 Float, allow varying no of digits after the decimal point.
Fixed allow only a fixed no of digits after the decimal points.

3. Floating point numbers
The term floating point is derived from the fact that there is a fixed number of digits before and after the decimal point i.e.., the decimal point can float.
The representation in which number of digit before and after the decimal number is set is called the fixed point representation.
generally floating point representations are slower and less accurate than fixed point representation, but they can handle a large range of numbers.

Distinguish between Analog computing and Digital computing

Analog computing
We refer to principles of solving problem using tools that are Analog in nature - e.g time, temperature, pressure and speed. The basic requirement in the application of analog computers is the writing down of differential equations describing the physical system of interest.

Digital Computing
Is a computing device that operates on inputs

$y = x^2 + 3x + 2$

2. System of linear algebraic equation

$2x + 3y = 7$

$5x + 8y = 18$

The values of x and y, that satisfies the above equation can be derived using numerical computation.

An approach is the used of direct method.

Direct method is complex, for number of variable

e.g $f(x) = 2x + 3y + 42$

$f(x) = 3x + 2y + 2z$

The best solution to these type of problem is the use of numerical computations implemented by

electronic situation.
numerical problems formulated from situation can be solved using numerical methods. The class method that solves a particular problem is dependent on that type of problem.
∴ mc is directly proportional to nm
where $Nc \neq 0$

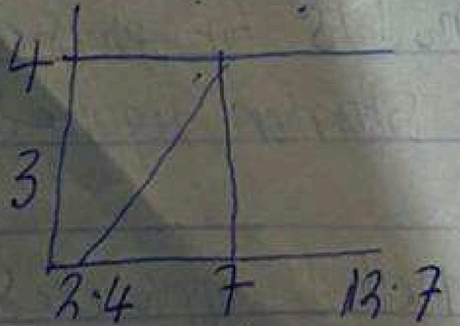
* Numerical methods are classified basically depending upon the type of problem.

1. Numerical methods to find roots of equations

Bisection method

In engineering, science and similar subject areas, algebraic expressions are used to explain concept in that area and that resolve in what we called transcendental equation.

eg $F(x) = x^2 + 3x + 2$



2·4 / 6·9 ⟹ root of the equation

$F(x) = x^2 + 3x + 2$

$F(x) - y$

$x$ - dependent
$t$ (time) - independent
capital F is the real function
$dy/dx = F(x)(y)$
Function of a function
$F(x)(y)$ is the small function of $f(x), f(y)$ means that we are taking the function of f and function of y and placing them in a set called

6/09/21 Numerical approach to computing

Numerical computing is a general approach for solving complex mathematical problems. This problems are solved using simple arithmetic operations. This approach involves formulation of simple mathematical models for physical situations in a way that such situation requires only arithmetic interpretation.

**Numerical methods**: method approaches used in numerical computing. The micro-electronic evolution and the development high and low medium level in computer are classical examples of numerical computation in

A diff equ that involves one or more dependent var with respect to to one or more independent variables.

Fields of scientific computations that require floating-point calculation.

Numerical operations

characteristic equation that is used to study the local variables of equilibrium.

qualitative analysis

$F(x) = 0$

Assignment

1. Write a short note on the application area of O.D.E.
2. Pick a specific area in engineering and discuss about the relationship with computer science and mathematical method.

6/09/

O D E

$$\frac{dy}{dx} = F(x), (y)$$

where $y(x)$ is a real value function

$F(x)(y)$ is a real function

$F(x)(y)$ is a real valued function of two real variable.

$y$ - dependent variable

$x$ - independent variable

e.g $\frac{dx}{dt} = -x^2$