

 **ANALISIS NUMERIK**
SEMESTER GASAL TAHUN AKADEMIK 2011/2012
PRODI TEKNIK KIMIA - FTI - UPN "VETERAN" YOGYAKARTA

PENENTUAN AKAR PERSAMAAN TAK LINIER TUNGGAL

Materi Kuliah:
PENGANTAR
BRACKETING METHODS
OPEN METHODS

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MAIN TOPIC & OBJECTIVES (1)

1 - Bracketing Methods for Finding the Root of a Single Nonlinear Equation

Specific objectives and topics:

- Understanding what roots problems are and where they occur in engineering and science
- Knowing how to determine a root graphically
- Understanding the incremental search method and its shortcomings
- Knowing how to solve a roots problem with the bisection method
- Knowing how to estimate the error of bisection and why it differs from error estimates for other types of root location algorithm
- Understanding false position and how it differs from bisection

MAIN TOPIC & OBJECTIVES (2)

2 - Open Methods for Finding the Root of a Single Nonlinear Equation

Objectives:

- Recognizing the difference between bracketing and open methods for root location
- Understanding the fixed-point iteration method and how you can evaluate its convergence characteristics
- Knowing how to solve a roots problem with the Newton-Raphson method and appreciating the concept of quadratic convergence
- Knowing how to implement both the secant and the modified secant methods

INTRODUCTION

- ▶ **What is a nonlinear equation?**
- ▶ **What are roots?**
Roots = zeros
- ▶ **Method/ approach for finding roots:**
 1. analytical method
 2. graphical method
 3. trial and error
 4. **numerical method → iterative**
- ▶ Function of $f(x)$: (1) **Explicit**, (2) **Implicit**
(based on the influence of independent variable on dependent variable)

GRAPHICAL METHODS

A simple method for obtaining an estimate of the root of the equation $f(x) = 0$ is to:

- ❖ **make a plot of the function**, and
- ❖ **observe where it crosses the x axis**
(x value for which $f(x) = 0$)

Advantages:

- ❖ provides a **rough approximation of the root** → can be employed as **starting guesses** for numerical methods
- ❖ useful for understanding **the properties of the functions**
- ❖ useful for anticipating the pitfalls of the numerical methods

Disadvantage:
not precise

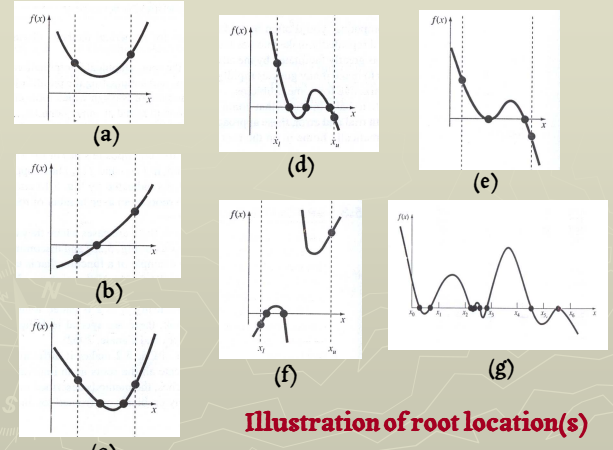


Illustration of root location(s)

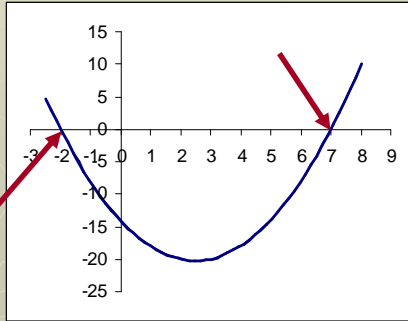
Contoh Ilustratif:

Persamaan: $f(x) = x^2 - 5x - 14 = 0$
 Akar persamaannya:?

Secara analitik:

→ Mudah...!

Secara grafik:



Secara Analitik:

Dengan menggunakan rumus abc untuk menentukan akar-akar persamaan kuadrat, diperoleh:

$$x_{1,2} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

Atau, dalam hal ini:

$$x_1 = \frac{5 - \sqrt{(-5)^2 - 4(1)(-14)}}{2(1)} = \frac{5 - 9}{2} = -2$$

$$x_2 = \frac{5 + \sqrt{(-5)^2 - 4(1)(-14)}}{2(1)} = \frac{5 + 9}{2} = 7$$

Secara numerik:

Misal, dipilih metode Newton-Raphson: $x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$

Iterasi ke-	x_i	$f(x_i)$	$f'(x_i)$	x_{i+1}
1	-4	22	-13	-2.30769
2	-2.30769	2.86391	-9.61336	-2.00985
3	-2.00985	0.08871	-9.01969	-2.00001
4	-2.00001	9.7E-05	-9.00002	-2
5	-2	1.2E-10	-9	-2
6	-2	0	-9	-2

Nilai tebakan awal

Iterasi ke-	x_i	$f(x_i)$	$f'(x_i)$	x_{i+1}
1	10	36	15	7.6
2	7.6	5.76	10.2	7.03529
3	7.03529	0.31889	9.07059	7.00014
4	7.00014	0.00124	9.00027	7
5	7	1.9E-08	9	7
6	7	0	9	7

Hasil

Hasil yang diperoleh dengan Polymath:

BRACKETING METHODS and INITIAL GUESSES

Two major classes of methods for finding the root of a single nonlinear equation (distinguished by the type of initial guess):

1. Bracketing methods
2. Open methods

❖ Based on two initial guesses that "bracket" the root
 ❖ Always work, but converge slowly (i.e. they typically take more iterations)

❖ Can involve one or more initial guesses, but there is no need for them to bracket the root
 ❖ Do not always work (i.e. they can diverge), but when they do they usually converge quicker

Bracketing Methods (Incremental Search Methods)

1. Metode Bisection
2. Metode False Position

INCREMENTAL SEARCH METHOD

In general, if $f(x)$ is real and continuous in the interval from x_1 to x_u and $f(x_1)$ and $f(x_u)$ have opposite signs, that is:

$$f(x_1) \cdot f(x_u) < 0$$

then there is **at least one real root** between x_1 and x_u .

Incremental search methods capitalize on this observation by locating an interval where the function changes sign. A potential problem with an incremental search is **the choice of the increment length**. If the length is too small, the search can be very time consuming. On the other hand, if the length is too great, there is a possibility that closely spaced roots might be missed. The problem is compounded by the possible existence of multiple roots.

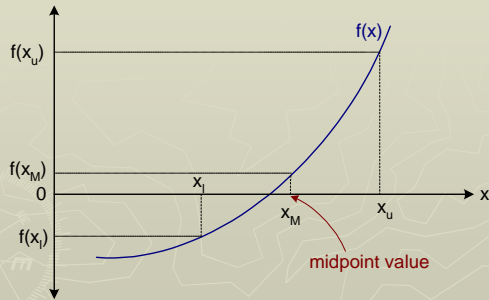
BISECTION METHOD

- Binary Search Method

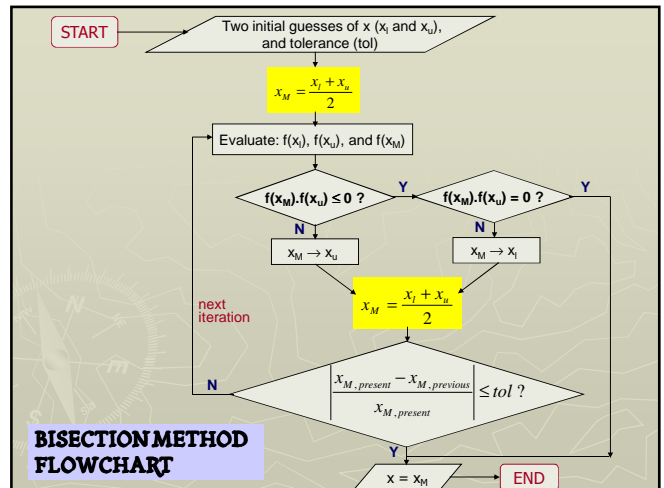
A "brute force" technique for root solving which is too inefficient for hand computation, but is ideally suited to machine computation.

An incremental search method in which **the interval is always divided in half**. If a function **changes sign** over an interval, the function value at the midpoint is evaluated. The location of the root is then determined as lying within the subinterval where the sign change occurs. The subinterval then becomes the interval for the next iteration. The process is repeated until the root is known to the required precision.

Consider: a function $f(x)$ which is known to have **one and only one real root** in the interval $x_1 < x < x_u$



Bisection formula:
$$x_M = \frac{x_l + x_u}{2}$$



BISECTION METHOD FLOWCHART

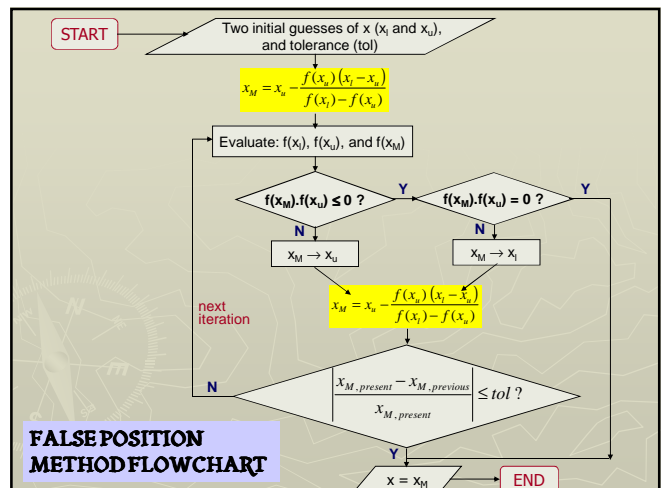
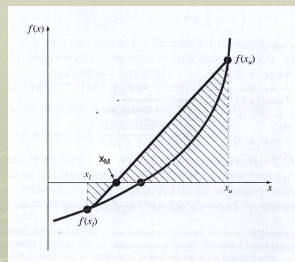
FALSE POSITION METHOD

= Linear Interpolation Method
= Regula-Falsi Method

It is **very similar to bisection method**, with the **exception that** it uses a different strategy to come up with its new root estimate.

False-position formula:

$$x_M = x_u - \frac{f(x_u)(x_l - x_u)}{f(x_l) - f(x_u)}$$



FALSE POSITION METHOD FLOWCHART

Example #1:

Use: (a) bisection method, and (b) false position method, to locate the root of: $f(x) = e^{-x} - x$

Use initial guesses of $x_l = 0$ and $x_u = 0,8$, and iterate until the approximate error falls below 1%

Graphically:

Calculation Results:

Bisection Method							
x_L	x_U	x_M	f_L	f_U	f_M	$f_M \cdot f_U$	ϵ_a (%)
0	0,8	0,4	1	-0,3507	0,2703	-0,0948	-
0,4	0,8	0,6	0,2703	-0,3507	-0,0512	0,0180	33,33
0,4	0,6	0,5	0,2703	-0,0512	0,1065	-0,0055	20,00
0,5	0,6	0,55	0,1065	-0,0512	0,0269	-0,0014	9,09
0,55	0,6	0,575	0,0269	-0,0512	-0,0123	0,0006	4,35
0,55	0,575	0,5625	0,0269	-0,0123	0,0073	-8,954E-05	2,22
0,5625	0,575	0,5688	0,0073	-0,0123	-0,0025	3,095E-05	1,10
0,5625	0,5688	0,5656	0,0073	-0,0025	0,0024	-5,991E-06	0,55

False Position Method							
x_L	x_U	x_M	f_L	f_U	f_M	$f_M \cdot f_U$	ϵ_a (%)
0	0,8	0,5923	1	-0,3507	-0,0392	0,0138	-
0	0,5923	0,5699	1,0000	-0,0392	-0,0044	0,0002	3,92
0	0,5699	0,5675	1,0000	-0,0044	-0,0005	0,0000	0,44

Example #2:

Use **bisection method** and **false position method** to determine the mass of the bungee jumper with a drag coefficient of $0,25 \text{ kg/m}$ to have a velocity of 36 m/s after 4 s of free fall. Note: The acceleration of gravity is $9,81 \text{ m/s}^2$

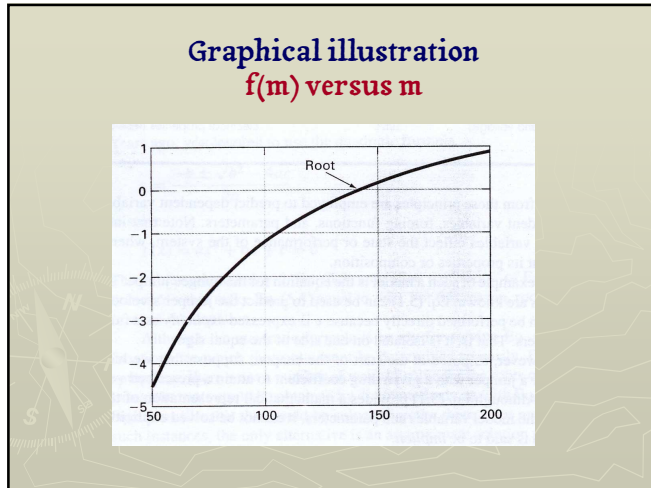
Free-fall velocity as a function of time:

$$v(t) = \sqrt{\frac{g m}{c_d}} \tanh\left(\sqrt{\frac{g c_d}{m}} t\right)$$

An alternative way to make the equation as a function of mass:

$$f(m) = \sqrt{\frac{g m}{c_d}} \tanh\left(\sqrt{\frac{g c_d}{m}} t\right) - v(t) = 0$$

Use initial guesses of $m_l = 50 \text{ kg}$ and $m_u = 200 \text{ kg}$, and iterate until the approximate error falls below 5% ($\epsilon_s = \text{stopping criterion} = 5\%$)



Calculation Results (by using MS Excel):

	A	B	C	D	E	F	G	H
11	BISECTION METHOD (until $\epsilon_a < 1\%$)							
12	m_L	m_U	m_M	F_L	F_U	F_M	$F_M \cdot F_U$	ϵ_a (%)
13	50	200	125	-4.5794	0.8603	-0.4086	-0.3515	-
14	125	200	162.5	-0.4086	0.8603	0.3594	0.3092	23.08
15	125	162.5	143.75	-0.4086	0.3594	0.0206	0.0074	13.04
16	125	143.75	134.38	-0.4086	0.0206	-0.1806	-0.0037	6.98
17	134.38	143.75	139.06	-0.1806	0.0206	-0.0770	-0.0016	3.37
18	139.06	143.75	141.41	-0.0770	0.0206	-0.0275	-0.0006	1.66
19	141.41	143.75	142.58	-0.0275	0.0206	-0.0033	-0.0001	0.82
22	FALSE POSITION METHOD (until $\epsilon_a < 1\%$)							
23	m_L	m_U	m_M	F_L	F_U	F_M	$F_M \cdot F_U$	ϵ_a (%)
24	50	200	176.28	-4.5794	0.8603	0.5662	0.4871	-
25	50	176.28	162.38	-4.5794	0.5662	0.3575	0.2024	8.56
26	50	162.38	154.24	-4.5794	0.3575	0.2194	0.0785	5.28
27	50	154.24	149.48	-4.5794	0.2194	0.1322	0.0290	3.19
28	50	149.48	146.69	-4.5794	0.1322	0.0788	0.0104	1.90
29	50	146.69	145.05	-4.5794	0.0788	0.0466	0.0037	1.13
30	50	145.05	144.09	-4.5794	0.0466	0.0275	0.0013	0.66

Calculation Results (by using Polymath):

POLYMATH Report
Nonlinear Equation

Calculated values of NLE variables

Variable	Value	$f(x)$	Initial Guess
1 m	142.7376	-1.284E-11	125. (50. < m < 200.)

Variable	Value
1 cd	0.25
2 g	9.81
3 t	4.
4 v	36.

Nonlinear equations

1 $f(m) = \text{sqrt}(g*m/cd) * \text{tanh}(\text{sqrt}(g*cd/m))*t - v = 0$

Explicit equations

1 $g = 9.81$
 2 $cd = 0.25$
 3 $v = 36$
 4 $t = 4$

General Settings

Total number of equations	5
Number of implicit equations	1
Number of explicit equations	4
Elapsed time	0.0000 sec
Solution method	SAFENEWT
Max iterations	150
Tolerance F	0.0000001
Tolerance X	0.0000001
Tolerance min	0.0000001

Open Methods

1. Metode Iterasi Satu Titik
– Metode Dua Kurva
2. Metode Newton-Raphson
3. Metode Secant

SIMPLE FIXED POINT ITERATION METHOD

It is also called:

- ☞ One point iteration method, or
- ☞ Successive substitution method

Rearranging the function $f(x) = 0$ so that x is on the left-hand side of the equation: $x = g(x)$

a formula to predict a new value of x as a function of an old value of x

This transformation can be accomplished either by:

- ☞ Algebraic manipulation, or
- ☞ Simply adding x to both sides of the original equation

Thus, given an initial guess at root x_i , the equation above can be used to compute a new estimate x_{i+1} as expressed by the iterative formula:

$x_{i+1} = g(x_i)$

The approximate error can be determined by:

$$\epsilon_a = \left| \frac{x_{i+1} - x_i}{x_{i+1}} \right| \cdot 100\%$$

Example:
Use the simple fixed-point iteration to locate the root of $f(x) = e^{-x} - x$

Solution:
The function can be separated directly and then expressed as: $x_{i+1} = e^{-x_i}$

Starting with an initial guess of $x_0 = 0$, this iterative equation can be applied to compute:

i	x_i	e^{-x_i}	$\epsilon_a, \%$	$\epsilon_t, \%$
0	0,0000	1,0000	-	-
1	1,0000	0,3679	100,000	76,322
2	0,3679	0,6922	171,828	35,135
3	0,6922	0,5005	46,854	22,050
4	0,5005	0,6062	38,309	11,755
5	0,6062	0,5454	17,447	6,894
6	0,5454	0,5796	11,157	3,835
7	0,5796	0,5601	5,903	2,199
8	0,5601	0,5711	3,481	1,239
9	0,5711	0,5649	1,931	0,705
10	0,5649	0,5684	1,109	0,399

Note: The true value of the root = 0,56714329

Two Curves Graphical Method

By graphical method, there are two alternatives for determining root of:

$$f(x) = e^{-x} - x$$

(a) Root at the point where it crosses the x axis

(b) Root at the intersection of the component functions

Two curves graphical method

FIXED-POINT ITERATION METHOD flowchart

```

    graph TD
      Start([START]) --> Init[/An initial guess of x (x_i = x_0), tol/]
      Init --> Calc[x_{i+1} = g(x_i)]
      Calc --> Error["\epsilon_a = \frac{x_i - x_{i+1}}{x_{i+1}} \cdot 100%"]
      Error --> Decision{ "\epsilon_a < tol ?" }
      Decision -- N --> Calc
      Decision -- Y --> Output[/x_i/]
      Output --> End([END])
  
```

CONVERGENCE OF SIMPLE FIXED-POINT ITERATION

(a) & (b) → **convergent**
 (c) & (d) → **divergent**

Note that convergence occurs when $|g'(x)| < 1$

NEWTON-RAPHSON METHOD

The most widely used of all root-locating formula

If the initial guess at the root is x_i , a tangent can be extended from the point $[x_i, f(x_i)]$. The point where this tangent crosses the x axis usually represents an improved estimate of the root.

The first derivative at x_i is equivalent to the slope: $f'(x_i) = \frac{f(x_i) - 0}{x_i - x_{i+1}}$

which can be rearranged to yield:

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

Newton-Raphson formula

Example:
 Use the Newton-Raphson method to estimate the root of $f(x) = e^{-x} - x$, employing an initial guess of $x_0 = 0$

Solution:
 The first derivative of the function can be evaluated as: $f'(x) = -e^{-x} - 1$

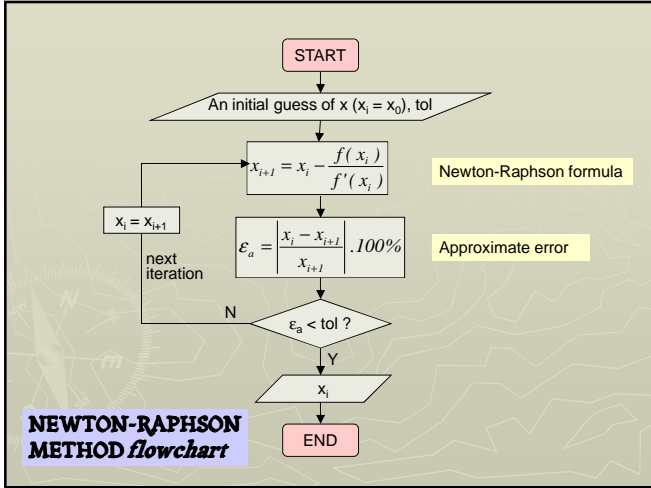
Then, by the Newton-Raphson formula:

$$x_{i+1} = x_i - \frac{e^{-x_i} - x_i}{-e^{-x_i} - 1}$$

Starting with an initial guess of $x_0 = 0$, this iterative equation can be applied to compute:

i	x_i	$\epsilon_a, \%$	$\epsilon_t, \%$
0	0	-	100
1	0,5	100	11,83886
2	0,566311003	11,70929	0,146751
3	0,567143165	0,146729	$2,2 \cdot 10^{-5}$
4	0,567143290	$2,21 \cdot 10^{-5}$	$7,23 \cdot 10^{-8}$

Comment:
 The approach **rapidly converges** on the true root. Notice that the true percent relative error at each iteration decreases much faster than it does in simple fixed-point iteration (in previous example)



FOUR CASES OF POOR CONVERGENCE OF THIS METHOD

There is **no general convergence criterion** for Newton-Raphson method. Its convergence depends on:

- the nature of the function, and
- the accuracy of the initial guess

SECANT METHOD

A potential problem in implementing the Newton-Raphson method is: **the evaluation of the derivative**. There are certain functions whose derivatives may be difficult or inconvenient to evaluate. For these cases, **the derivative can be approximated by a backward finite divided difference:**

$$f'(x_i) \cong \frac{f(x_{i-1}) - f(x_i)}{x_{i-1} - x_i}$$

This approximation can be substituted into Newton-Raphson formula to yield the following iterative equation:

$$x_{i+1} = x_i - \frac{f(x_i)(x_{i-1} - x_i)}{f(x_{i-1}) - f(x_i)}$$

Secant method formula

Notice that this approach **requires two initial estimates of x**. However, because $f(x)$ is not required to change signs between the estimates, it is not classified as a bracketing method.

Rather than using two arbitrary values to estimate the derivative, **an alternative approach** involves a fractional perturbation of the independent variable to estimate $f'(x)$:

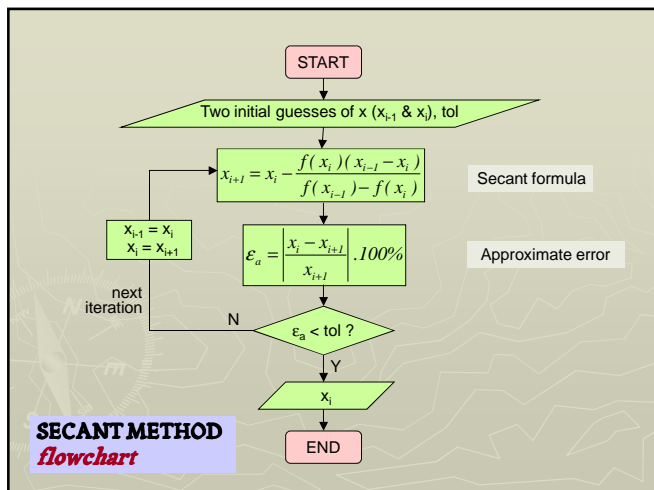
$$f'(x_i) \cong \frac{f(x_i + \delta x_i) - f(x_i)}{\delta x_i}$$

where δ = a small **perturbation fraction**

This approximation can be substituted into Newton-Raphson formula to yield the following iterative equation:

$$x_{i+1} = x_i - \frac{\delta x_i f(x_i)}{f(x_i + \delta x_i) - f(x_i)}$$

Modified secant method

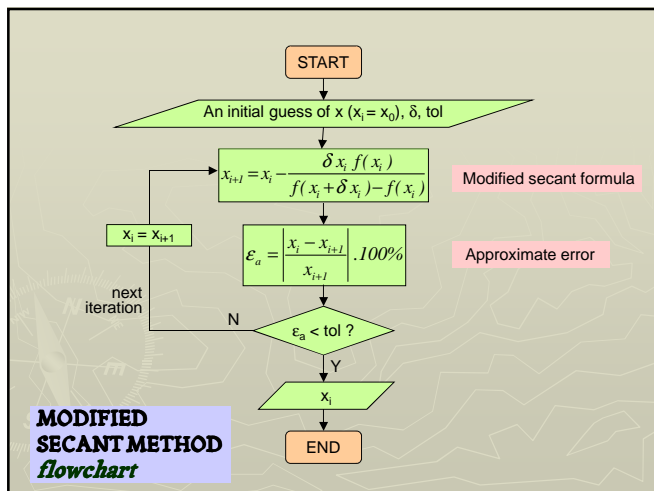


Hasil Penyelesaian Contoh Soal yang Sama dengan Sebelumnya (Metode Secant):

	A	B	C	D	E
1	xi-1	xi	fi-1	fi	xi+1
2	1	2	-0.632121	-1.86466	0.487142
3	2	0.487142	-1.864665	0.127238	0.583780
4	0.487142	0.583780	0.127238	-0.02599	0.567386
5	0.583780	0.567386	-0.025994	-0.00038	0.567143
6	0.567386	0.567143	-0.000381	1.14E-06	0.567143
7	0.567143	0.567143	1.14E-06	-5E-11	0.567143
8	0.567143	0.567143	-5.03E-11	0	0.567143

↑ ↑ ↑

Konvergen!



Example:
Use **the modified secant method** to determine the mass of the bungee jumper with a drag coefficient of 0,25 kg/m to have a velocity of 36 m/s after 4 s of free fall. Note: The acceleration of gravity is 9,81 m/s². Use an initial guess of 50 kg and a value of 10⁻⁶ for the perturbation factor.

Solution:

First iteration:

$x_0 = 50$	$f(x_0) = -4,57938708$
$x_0 + \delta x_0 = 50,00005$	$f(x_0 + \delta x_0) = -4,5793381118$

$$x_1 = 50 - \frac{10^{-6}(50)(-4,57938708)}{-4,579381118 - (-4,57938708)} = 88,39931$$

$|\epsilon_r| = 38,07\%$; $|\epsilon_a| = 43,44\%$

Second iteration:

$$x_1 = 88,39931 \quad f(x_1) = -1,69220771$$

$$x_1 + \delta x_1 = 88,39940 \quad f(x_1 + \delta x_1) = -1,692203516$$

$$x_2 = 88,39931 - \frac{10^{-6}(88,39931)(-1,69220771)}{-1,692203516 - (-1,69220771)} = 124,08970$$

$|\epsilon_r| = 13,06\%$; $|\epsilon_a| = 28,76\%$

The calculation can be continued to yield:

i	x_i	$x_i + \delta x_i$	$f(x_i)$	$f(x_i + \delta x_i)$	$ \epsilon_r $ (%)	$ \epsilon_a $ (%)
0	50	50,00005	-4,57938708	-4,579381118	64,97	-
1	88,39931	88,39940	-1,692207707	-1,692203516	38,07	43,44
2	124,08970	124,08982	-0,432369881	-0,43236662	13,06	28,76
3	140,54172	140,54186	-0,045550483	-0,045547526	1,54	11,71
4	142,70719	142,70733	-0,000622927	-0,000620007	0,02	1,52
5	142,73763	142,73777	$-1,19176 \cdot 10^{-7}$	$2,80062 \cdot 10^{-6}$	0,00	0,02
6	142,73763	142,73778	$9,9476 \cdot 10^{-14}$	$2,9198 \cdot 10^{-6}$	0,00	0,00

Comment:
The choice of a proper value for δ is not automatic.
If δ is too small :
If δ is too big :

PROBLEMS

Problem #1:

(a) $f(x) = \sin(\sqrt{x}) - x \quad x_0 = 0,5$

(b) $f(x) = -11 - 22x + 17x^2 - 2,5x^3$
Carilah nilai x pada interval $x = 1$ dan $x = 3$

Problem #2:

Using $x = 1$ as the starting point, find a root of the following equation to three significant figures:

$$f(x) = x^2 e^x - 1 = 0$$

using:

- successive substitution
- Newton's method
- the secant method (use $x = 1,01$ as your second point)

Problem #3:

Using $x = 4$ as the starting point, find a root of the following equation:

$$f(x) = x e^x + x - 5e^x - 5 = 0$$

using:

- Newton's method
- the secant method (use $x = 4,1$ as your second point)
- the regula falsi method

Problem #4:

Consider the following nonlinear equation:

$$f(x) = x^2 - e^x = 0$$

Show at least three cycles of search using a starting point of $x = 1$ for:

- Newton's method
- regula falsi method

Problem #5:

Water is flowing in a trapezoidal channel at a rate of $Q = 20 \text{ m}^3/\text{s}$. The critical depth y for such a channel must satisfy the equation:

$$0 = 1 - \frac{Q^2}{g A_c^3} B$$

where $g = 9,81 \text{ m/s}^2$, A_c = the cross-sectional area (m^2), and B = the width of the channel at the surface (m). For this case, the width and the cross-sectional area can be related to depth y by:

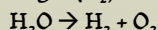
$$B = 3 + y$$

$$\text{and } A_c = 3y + \frac{y^2}{2}$$

Solve for the critical depth using: (a) the graphical method, (b) bisection, and (c) false position. For (b) and (c), use **initial guesses of $y_1 = 0,5$ and $y_2 = 2,5$** , and iterate until the approximate error falls below 1% or the number of iterations exceeds 10. Discuss your results.

Problem #6:

In a chemical engineering process, water vapor (H_2O) is heated to sufficiently high temperatures that a significant portion of the water dissociates, or splits apart, to form oxygen (O_2) and hydrogen (H_2):



If it assumed that this is the only reaction involved, the mole fraction x of H_2O that dissociates can be represented by:

$$K = \frac{x}{1-x} \sqrt{\frac{2 P_t}{2+x}}$$

where K is the reaction's equilibrium constant and P_t is the total pressure of the mixture. If $P_t = 3 \text{ atm}$ and $K = 0,05$, determine the value of x that satisfies the equation above.

Problem #7:

The Redlich-Kwong equation of state is given by:

$$p = \frac{RT}{v-b} - \frac{a}{v(v+b)\sqrt{T}}$$

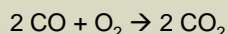
where R = the universal gas constant [$= 0,518 \text{ kJ/kg.K}$], T = absolute temperature (K), p = absolute pressure (kPa), and v = the volume of a kg of gas (m^3/kg). The parameter a and b are calculated by:

$$a = 0,427 \frac{R^2 T_c^{2,5}}{P_c} \quad \text{and} \quad b = 0,0866 R \frac{T_c}{P_c}$$

where $p_c = 4600 \text{ kPa}$ and $T_c = 191 \text{ K}$. As a chemical engineer, you are asked to determine the amount of methane fuel that can be held in a 3-m^3 tank at a temperature of -40°C with a pressure of 65000 kPa . Use a root locating method of your choice to calculate v and then determine the mass of methane contained in the tank.

Problem #8:

Determine the equilibrium conversion for:



if stoichiometric amounts of CO and air are reacted at 2000 K and 1 atmosphere pressure. At 2000 K the equilibrium constant for this reaction is $62,4 \times 10^6 \text{ atm}^{-1}$. As a basis, consider 2 gmole of CO. Then there would be 1 gmole of O_2 and $3,76 \text{ gmole}$ of N_2 . Performing a mole balance on each species and defining x as the amount of CO that reacts yields:

$$N_{\text{CO}} = 2 - x$$

$$N_{\text{O}_2} = 1 - 0,5 x$$

$$N_{\text{CO}_2} = x$$

$$N_{\text{N}_2} = 3,76$$

Then the partial pressures are given as:

$$p_{\text{CO}} = \frac{N_{\text{CO}}}{N_T} = \frac{2-x}{6,76-0,5x}$$

$$p_{\text{O}_2} = \frac{N_{\text{O}_2}}{N_T} = \frac{1-0,5x}{6,76-0,5x}$$

$$p_{\text{CO}_2} = \frac{N_{\text{CO}_2}}{N_T} = \frac{x}{6,76-0,5x}$$

The equilibrium relationship is given by: $K = \frac{P_{CO_2}^2 P_T}{P_{CO}^2 P_{O_2}}$

where P_T is the total pressure and remembering that the standard state fugacities of CO_2 , CO , and O_2 are unity. Substituting yields:

$$\frac{x^2 (6,76 - 0,5 x)}{(1 - 0,5 x) (2 - x)^2} = 62,4 \cdot 10^6$$

Rearranging into a normalized form:

$$\frac{x^2 (6,76 - 0,5 x)}{62,4 \cdot 10^6 (1 - 0,5 x) (2 - x)^2} - 1 = 0$$

- Solve for the equilibrium composition using Newton's method with a starting point of $x_0 = 1,0$ gmole.
- Solve this problem using the regula falsi method.

Problem #9:

Van der Waals equation of state is given as:

$$\left(P + \frac{a}{V^2} \right) (\bar{V} - b) = R T$$

where: $P \equiv$ pressure (10 atm), $T \equiv$ temperature (250 K)
 $R \equiv$ gas constant (0,082 liter.atm/gmole.K), $V \equiv$ specific volume (liter/gmole)

Determine the specific volume for ammonia using:

- successive substitution
- Newton's method
- Secant method

The Van der Waals constants for ammonia are:
 $a = 4,19 \times 10^6 \text{ atm (cm}^3/\text{gmole)}^2$ and $b = 37,2 \text{ cm}^3/\text{gmole}$.
 (Beware of the units!)

Problem #10:

Pendirian suatu pabrik kimia memerlukan *fixed capital* (FC) = Rp 700 milyar dan *working capital* (WC) = Rp 300 milyar.

Nilai *annual cash flow* (C) = Rp 250 milyar.

Umur pabrik diperkirakan selama 10 tahun dengan *salvage value* (SV) = Rp 70 milyar.

Jika i menyatakan nilai suku bunga investasi ini yang diekivalensikan dengan jika disimpan di bank, **tentukan nilai i !**

Jika digunakan *present value analysis*, maka nilai i dapat dihitung dari persamaan berikut ini:

$$FC + WC = \frac{C}{1+i} + \frac{C}{(1+i)^2} + \frac{C}{(1+i)^3} + \dots + \frac{C}{(1+i)^{10}} + \frac{WC + SV}{(1+i)^{10}}$$

Problem #11:

The saturation concentration of dissolved oxygen in fresh water can be calculated with the equation:

$$\ln o_{sf} = -139,34411 + \frac{1,575701 \times 10^5}{T_a} - \frac{6,642308 \times 10^7}{T_a^2} + \frac{1,243800 \times 10^{10}}{T_a^3} - \frac{8,621949 \times 10^{11}}{T_a^4}$$

where o_{sf} = the saturation concentration of dissolved oxygen in fresh water at 1 atm (mg L^{-1}); and T_a = absolute temperature (K). Remember that $T_a = T + 273,15$, where T = temperature ($^{\circ}\text{C}$). According to this equation, saturation decreases with increasing temperature. For typical natural waters in temperate climates, the equation can be used to determine that oxygen concentration ranges from 14.621 mg/L at 0°C to 6.949 mg/L at 35°C . Given a value of oxygen concentration, this formula and the bisection method can be used to solve for temperature in $^{\circ}\text{C}$. If the initial guesses are set as 0 and 35°C , how many bisection iterations would be required to determine temperature to an absolute error of 0.005°C ?

