MTS2A1
Komputer & Simulasi

Model Matematik (Analitis)

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Model Matematik (Mathematical Model)

Mathematical model: a formulation that expresses the essential features of a physical system or process in mathematical terms.

Dependent variable = *f* (independent variables, parameters)

Dependent variable = a characteristic that reflects the behavior or state of the system.

Independent variables = dimensions, such as time and space, along which the system's behaviour is being determined.

Parameters = the system's properties or composition.

The actual mathematical expression of the mathematical model can range from a **simple algebraic relationship** to large complicated sets of **differential equations.**

Contoh Model Matematik

Ideal Gas Law

$$pV = nRT$$

where

p is pressure

V is volume

n is the number of moles

R is the universal gas constant

T is temperature (K)

Schrodinger Equation (Quantum Physics)

Time-independent Schrödinger equation (*single non-relativistic particle*)

$$E\Psi(\mathbf{r}) = \left[\frac{-\hbar^2}{2\mu}\nabla^2 + V(\mathbf{r})\right]\Psi(\mathbf{r})$$

where i = imaginary unit, ħ=the Planck constant divided by 2π, ∂/∂t = partial derivative with respect to time t, Ψ =the wave function of the quantum system, and Ĥ = Hamiltonian operator (which characterizes the total energy of any given wave function and takes different forms depending on the situation).

Maxwell Equation (Thermodynamics)

$$dU = TdS - PdV \implies \left(\frac{\partial T}{\partial V}\right)_S = -\left(\frac{\partial P}{\partial S}\right)_V$$

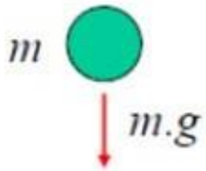
$$dA = -SdT - PdV \implies \left(\frac{\partial S}{\partial V}\right)_T = \left(\frac{\partial P}{\partial T}\right)_V$$

$$dH = TdS + VdP \implies \left(\frac{\partial T}{\partial P}\right)_S = \left(\frac{\partial V}{\partial S}\right)_P$$

$$dG = -SdT + VdP \implies -\left(\frac{\partial S}{\partial P}\right)_T = \left(\frac{\partial V}{\partial T}\right)_P$$

The characteristic functions are: U (internal energy), A (Helmholtz free energy), H (enthalpy), and G (Gibbs free energy). The thermodynamic parameters are: T (temperature), S (entropy), P (pressure), and V (volume).

Contoh sederhana



The velocity of a free-falling object, neglecting any air friction, is governed by Newton's second law of motion:

v at time *t*?

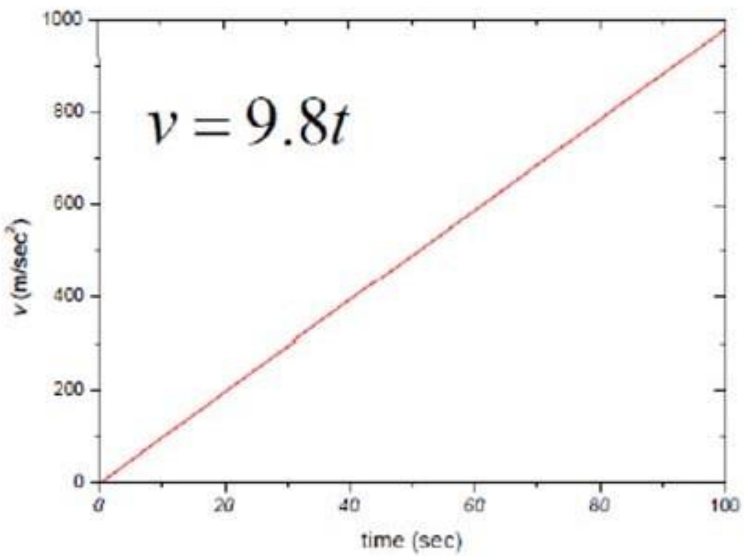
$$F = ma$$

$$mg = m\frac{dv}{dt}$$

$$dv = gdt$$

$$v = \int gdt$$

for v_0 = *0 and g = 9.8 m/sec*^{2}



$$\boxed{v = v_0 + gt}$$ → a simple mathematical model

v = dependent variable
t = independent variable
g, v_o = parameters

Contoh agak rumit

The net force is composed of two opposing forces: the downward pull of gravity F_D and the upward force of air resistance F_U.

$$F_D = mg$$

$$F_U = -cv$$

c = drag coefficient, depending on properties of the falling object

$$F = ma$$

$$mg - cv = m\frac{dv}{dt}$$

v at time t?

$$\frac{dv}{dt} = g - \frac{c}{m}v$$

a differential equation

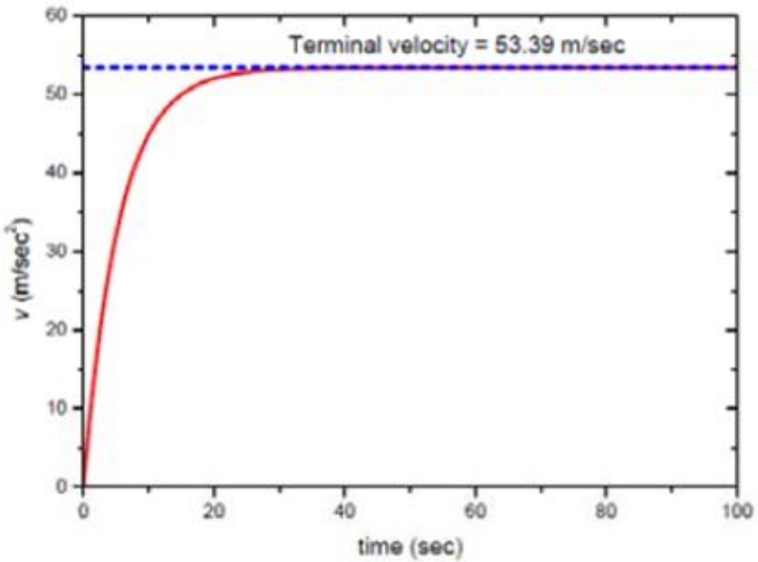
Calculus is required to obtain a closed-form solution of v.

If the parachutist is initially at rest (*v = 0 at t = 0), calculus can be used* to obtained the closed-form solution:

$$v(t) = \frac{gm}{c}(1 - e^{-(c/m)t})$$

t = independent variable
v = dependent variable
g, c, m = parameters

Example: A parachutist of mass 68.1 kg jumps out of a stationary hot air balloon. Compute the velocity if the drag coefficient is 12.5 kg/sec.



$$v(t) = \frac{gm}{c}(1 - e^{-(c/m)t})$$

$$v(t) = \frac{9.8(68.1)}{12.5}(1 - e^{-(12.5/68.1)t})$$

$$v(t) = 53.39(1 - e^{-0.18355t})$$

Metode Numerik

Ada model matematik yang tidak dapat diselesaikan dengan mudah seperti pada ke dua contoh soal yang telah diberikan.

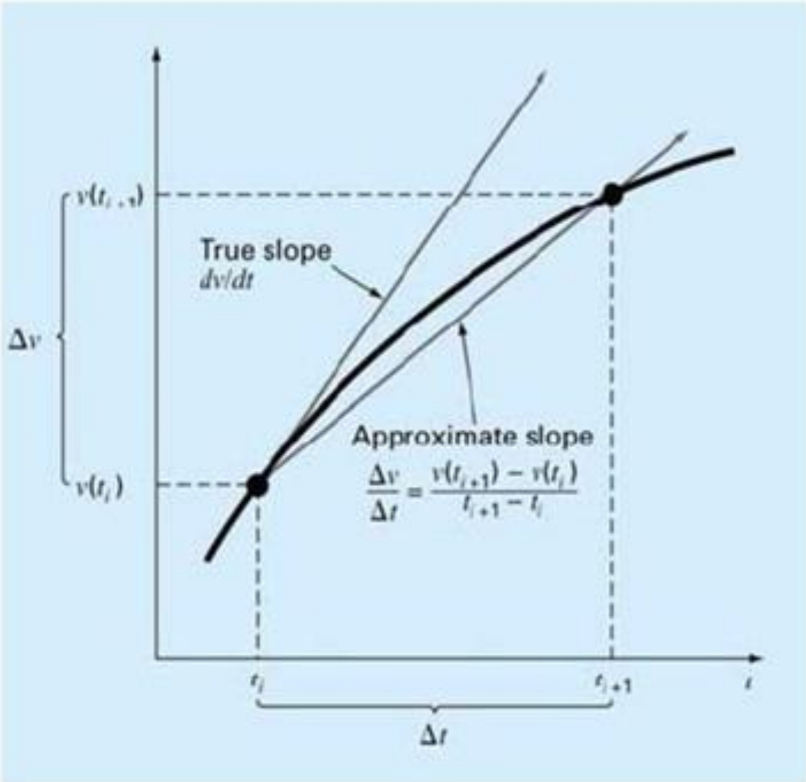
Oleh karena itu perlu untuk mengembangkan solusi numerik yang mendekati solusi analitis (exact)

Metode ini disebut **Metode Numerik** dimana suatu problem matematik di formulasikan sehingga dapat diselesaikan menggunakan operasi aritmetik yati +, - , x dan :

Operasi ini akan menghasilkan numerical error / galat yang disebabkan oleh pendekatan, interval, satuan/dimensi serta desimal yang digunakan.

Oleh karena itu penggunaan satuan dan decimal yang tepat sangat mempengaruhi hasil

Contoh Metode Numerik 1



For example, the time rate of change of velocity can be approximated by:

$$\frac{dv}{dt} \cong \frac{\Delta v}{\Delta t} = \frac{v(t_{i+1}) - v(t_i)}{t_{i+1} - t_i}$$

$$\frac{dv}{dt} = g - \frac{c}{m} v$$

$$\frac{v(t_{i+1}) - v(t_i)}{t_{i+1} - t_i} = g - \frac{c}{m} v(t_i)$$

$$v(t_{i+1}) = v(t_i) + [g - \frac{c}{m} v(t_i)](t_{i+1} - t_i)$$

Contoh 2 Metode Numerik

A parachutist of mass 68.1 kg jumps out of a stationary hot air balloon. Compute the velocity if the drag coefficient is 12.5 kg/sec.

$$v(t_i + 1) = v(t_i) + [g - \frac{c}{m} v(t_i)](t_{i+1} - t_i)$$

$$v(t_i + 1) = v(t_i) + [9.8 - 0.18355 v(t_i)](t_{i+1} - t_i)$$

Initial condition: $t_0 = 0 \rightarrow v_0 = 0$

Take $\Delta t = 2 \sec$

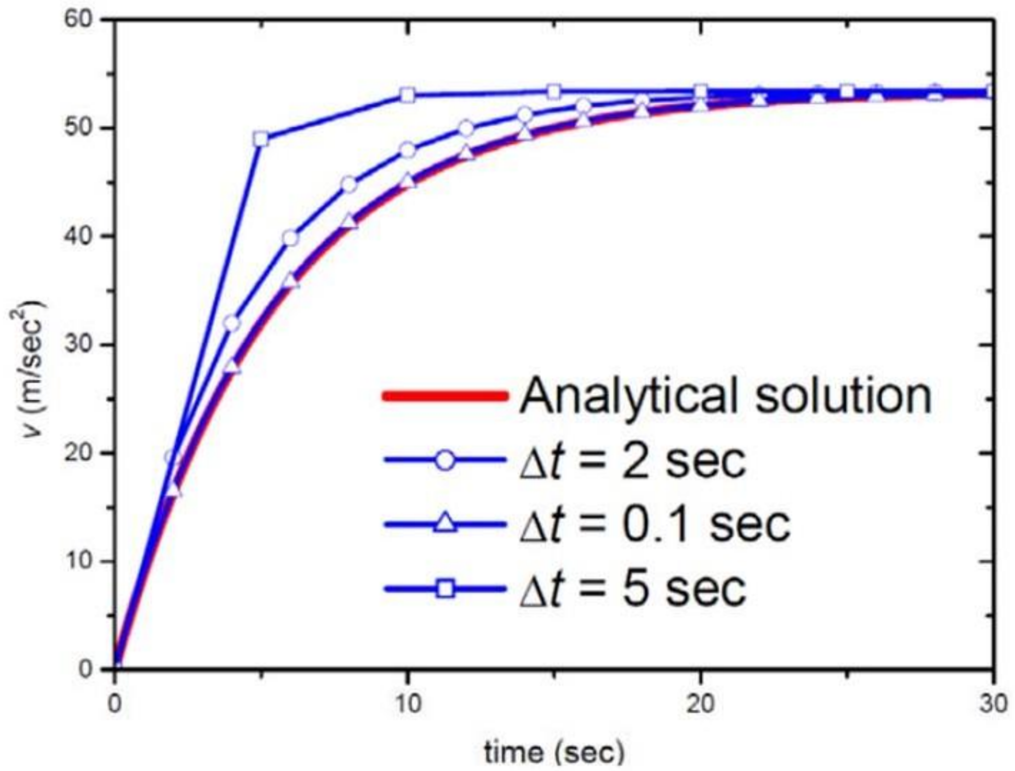
At $t_1 = 2 \sec$

$$v(t_1) = v(t_0) + [9.8 - 0.18355 v(t_0)](t_1 - t_0)$$
$$= 0 + [9.8 - 0.18355(0)](2 - 0) = 19.60 m / \sec$$

At $t_2 = 4 \sec$

$$v(t_2) = v(t_1) + [9.8 - 0.18355 v(t_1)](t_2 - t_1)$$
$$= 19.6 + [9.8 - 0.18355(19.6)](4 - 2) = 32.00 m / \sec$$

i	t	v
0	0	0
1	2	19.6
2	4	32.00
3	6	39.86
4	8	44.82
5	10	47.97
6	12	49.96
7	14	51.22
8	16	52.02
9	18	52.52
10	20	52.84
11	22	53.04
12	24	53.17
13	26	53.25
14	28	53.30
15	30	53.33
16	32	53.36
17	34	53.37
18	36	53.38
19	38	53.38
20	40	53.38
21	42	53.39
22	44	53.39
23	46	53.39
24	48	53.39
25	50	53.39



Error becomes smaller for smaller Δt

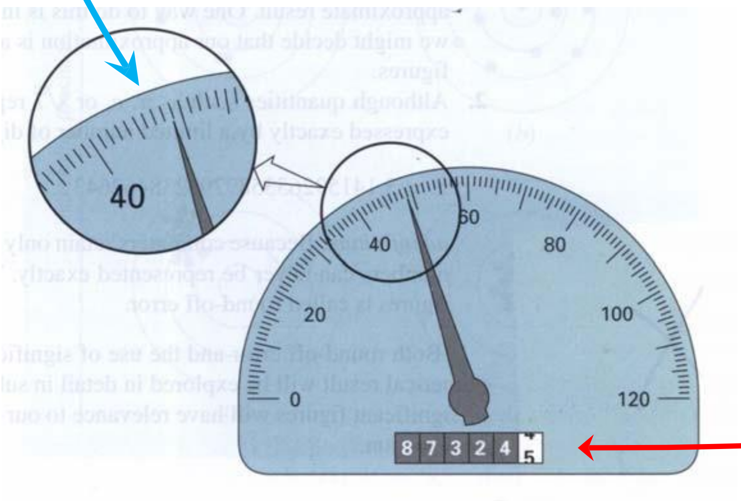
Use EXCEL

Digit (Significant Figures)

Speedomter: between 48 and 49 km/h
If insist on estimating up to 1 decimal place, one person might say 48.8 km/h and another might say 48.9 km/h.

But only the first two digits can be used with confidence.

On the basis of the speedometer, it is ridiculous to give the speed as 48.8642138 km/h.



From Odometer, we can conclude car has traveled slightly less than 87,324.5 km; in this case, the seventh digit is uncertain.

A car speedometer and odometer illustrating the concept of significant figures

Digit (Significant Figures)

Number of significant figures indicates precision. Significant digits of a number are those that can be *used* with *confidence*.

53,800 How many significant figures?

5.38×10^4	3	53800, 53802, ..., 53849
5.380×10^4	4	53800, 53801, 53802, 53803, 53804
5.3800×10^4	5	53800

Zeros are sometimes used to locate the decimal point and are not significant figures.

0.00001753	4	1.753×10^{-5}
0.0001753	4	1.753×10^{-4}
0.001753	4	1.753×10^{-3}

Quantifies such as π, e, $\sqrt{7}$ etc. cannot be expressed exactly by finite number of digits.

$\pi = 3.14159265358979323846 2643...$

Round-off, Truncation and Discretization Errors

Round-off errors arise because computers cannot represent real number exactly with a finite number of binary bits.

Truncation errors are committed when an iterative method is terminated or a mathematical procedure is approximated, and the approximate solution differs from the exact solution.

Discretization errors occur because the solution of the *discrete representation* of a problem does not coincide with the solution of the continuous problem.

Example: replacing derivative of a function by its finite difference representation.

Numerical Error (Galat)

Numerical errors arise from the use of approximations to represent exact mathematical operations and quantities.

True error: E_t = *true value – approximation* (may be **+** *or* **-**)

True fractional relative error: $\varepsilon_t = \frac{\text{true error}}{\text{true value}} \times 100\%$ (may be + or -)

Example: The measured lengths of a bridge and a rivet are 9999 and 9 cm, respectively. If the true values are 10,000 and 10 cm, respectively, compute the true error and the true percent relative error.

	Bridge	Rivet
E_t	$10{,}000 - 9999 = 1$ cm	$10 - 9 = 1$ cm
ε_t	$\frac{1}{10000} \times 100\% = 0.01\%$	$\frac{1}{10} \times 100\% = 10\%$

Numerical Error (Galat)

In reality, true value or analytical solution of a mathematical model may not be available. For this case, an alternative is to normalize the error using the best available estimate of the true value.

Approximate error: $$\varepsilon_a = \frac{\text{approximate error}}{\text{approximation}} \times 100\%$$ (may be + or -)

Certain numerical methods use an iterative approach to compute answers.

$$\varepsilon_a = \frac{\text{current approximation - previous approximation}}{\text{current approximation}} \times 100\%$$ (may be + or -)

In computation, we are interested in whether the absolute value of error is lower than a prescribed value.

$$|\varepsilon_a| < \varepsilon_s$$

If the following criterion is met, we can be assured that the result is correct to at least *n significant figures.*

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

Contoh 1

In mathematics, functions can often be represented by infinite series. Maclaurin series of expansion:

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + . \cdots + \frac{x^n}{n!}$$

Starting with the simplest version, $e^x = 1$, add one term at a time to estimate $e^{0.5}$. Compute the true and approximate percent relative errors. Add terms until the approximate error falls below a pre-specified error criterion ε_s conforming to 3 significant figures. The true value of $e^{0.5} = 1.648721$.

Solution:

$$\varepsilon_s = (0.5 \times 10^{2-n})\% = (0.5 \times 10^{2-3})\% = 0.05\%$$

One term:

$$e^{0.5} = 1 \qquad \varepsilon_t = \frac{1.648721 - 1}{1.648721} \times 100\% = 39.3\% \qquad \varepsilon_a \rightarrow undefined$$

Contoh 1 (cont'd)

Two terms:

$$e^{0.5} = 1 + 0.5 = 1.5 \qquad \varepsilon_t = \frac{1.648721 - 1.5}{1.648721} \times 100\% = 9.02\% \qquad \varepsilon_a = \frac{1.5 - 1}{1.5} \times 100\% = 33.3\%$$

Three terms:

$$e^{0.5} = 1 + 0.5 + \frac{0.5^2}{2!} = 1.625 \qquad \varepsilon_t = \frac{1.648721 - 1.625}{1.648721} \times 100\% = 1.44\% \qquad \varepsilon_a = \frac{1.625 - 1.5}{1.625} \times 100\% = 7.69\%$$

Terms	Result	ε_t (%)	ε_a (%)
1	1	39.3	
2	1.5	9.02	33.3
3	1.625	1.44	7.69
4	1.645833333	0.175	1.27
5	1.648437500	0.0172	0.158
6	1.648697917	0.00142	0.0158

$e^{0.5} \approx 1.65$

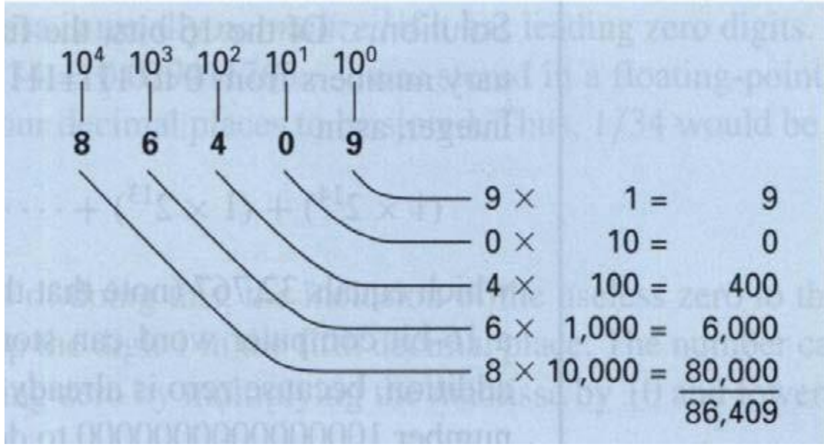
3 significant figures

$\varepsilon_a < \varepsilon_s$

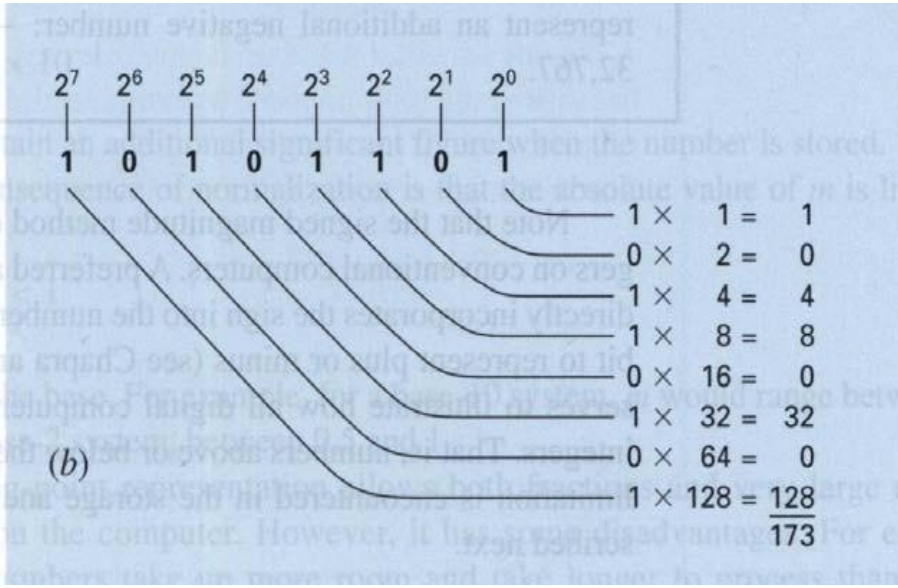
Computer Representation of Numbers

- Integer Representation

Decimal value 86,409

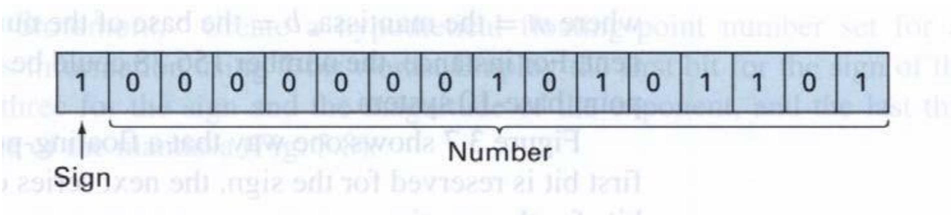


Binary representation of decimal integer of 173 on a 8-bit computer.



Computer Representation of Numbers (1)

Representation of the integer 173 (base-10) on a 16-bit computer using signed magnitude method



Max and Min number represented by 16-bits with 1 sign bit Max

value: 0111111111111111 = $(32,767)_{\text{Base-10}}$

Min value: 1111111111111111 = $(-32,767)_{\text{Base-10}}$

Since ‘minus’ zero is redundant,

1000000000000000 is taken to mean -32768

Computer Representation of Numbers (2)

Floating-Point representation in scientific format: **$m.b^e$**

b = base of number system

m = mantissa, usually normalized to lie between $1/b \leq m < 1$

$$\text{if } b=2, \quad (0.5)_{10} \leq m < (1)_{10}$$
$$\text{if } b=10, \; 0.1 \leq m < 1$$

e = exponent, a signed integer (can be either negative or positive)

For example, in the base-10 system

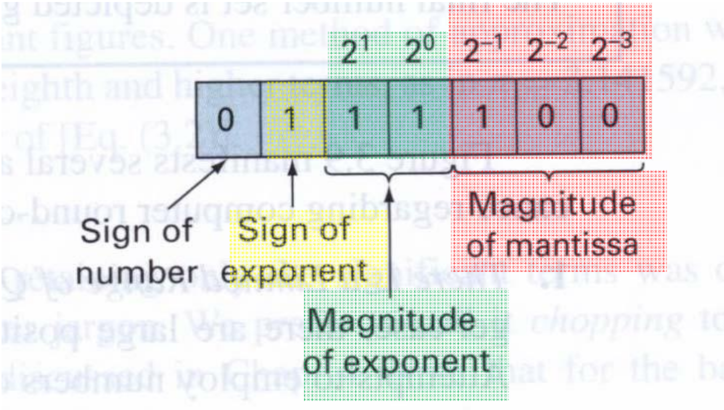
156.78 is represented as 0.15678×10^{3}

0.0015678 is represented as 0.15678×10^{-3}

} Same significant figures

Floating-point system allows very large numbers to be represented with finite number of bits in a computer. Its adoption introduces a source of error because the mantissa holds only a finite number of significant figures.

Hypothetical Set of Floating-Point Number Using Only 7-bits



Smallest positive number = +0.5 x $2^{(-3)}$ = 0.0625 in the base-10 system Although a smaller mantissa is possible (eg. 001, 010, 011), the value of 100 is used because of normalization rule (1/b minimum)

The next higher number is

$$0111101 = (1\text{x}2^{-1} + 1\text{x}2^{-2} + 1\text{x}2^{-3}) \text{ x } 2^{-3} = (0.078125)_{10}$$

Highest positive number is

$$0011111 = (1\text{x}2^{-1} + 1\text{x}2^{-2} + 1\text{x}2^{-3}) \text{ x } 2^{3} = (7.0)_{10}$$

Range and Limitation of Floating-Point Representation

1. There is a limited range of values that may be represented.

   In the 7-bits system, the range of positive numbers are 0.0625 to 7.0

2. Not all values can be represented within the range. In the hypothetical example, nothing can be represented between the smallest binary number 0111100 (0.0625) and the next bigger binary number 0111101 (0.078125).

$$\Delta x = 0.078125 - 0.0625 = 0.015625$$

3. The interval $\otimes x$ increases as the number grows in magnitude. This results from the preservation of significant figures in the mantissa.

The ratio $\frac{|\Delta x|}{|x|} \leq E$ is referred to as the machine epsilon which can be computed as

$$E = b^{1-t}$$

where b is the base and ***t*** is the number of significant digit in the mantissa.

Further Readings:

Numerical Methods for Engineers by SC Chapra and RP Canale, 2010
Sixth Edition, McGraw-Hill International Edition.

Chapters 1, 2, 3 and 4.