NUMERICAL METHODS

Lecture 0

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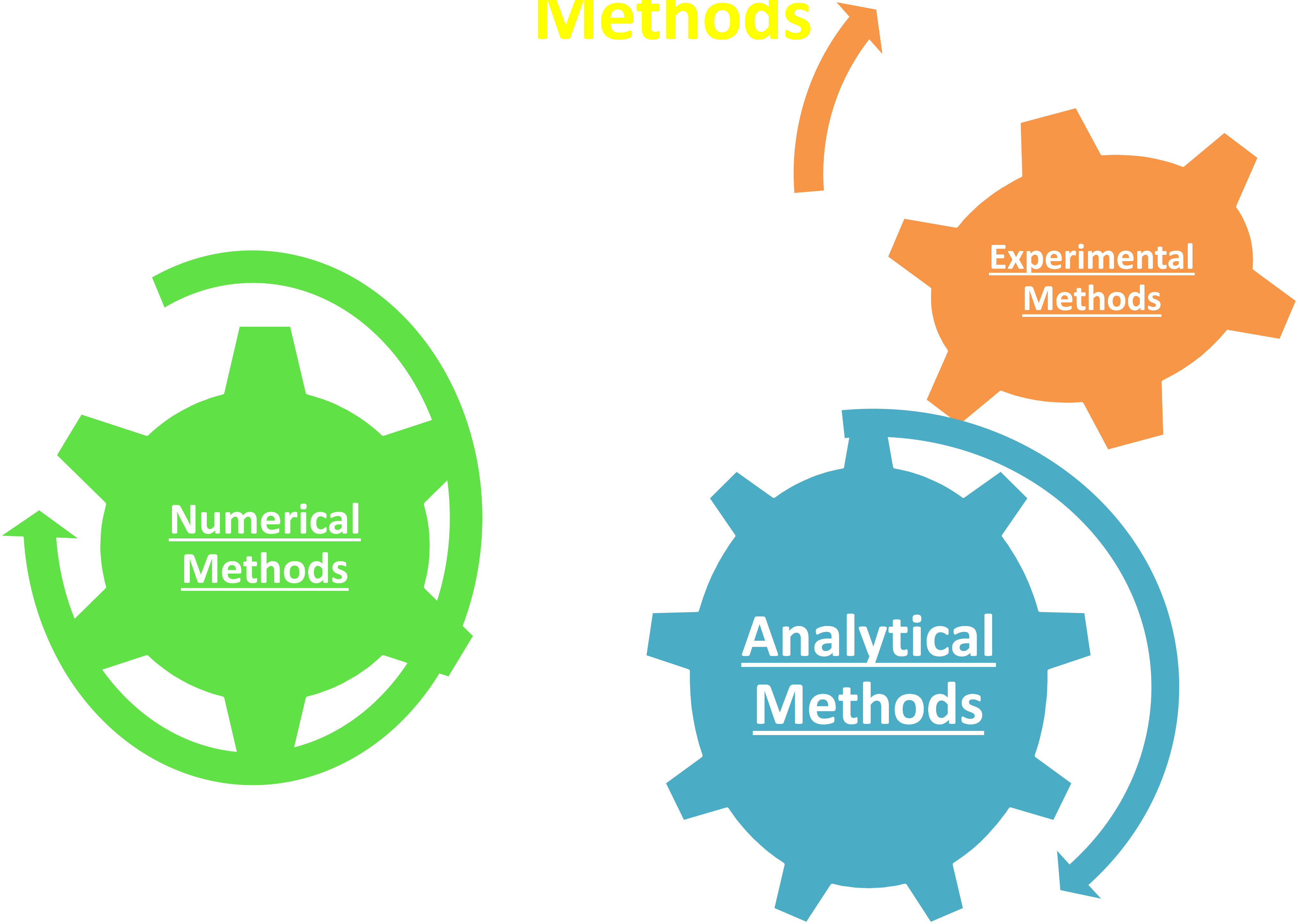
Methods



Experimental Methods
Numerical Methods
Analytical Methods

Methods

Analytical Methods

$EI\, d^2 u/ dx^2 = M$, $EI\, d^4 u/ dx^4 = w$

$D\,(\delta^4 u/ \delta x^4 + 2\, \delta^4 u/ \delta x^2 \delta y^2 + \delta^4 u/ \delta y^4) = w$

$D\,(\delta^4 u/ \delta x^4 + \delta^4 u/ \delta y^4 + \delta^4 u/ \delta z^4 + 2\, \delta^4 u/ \delta x^2 \delta y^2 + 2\, \delta^4 u/ \delta y^2 \delta z^2 + 2\, \delta^4 u/ \delta x^2 \delta z^2) = w$

Numerical Methods

Finite Element/Strip/Difference/Volume Methods

Boundary Element/Knot/Particle Methods

Domain Decomposition / Neumann & Neumann Methods

Experimental Methods

Can’t Simulate

Skilled persons required

What do we need?

Basic Needs in the Numerical Methods:

Practical:

Can be computed in a reasonable amount of time.

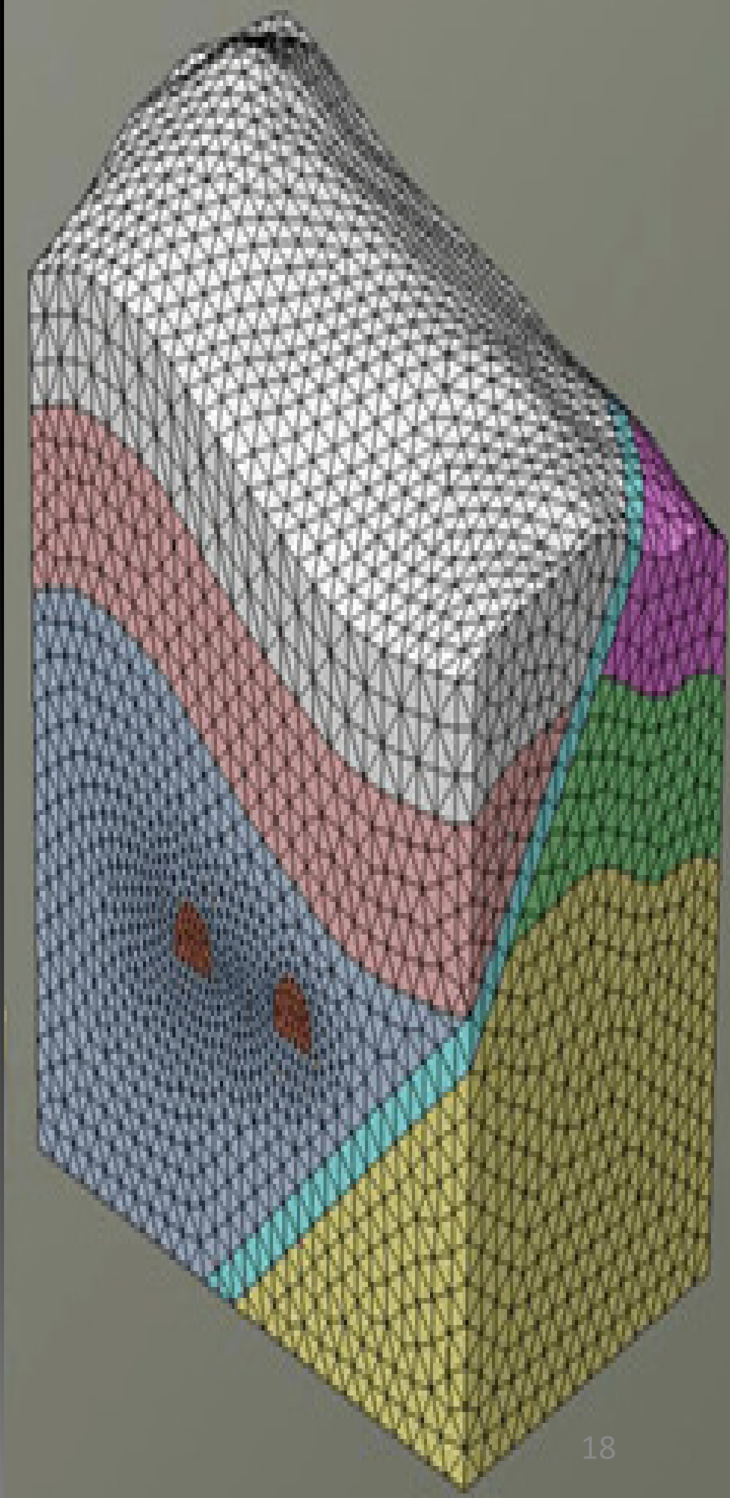
Accurate:

Good approximate to the true value,

Information about the approximation error (Bounds, error order,...).

Solution of Linear Equation y = mx + c

$$4x + 3 = 0$$



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:

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

Find the minimum of the following function both analytically and numerically:

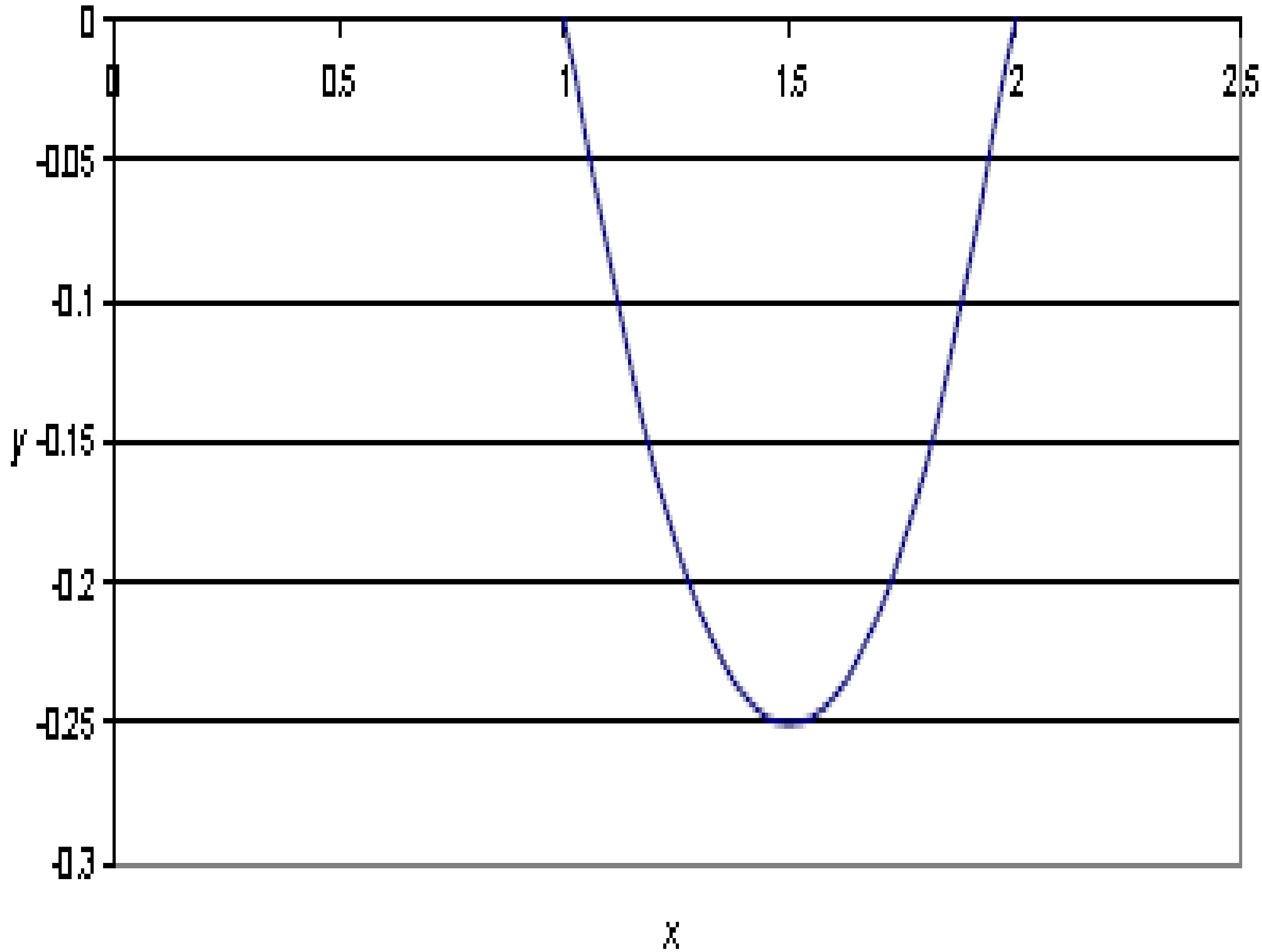
$$y = x^2 - 3x + 2$$

Analytical Solution:

$$\frac{dy}{dx} = 2x - 3 = 0 \qquad \Rightarrow \; x = \frac{3}{2} = 1.5$$

$$\text{Therefore,} \quad y_{\min} = (1.5)^2 - 3(1.5) + 2 = -0.25$$

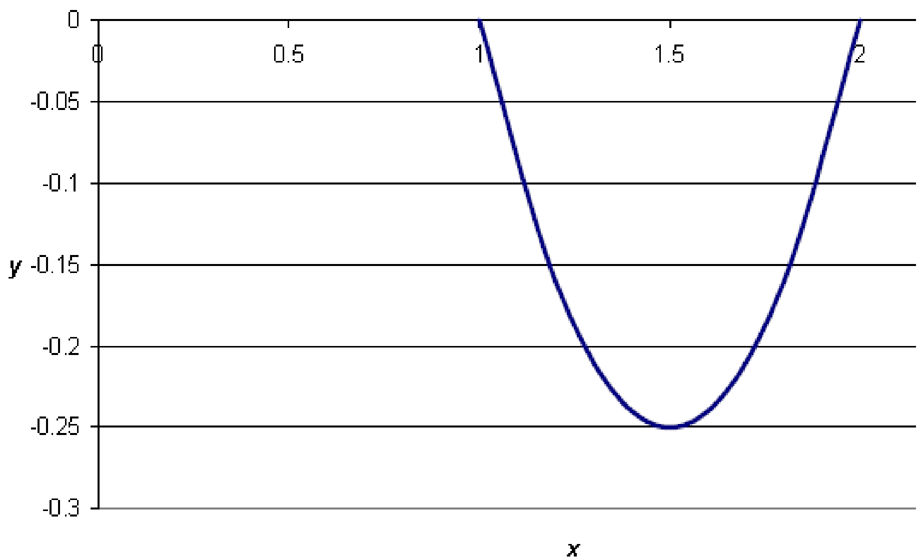
x	y
1	0
1.2	-0.16
1.4	-0.24
1.6	-0.24
1.8	-0.16
2	0



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

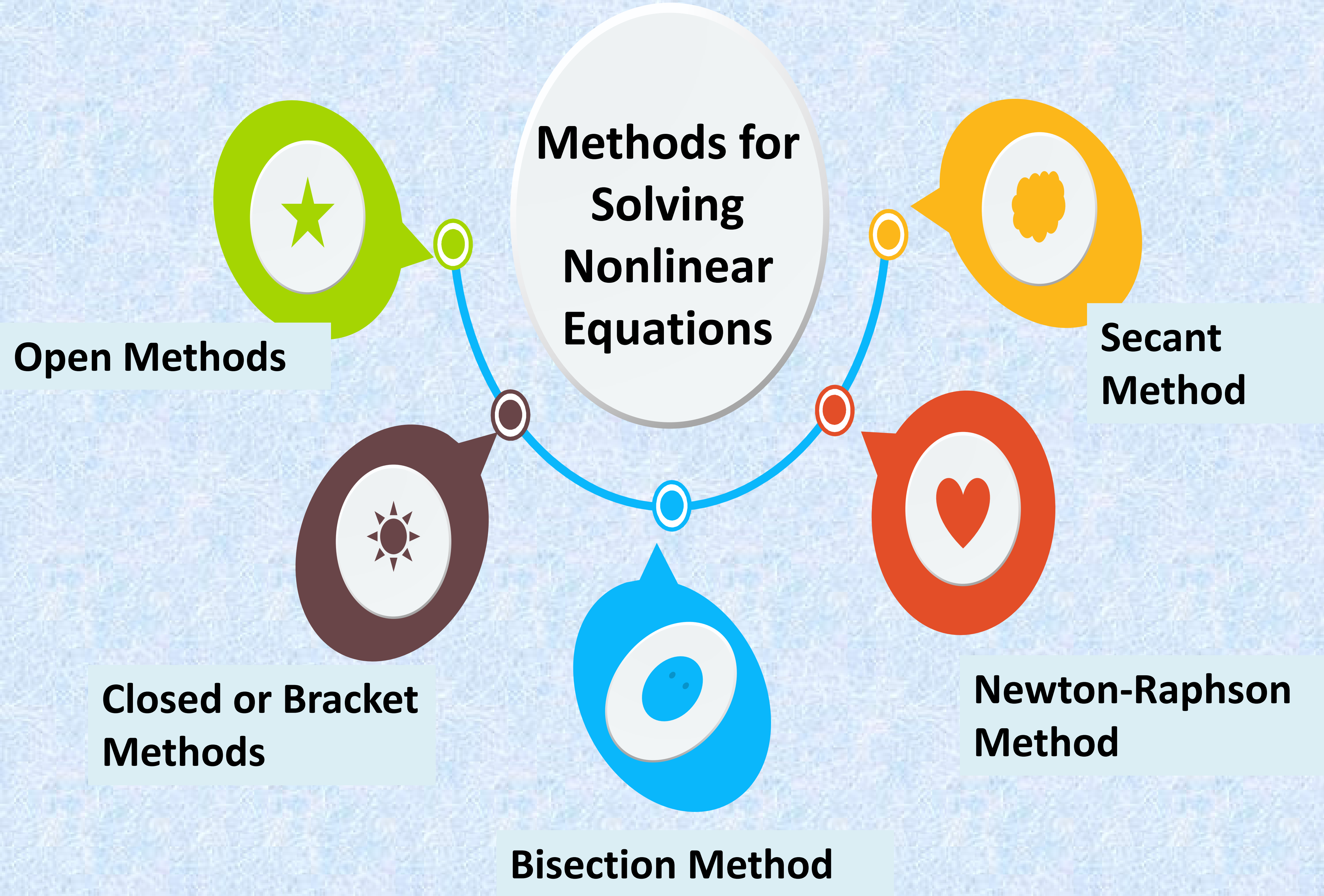
Example (cont'd): Analytical Vs. Numerical

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



x	y
1.4	-0.24
1.42	-0.2436
1.44	-0.2464
1.46	-0.2484
1.48	-0.2496
1.5	-0.25
1.52	-0.2496
1.54	-0.2484
1.56	-0.2464
1.58	-0.2436
1.6	-0.24

y_{min}


Methods for Solving Nonlinear Equations
Open Methods
Closed or Bracket Methods
Bisection Method
Newton-Raphson Method
Secant Method

Solution of Systems of Linear Equations

$$x_1 + x_2 = 3$$
$$x_1 + 2x_2 = 5$$

$$\begin{bmatrix} 1 & 1 \\ 1 & 2 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} = \begin{bmatrix} 3 \\ 5 \end{bmatrix}$$

One can solve it as :

$$x_1 = 3 - x_2 , \qquad 3 - x_2 + 2x_2 = 5$$
$$\Rightarrow x_2 = 2,\ x_1 = 3 - 2 = 1$$

$$\begin{Bmatrix} x_1 \\ x_2 \end{Bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

What to do if we have

1000 equations in 1000 unknowns.

Methods for Solving Systems of Linear Equations

$$\left[\begin{array}{ccccc|c} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} & c_1 \\ & a''_{22} & a''_{23} & \cdots & a''_{2n} & c''_2 \\ & & a'''_{33} & \cdots & a'''_{3n} & c'''_3 \\ & & & & & \vdots \\ & & & & a_{nn}^{\text{n dashes}} & c_n \end{array}\right]$$

$$x_1^{(k+1)} = \frac{1}{a_{11}}\left[b_1 - a_{12}x_2^{(k)} - a_{13}x_3^{(k)} - \dots - a_{1n}x_n^{(k)}\right]$$

$$x_2^{(k+1)} = \frac{1}{a_{22}}\left[b_2 - a_{21}x_1^{(k+1)} - a_{23}x_3^{(k)} - \dots - a_{2n}x_n^{(k)}\right]$$

$$x_3^{(k+1)} = \frac{1}{a_{33}}\left[b_3 - a_{31}x_1^{(k+1)} - a_{32}x_2^{(k+1)} - \dots - a_{3n}x_n^{(k)}\right]$$

$$\vdots$$

$$x_n^{(k+1)} = \frac{1}{a_{nn}}\left[b_n - a_{n1}x_1^{(k+1)} - a_{n2}x_2^{(k+1)} - \dots - a_{n,n-1}x_{n-1}^{(k)}\right]$$

$$\begin{bmatrix} f_1 & g_1 & & & & & \\ e_2 & f_2 & g_2 & & & & \\ & e_3 & f_3 & g_3 & & & \\ & & \cdot & \cdot & \cdot & & \\ & & & \cdot & \cdot & \cdot & \\ & & & & \cdot & \cdot & \cdot \\ & & & & e_{n-1} & f_{n-1} & g_{n-1} \\ & & & & & e_n & f_n \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \\ \cdot \\ \cdot \\ \cdot \\ x_{n-1} \\ x_n \end{Bmatrix} = \begin{Bmatrix} r_1 \\ r_2 \\ r_3 \\ \cdot \\ \cdot \\ \cdot \\ r_{n-1} \\ r_n \end{Bmatrix}$$

Naive Gaussian Elimination

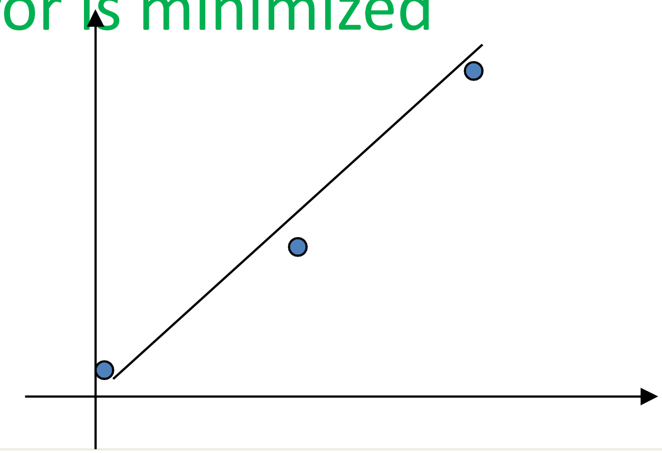
Gaussian Seidel

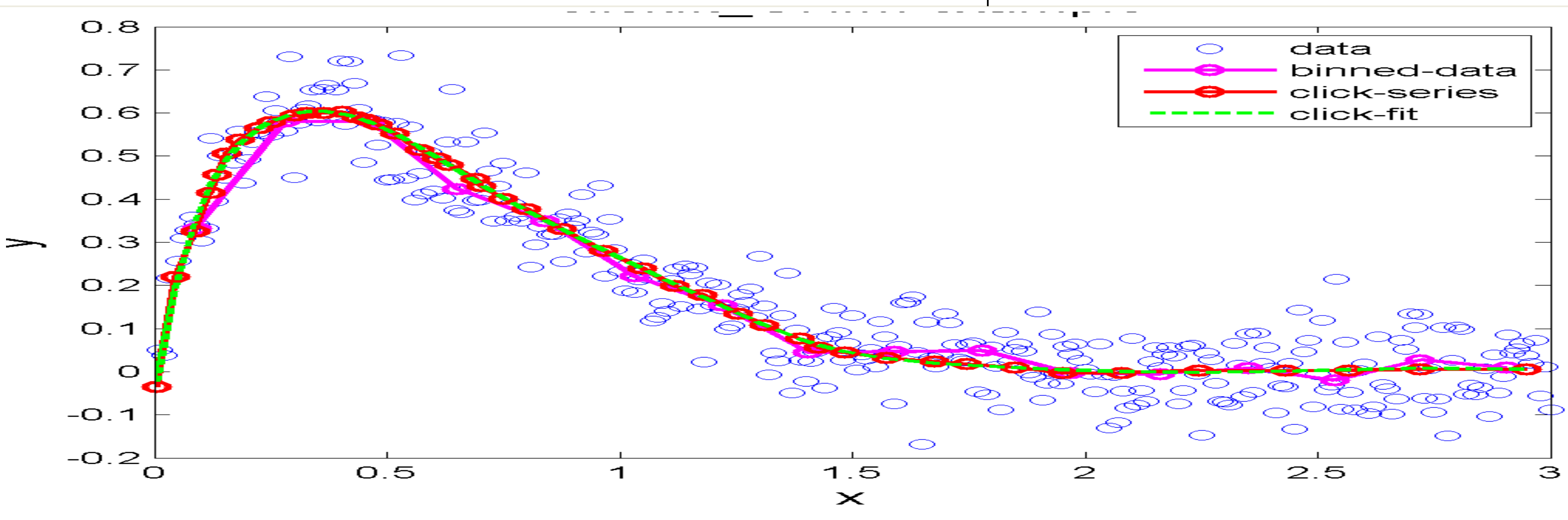
Algorithm for Tri-diagonal Equations

Curve Fitting

- Given a set of data:
- 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

x	0	1	2
y	0.5	10.3	21.3

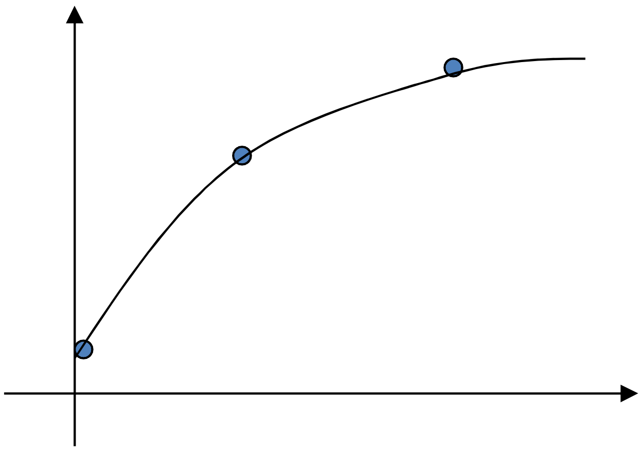




Interpolation

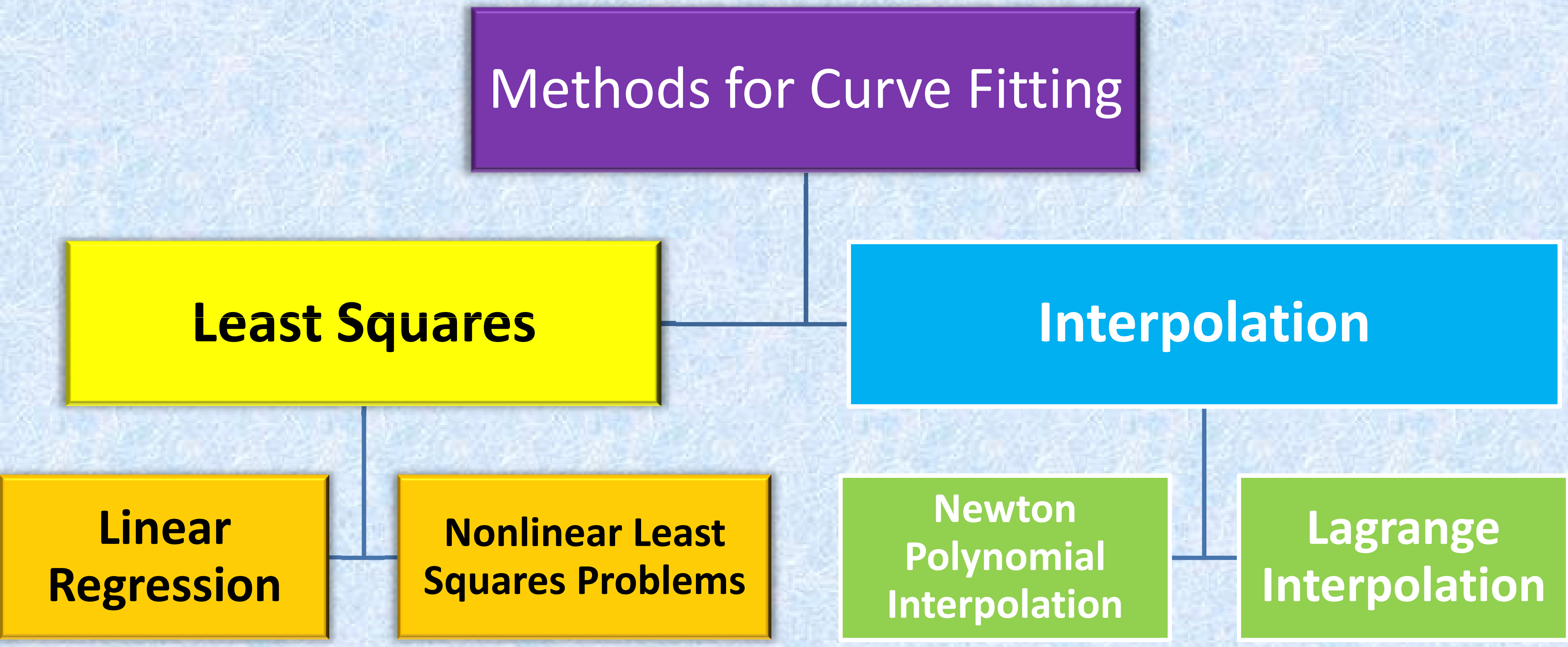
- Given a set of data:

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
Interpolation
Linear Regression
Nonlinear Least Squares Problems
Newton Polynomial Interpolation
Lagrange Interpolation

Integration

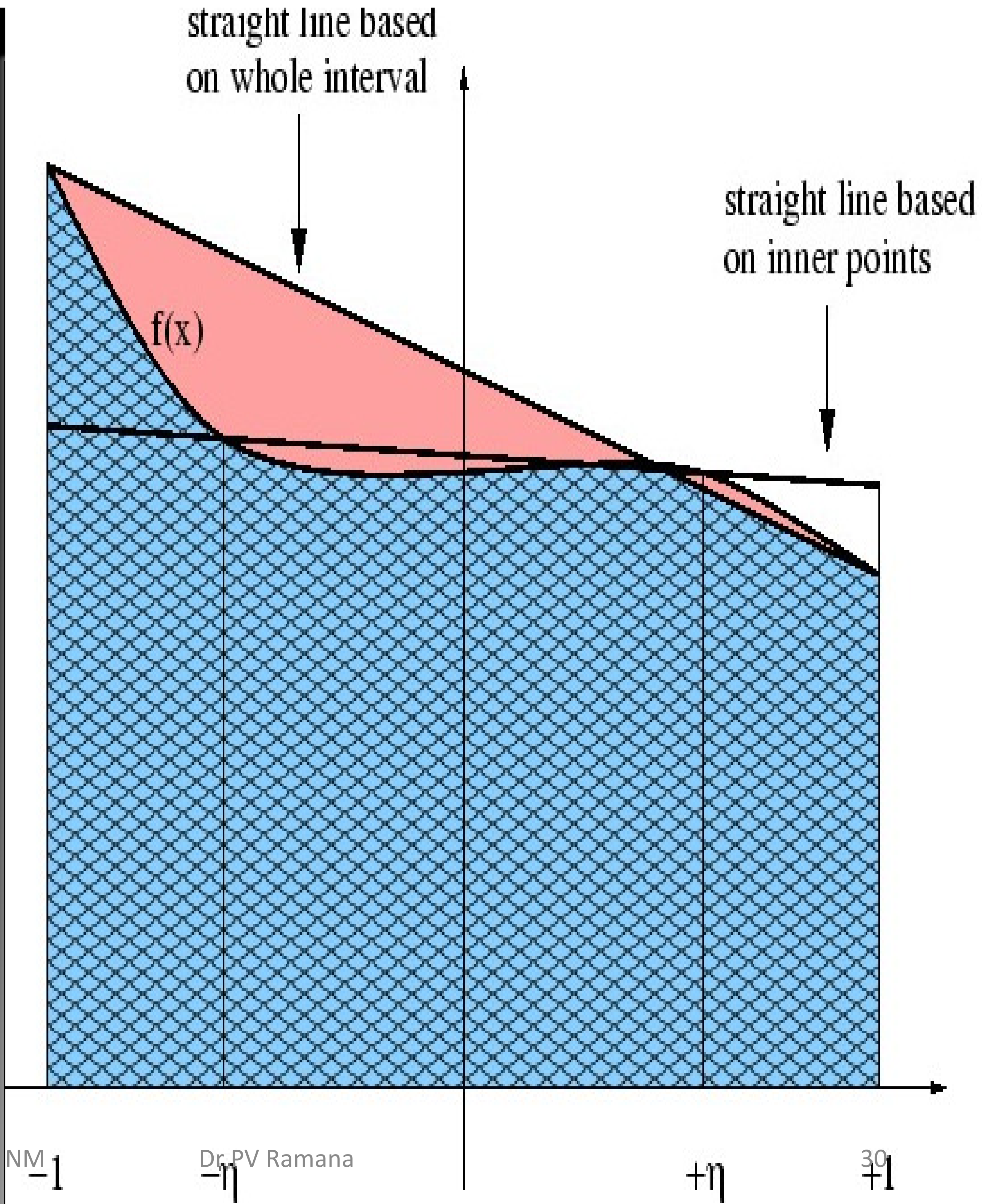
$$\int_1^3 x\,dx = \frac{1}{2}x^2\Big|_1^3 = \frac{9}{2} - \frac{1}{2} = 4$$

But many functions have no analytical solutions :

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

Methods for Numerical Integration

- ✓ **Gauss Quadrature**
- ✓ **Trapezoid Method**
- ✓ **Romberg Method**



Differentiation

$f(x) = x^3$ $(\therefore f'(x) = 3x^2$ $f'(1) = 3)$

f(x) = $-0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$

f'(x) = $-0.4x^3 - 0.45x^2 - 1.0x - 0.25$

But many functions have no analytical solutions :

$$f(x) = \frac{\left(\cos(100x^2)\right)^5}{x^3}$$

Solution of Ordinary Differential Equations

A solution to the differential equation:

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

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

$$\frac{2}{\sqrt{3}} e^{3t/2} \sin\left(\sqrt{3}t \big/ 2 \right)$$

Non linear ODE:

$$\ddot{x}(t) + 3\dot{x}(t) + 3x^2(t) = 0;\ \dot{x}(0) = 1;\ x(0) = 0$$

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:

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

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

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

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

Representing Real Numbers, Precision & Accuracy

- The decimal system as

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

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

- Standard Representations:

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

Normalized Floating Point Representation

- Normalized Floating Point Representation:

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

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 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}

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

sign mantissa exponent

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

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

Remarks

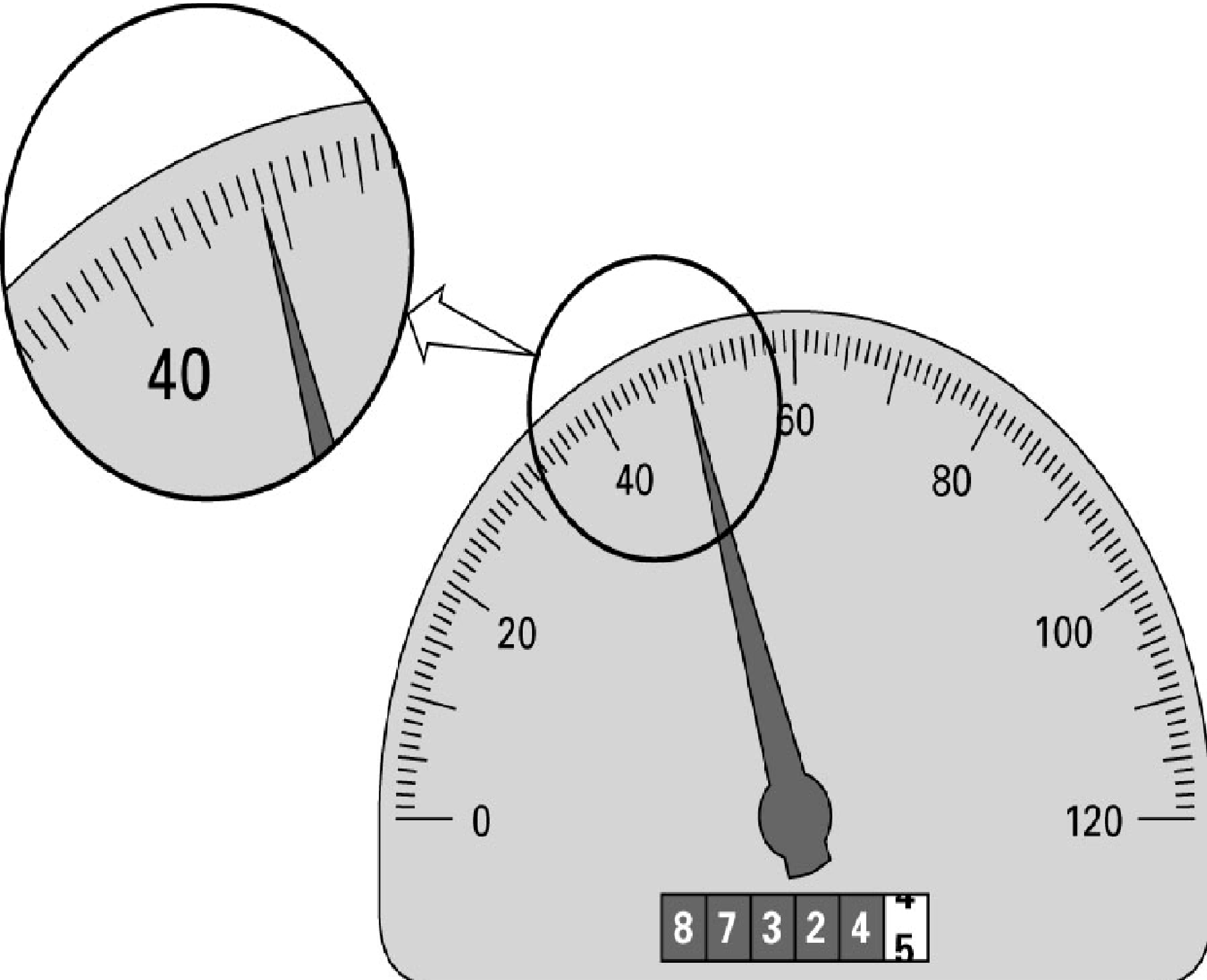
- Numbers that can be exactly represented are called machine numbers.

- 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.



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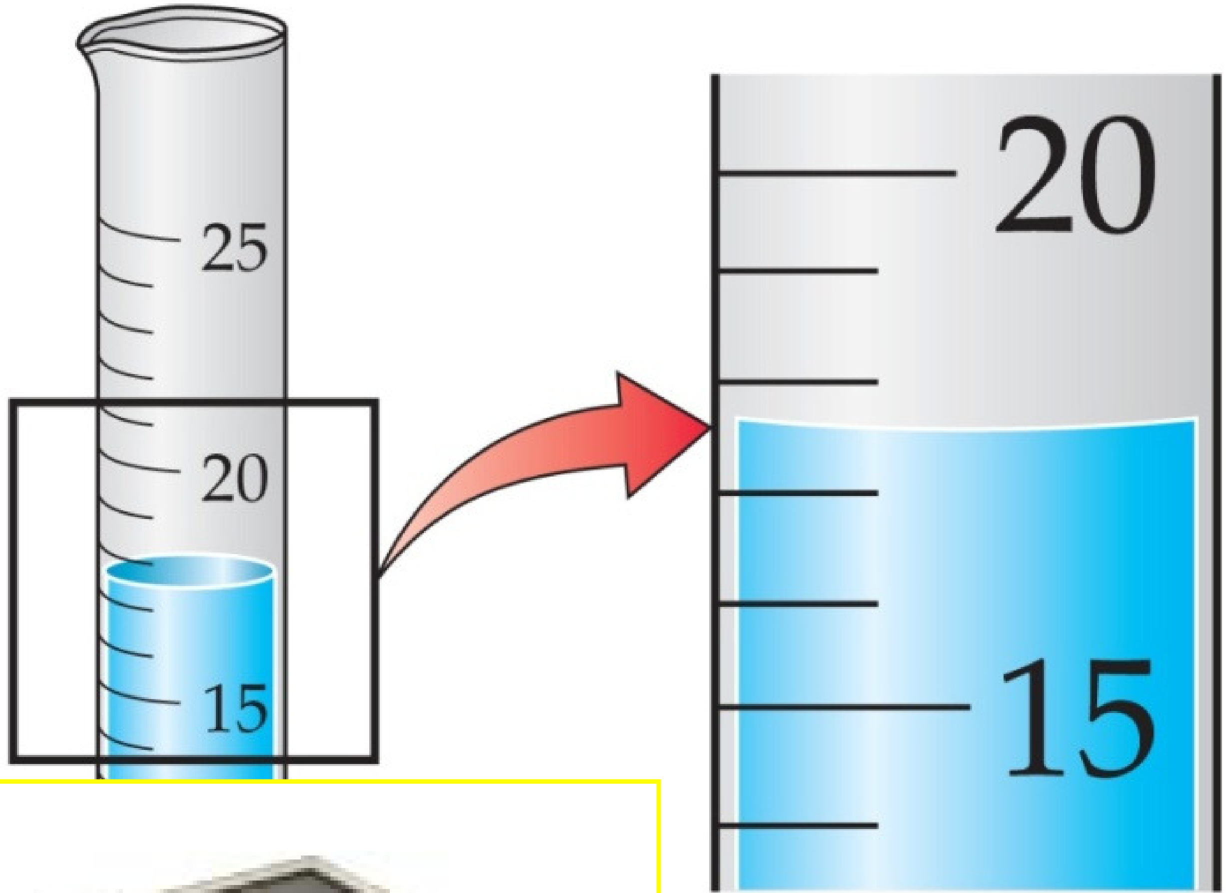

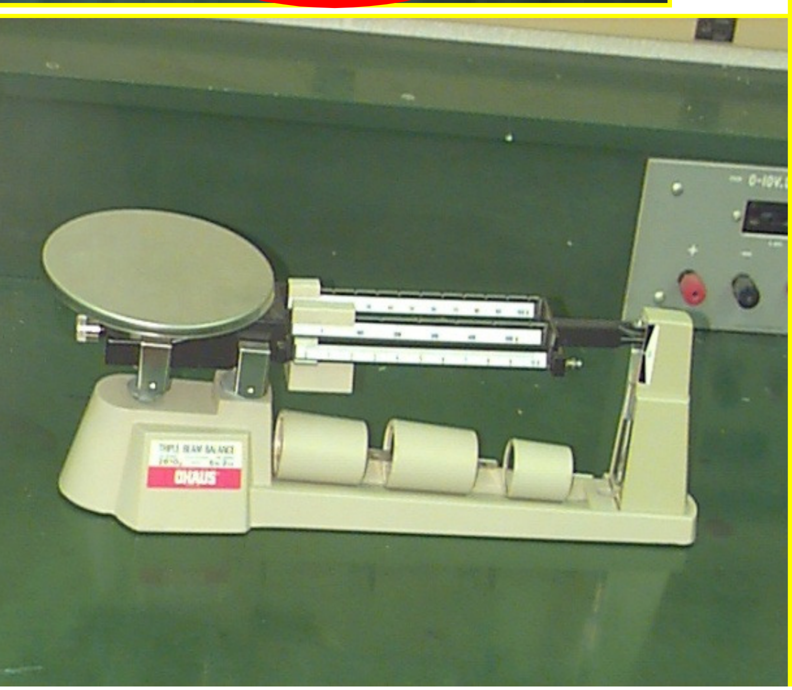

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Accuracy and Precision

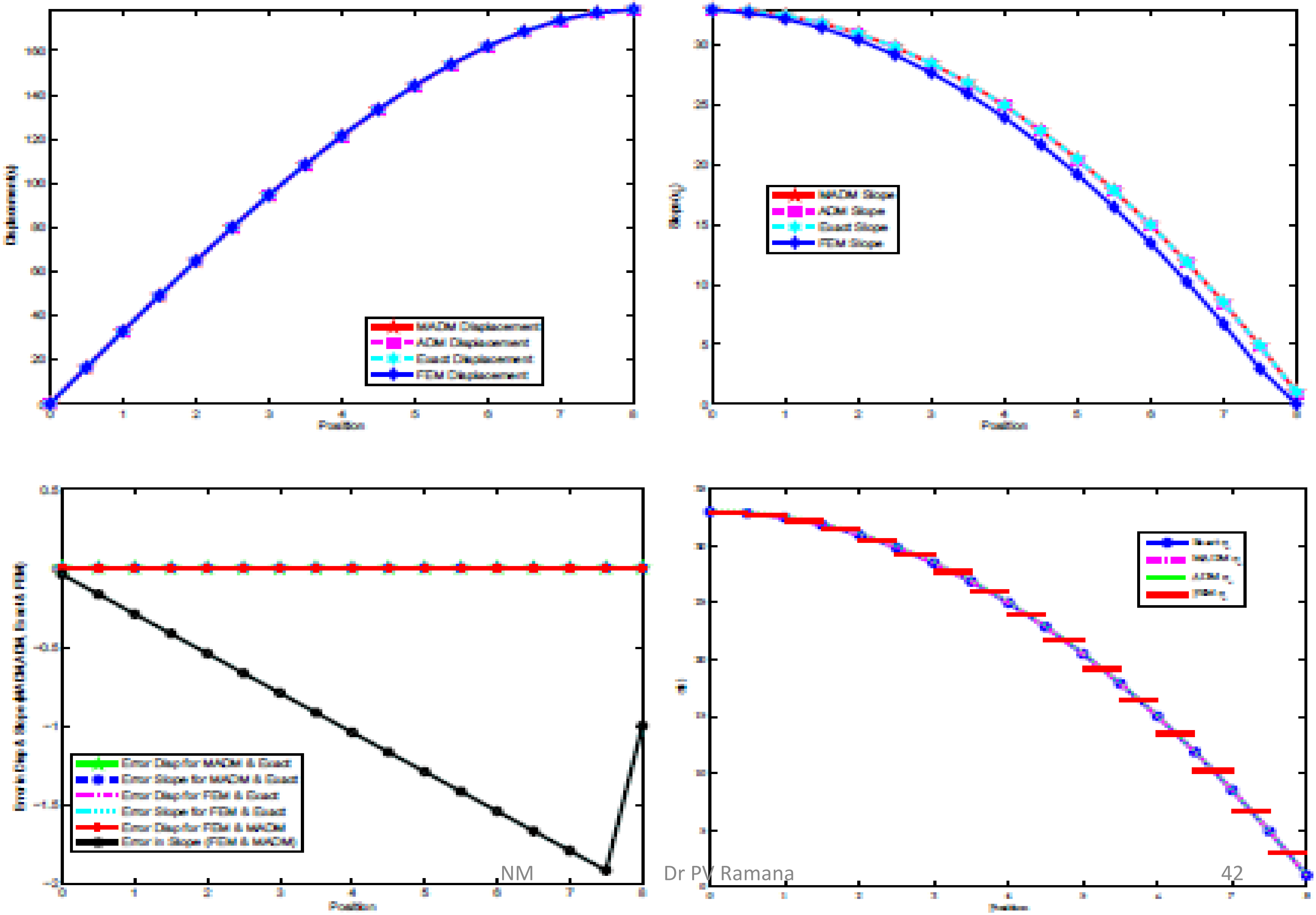
Accuracy is related to the closeness to the true value.

Accuracy and Precision: **Accuracy** refers to the closeness of a measured value to a standard or known value. For example, if in lab you obtain a weight measurement of 8.2 kg for a given substance, but the actual or known weight is 10 kg, then your measurement is not **accurate**.

Precision is related to the closeness to other estimated values.

Precision is a description of *random errors*, a measure of statistical variability.
Accuracy is a description of *systematic errors*, a measure of statistical bias;

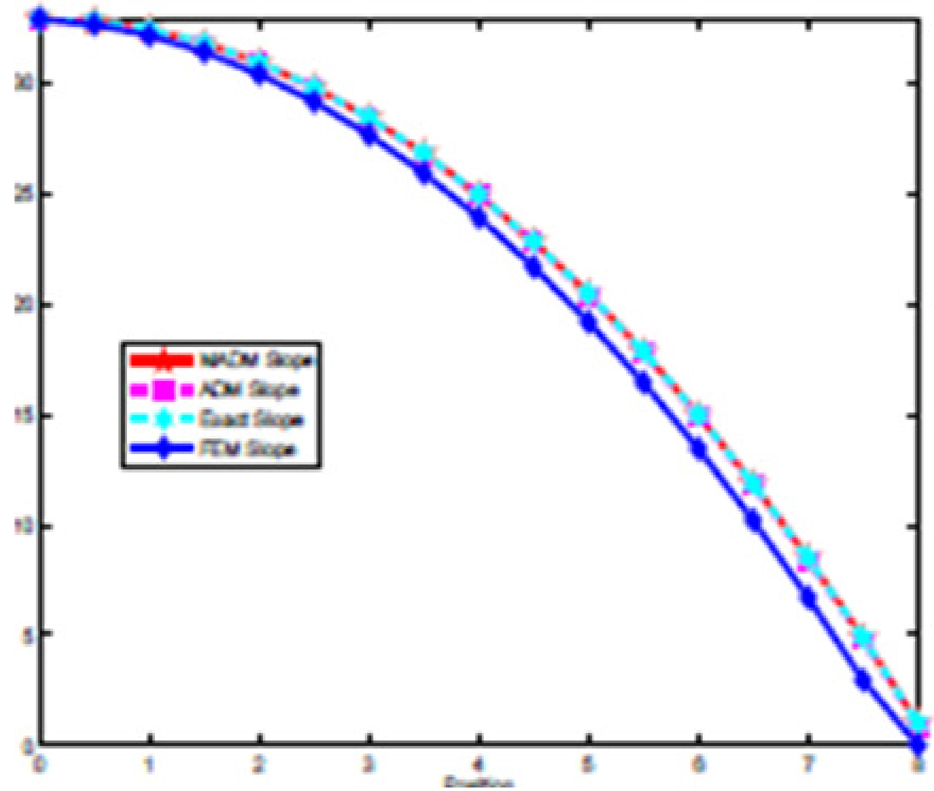
Errors in Round off & Truncation



Absolute or True Error:

True Fractional Relative Error:

True Percent Relative Error:



E_t = True value – Approximation value

$$\epsilon_t = \frac{\text{True value} - \text{Approximate value}}{\text{True value}}$$

$$\epsilon_t = \frac{\text{True value} - \text{Approximate value}}{\text{True value}} * 100\%$$

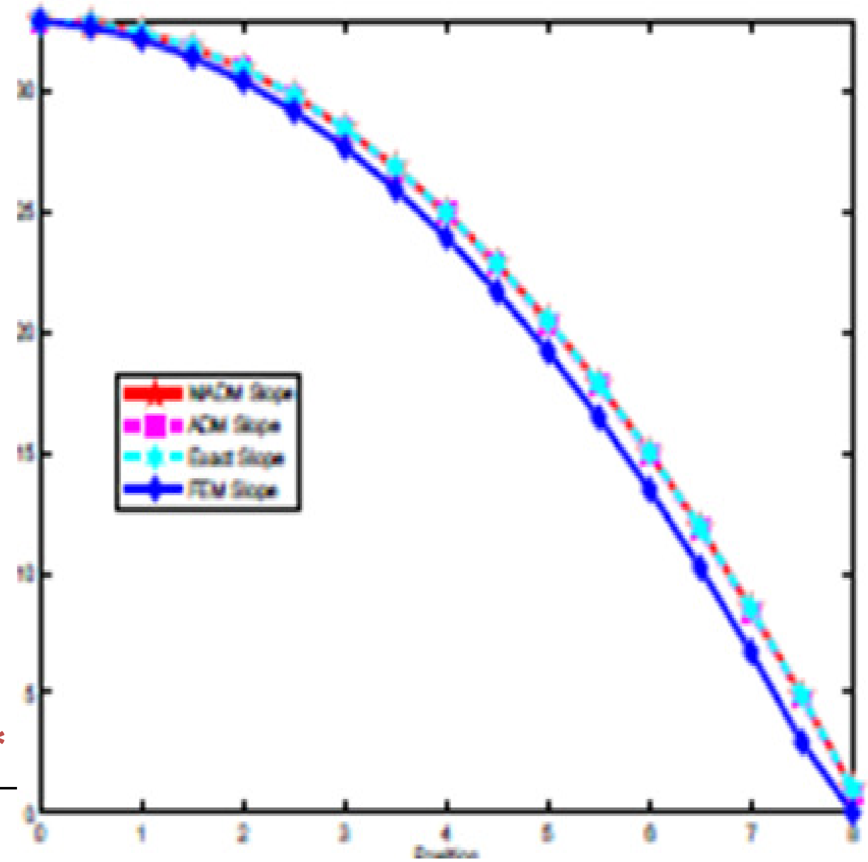
When true value is not known

- *Approximate relative error:*

$$\epsilon_a = \frac{\text{approximate error} * 100\%}{\text{approximation}}$$

- Numerical methods using *iteration*

$$\epsilon_a = \frac{(\text{present approximate} - \text{previous approximate})*}{\text{present approximation}}$$

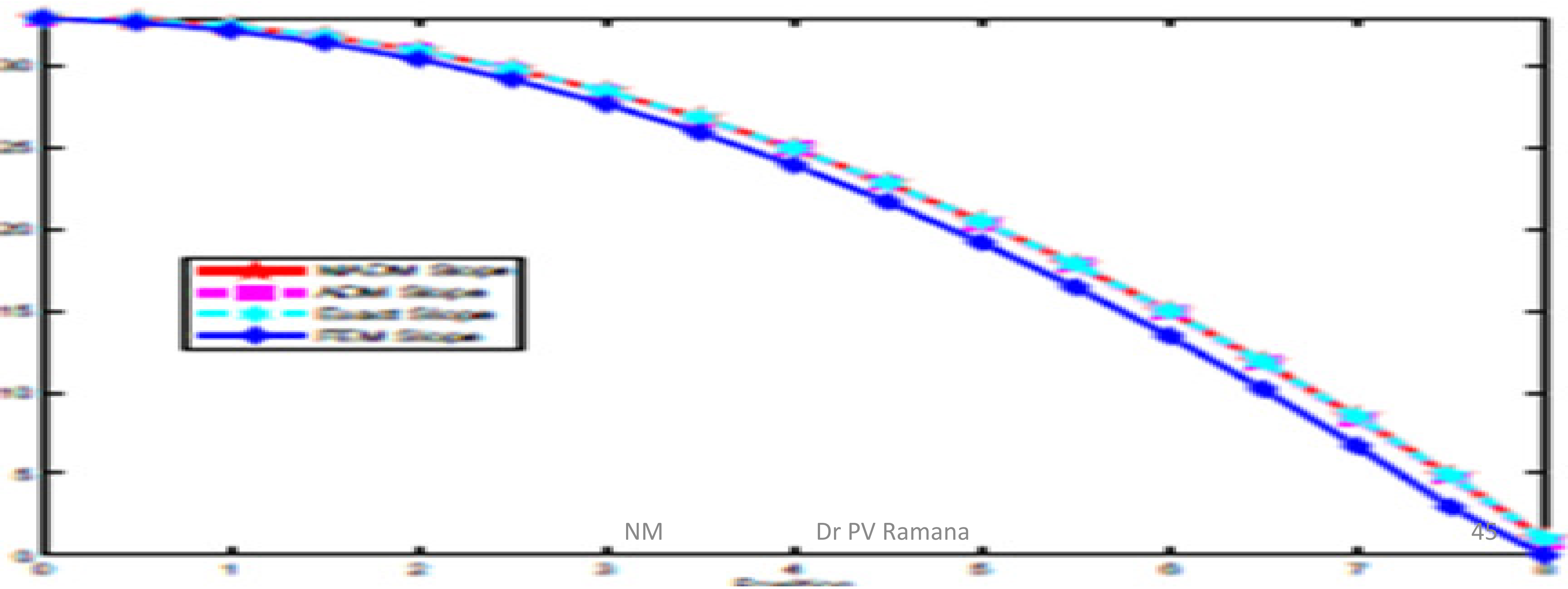


- Stopping criterion: Relative error is less than some tolerance value

- *Accuracy of result up to n significant digits*

  $\epsilon_s = (0.5 \times 10^{2-n})\ \%$

- **When $|\epsilon_a| < \epsilon_s$ then the result is correct up to n significant digits**



Error Estimation

01

Errors **are mainly associated with calculations and measurements**

02

***Accuracy*: How closely a computed value or measured value agrees with true value**

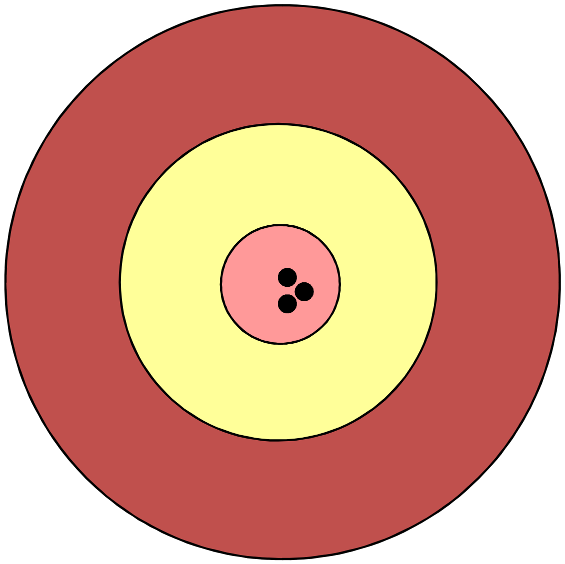
03

***Precision:* How individual computed values or measured values agree with one another**

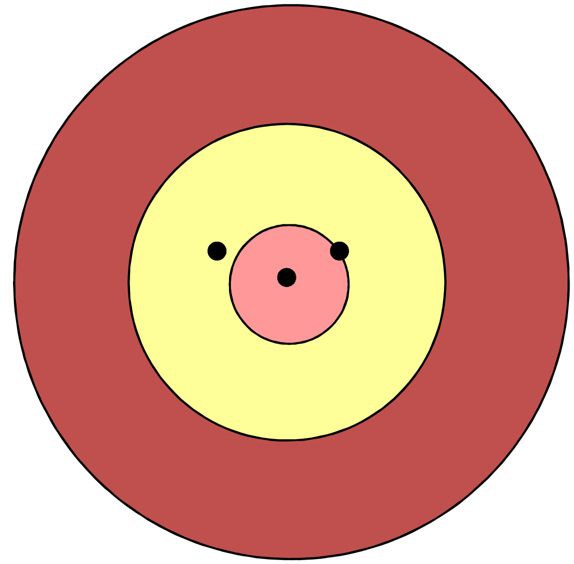
04

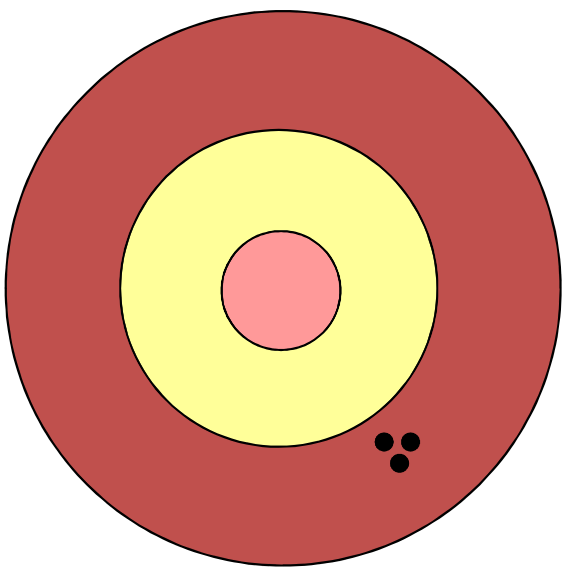
- **Inaccuracy is also called *bias***
- **Imprecision is also called *uncertainty***

Accuracy & Precision

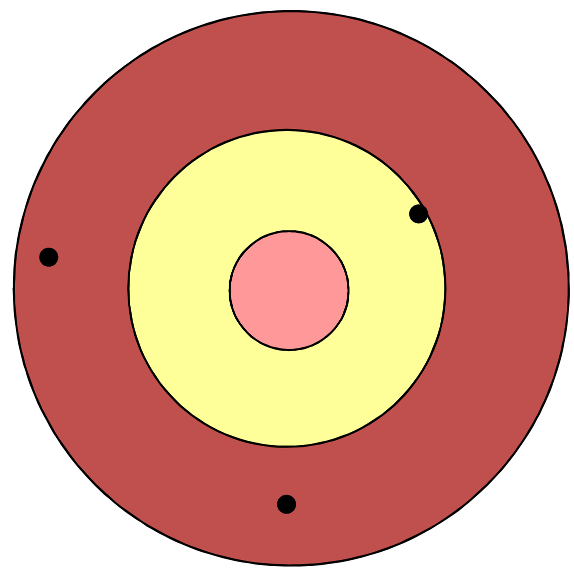


Accuracy without Precision

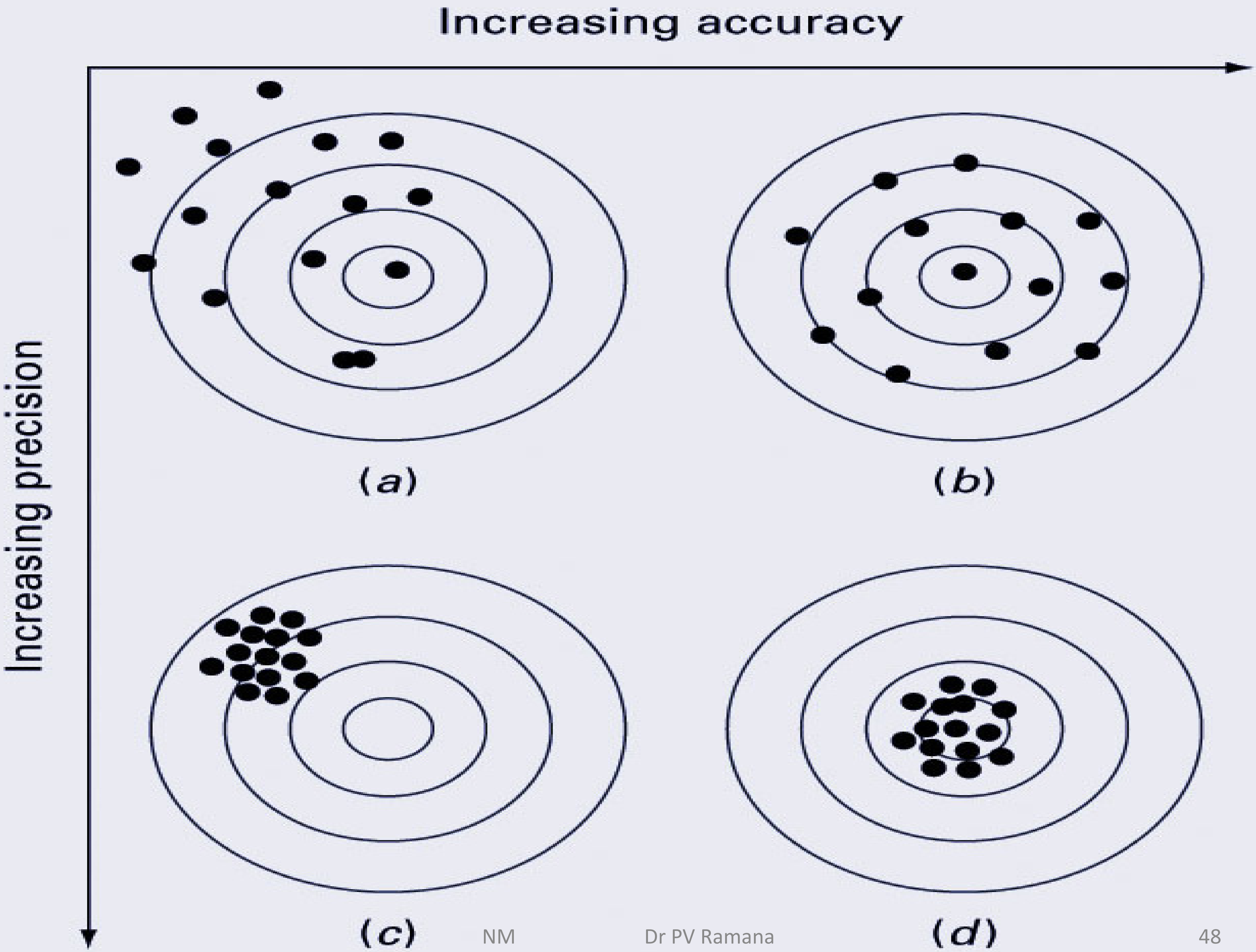




Precision without Accuracy



No Precision & No Accuracy


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

Types of Errors

- **Round-off errors:** 10/3, π, $7^{1/2}$, e, etc. cannot be represented exactly
- **Truncation errors:** These errors are related to Taylor series
- **Blunders:** Due to human errors and machine imperfections
- **Formulation errors**
- **Errors due to assumptions and data uncertainty**

ROUND OFF ERRORS

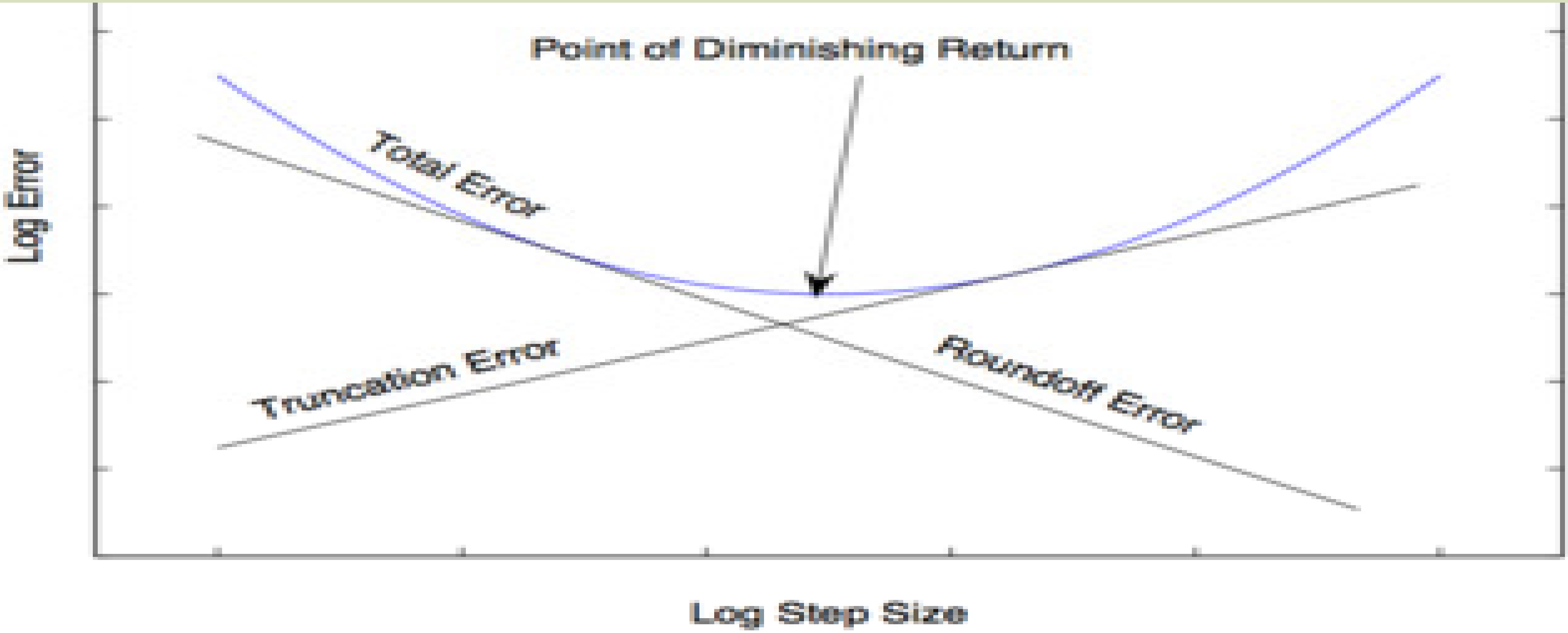
Size and Precision limitations

- Integer representation
- Floating point representation
- Machine epsilon (machine precision)

Numerical manipulations are sensitive to round off errors

- Subtractive cancellation
- Large computations

TRUNCTION ERRORS

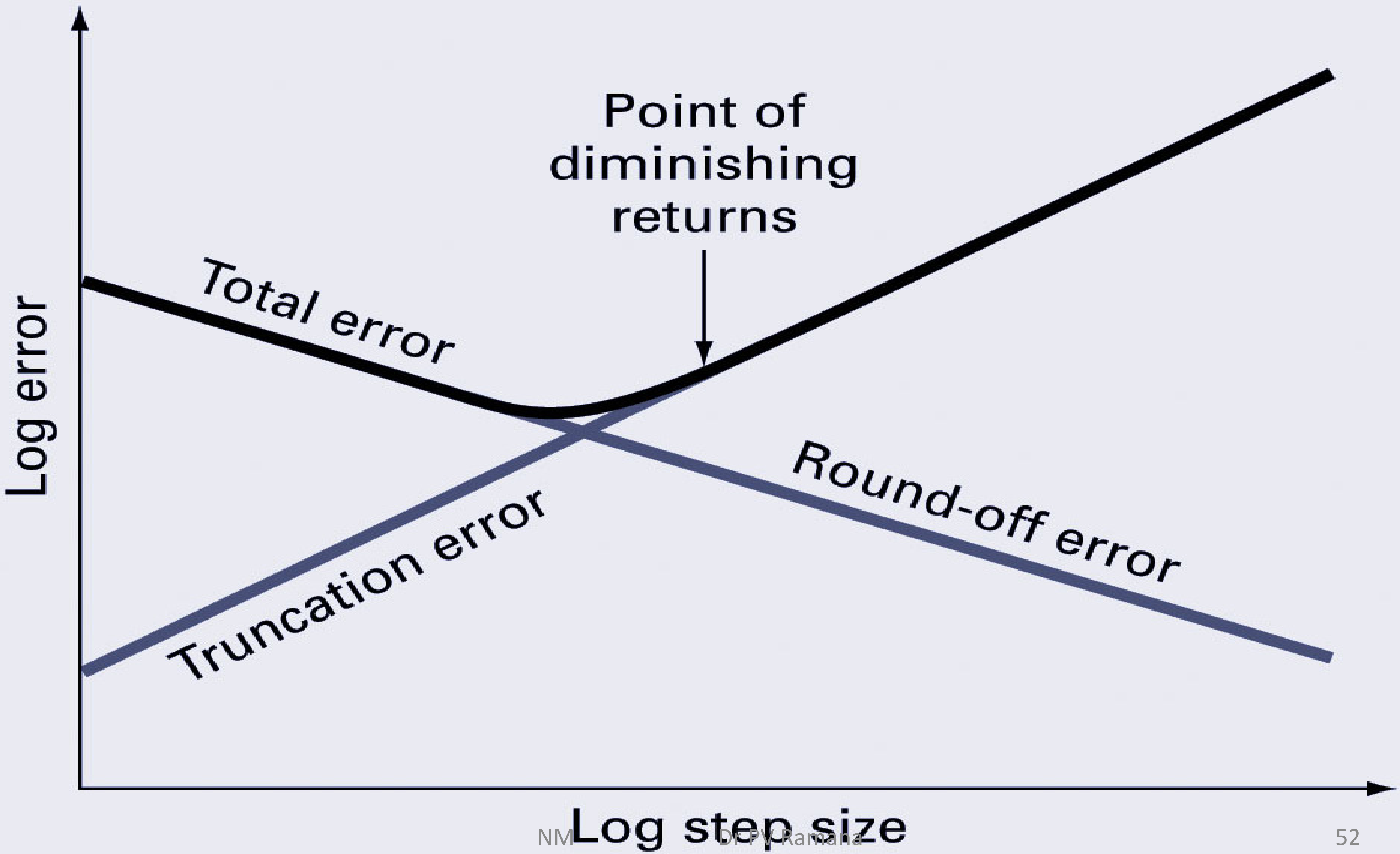


Result of using an approximation instead of exact mathematical procedure

- Using Taylor series to approximate a polynomial function

TOTAL NUMERICAL ERROR

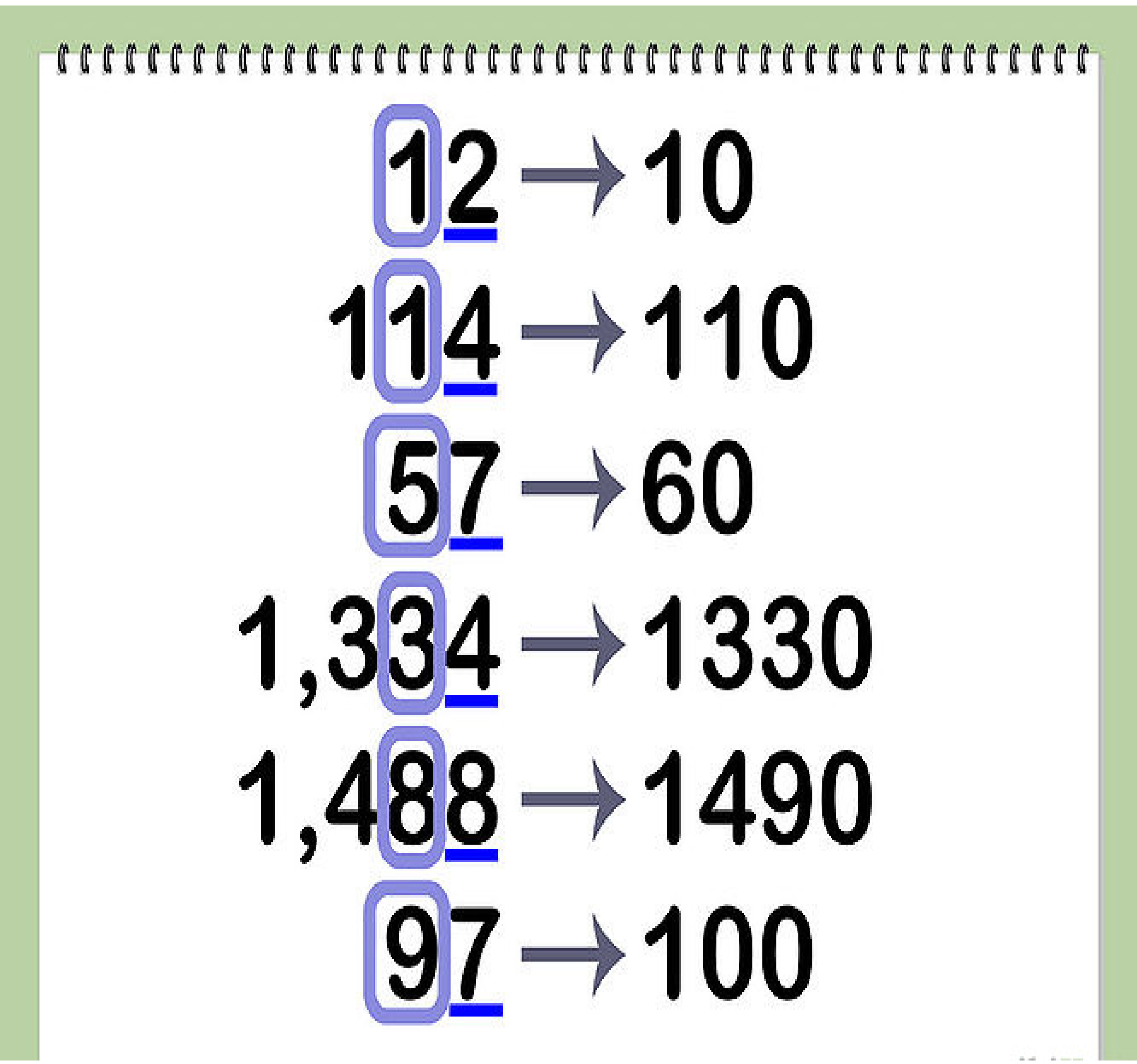
- Summation of truncation and roundoff errors



Rounding and Chopping

- Rounding: Replace the number by the nearest machine number.

- Chopping: Throw all extra digits.



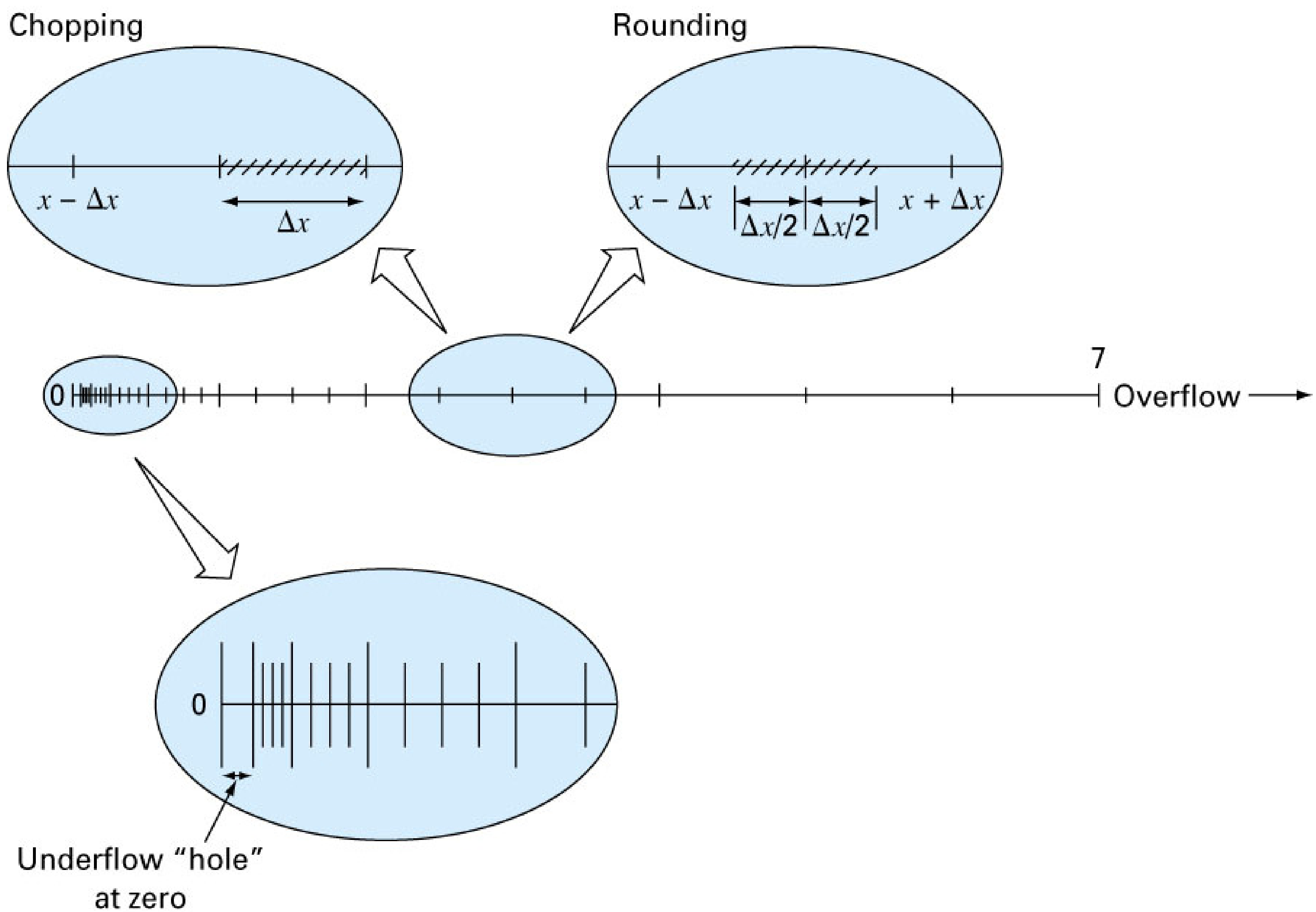
$$x = 72.32451 = 0.7232451 \times 10^2$$

$$= (0.7232 + 0.0000451) \times 10^2$$

$$= (0.7232 + 0.451 \times 10^{-4}) \times 10^2$$

$\therefore$ chopping error in representing $x = 0.451 \times 10^{2-4}$.

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

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

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

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

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

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

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

Taylor Theorem
Motivation

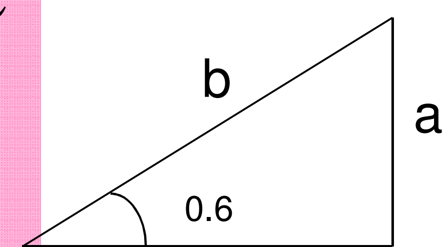
- One can easily compute expressions like:

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

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

One can use the definition to compute $\sin(0.6)$?

is this a practical way?



Taylor Series

n^{th} order Taylor series: $$f(x_{i+1}) \approx f(x_i) + f'(x_i)(x_{i+1} - x_i) + \frac{f''(x_i)}{2!}(x_{i+1} - x_i)^2 + \frac{f'''(x_i)}{3!}(x_{i+1} - x_i)^3$$

$$+ \ldots \frac{f^n(x_i)}{n!}(x_{i+1} - x_i)^n$$

$$f(a) + \frac{f'(a)}{1!}(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \frac{f'''(a)}{3!}(x-a)^3 + \cdots . \qquad \rightleftharpoons \sum_{n=0}^{\infty} \frac{f^{(n)}(a)}{n!}(x-a)^n$$

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(x) + \cdots + \frac{h^{(n-1)}}{(n-1)!} f^{(n-1)}(x) + \frac{h^n}{n!} f^n(x + \lambda h).$$

Zero order Taylor series: $$\boxed{f(x_{i+1}) \approx f(x_i)}$$

1^{st} order Taylor series: $$f(x_{i+1}) \approx f(x_i) + f'(x_i)(x_{i+1} - x_i)$$

2^{nd} order Taylor series: $$f(x_{i+1}) \approx f(x_i) + f'(x_i)(x_{i+1} - x_i) + \frac{f''(x_i)}{2!}(x_{i+1} - x_i)^2$$

$$e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!} = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots \quad \text{for all } x$$

$$\log(1 - x) = -\sum_{n=1}^{\infty} \frac{x^n}{n} \quad \text{for } -1 \le x < 1$$

$$\log(1 + x) = \sum_{n=1}^{\infty} (-1)^{n+1} \frac{x^n}{n} \quad \text{for } -1 < x \le 1$$

$$\frac{1 - x^{m+1}}{1 - x} = \sum_{n=0}^{m} x^n \quad \text{for } x \ne 1 \text{ and } m \in \mathbb{N}_0$$

$$\frac{1}{1 - x} = \sum_{n=0}^{\infty} x^n \quad \text{for } |x| < 1$$

$$\sin x = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!} x^{2n+1} = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \cdots \quad \text{for all } x$$

$$\cos x = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} x^{2n} = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \cdots \quad \text{for all } x$$

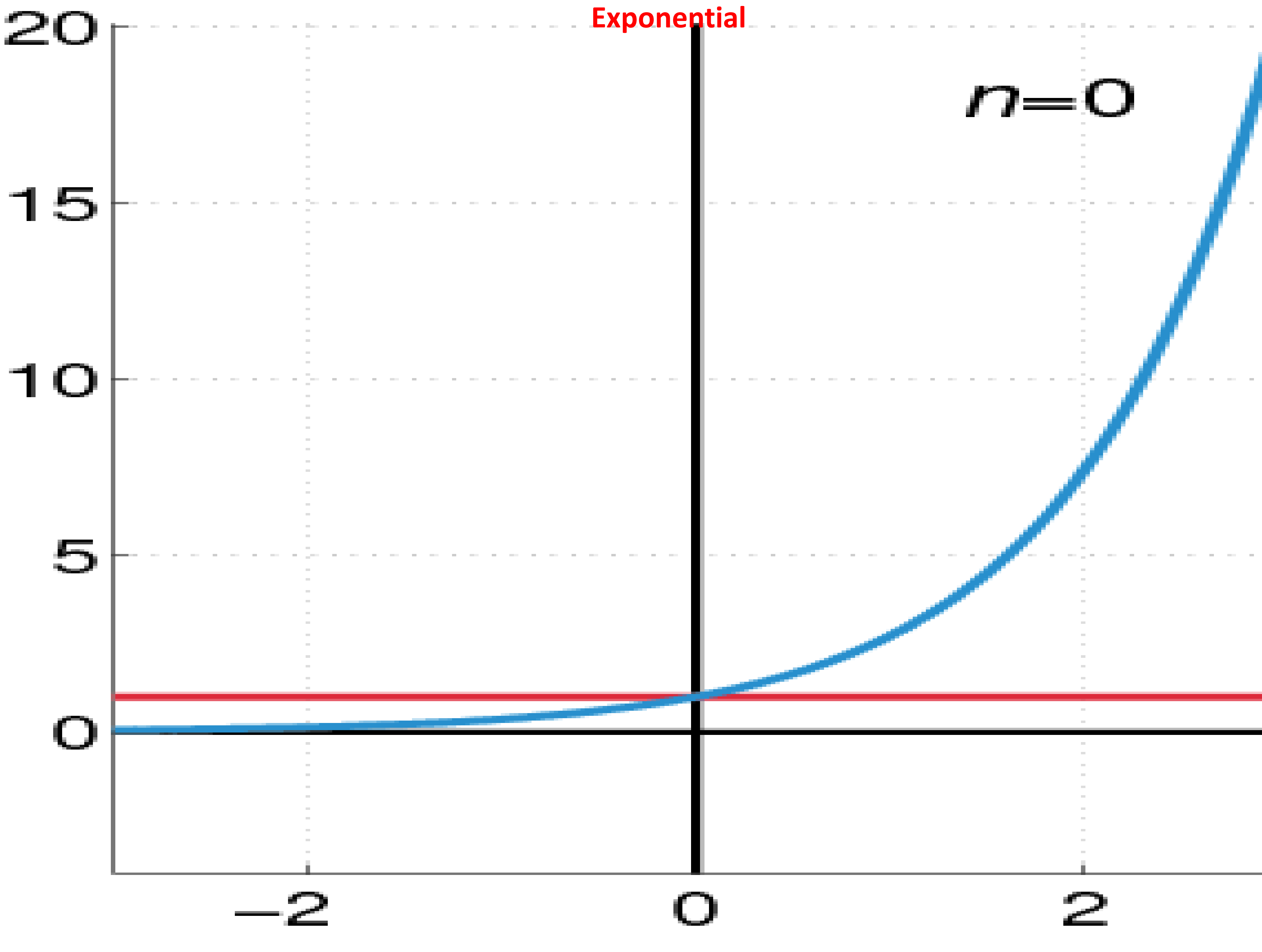
$$\tan x = \sum_{n=1}^{\infty} \frac{B_{2n}(-4)^n(1-4^n)}{(2n)!} x^{2n-1} = x + \frac{x^3}{3} + \frac{2x^5}{15} + \cdots \quad \text{for } |x| < \frac{\pi}{2}$$

$$\sec x = \sum_{n=0}^{\infty} \frac{(-1)^n E_{2n}}{(2n)!} x^{2n} \quad \text{for } |x| < \frac{\pi}{2}$$

$$\arcsin x = \sum_{n=0}^{\infty} \frac{(2n)!}{4^n (n!)^2 (2n+1)} x^{2n+1} \quad \text{for } |x| \le 1$$

$$\arccos x = \frac{\pi}{2} - \arcsin x = \frac{\pi}{2} - \sum_{n=0}^{\infty} \frac{(2n)!}{4^n (n!)^2 (2n+1)} x^{2n+1} \quad \text{for } |x| \le 1$$

$$\arctan x = \sum_{n=0}^{\infty} \frac{(-1)^n}{2n+1} x^{2n+1} \quad \text{for } |x| < 1$$



Exponential
n=0
20
15
10
5
0
−2
0
2

Taylor Series

$$f(x) = c_0 + c_1 x + c_2 x^2 + c_3 x^3 + c_4 x^4 + \cdots,$$

$$f(x) = 3 + 5x + 7x^2 + 9x^3 + 11x^4 + \cdots,$$

$$f(0) = 3 + 0 + 0 + 0 + 0 + \cdots = 3.$$

$$f'(x) = 5 + 14x + 27x^2 + 44x^3 + \cdots,$$

$$\begin{array}{lcccccccc} f(x) = & 3 & + & 5x & + & 7x^2 & + & 9x^3 & + \cdots \\ & & & \downarrow & & \downarrow & & \downarrow & \cdots \\ f'(x) = & & & 5 & + & 14x & + & 27x^2 & + \cdots \end{array}$$