Assignment 1

Himanshu Choudhary (20002005g)

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Problem 1 - Solution to non-linear equation

- Problem statement

Write a program to generate a P-V isotherm for given conditions from van der waals equation for designing a system to capture and store gaseous CO_2, at sub surface conditions.

- DESCRIPTION OF METHOD

Since we have to plot a graph, we will need values of P (x axis) and V (y axis). And since we are required to get V from given P, we need to solve the non linear equation of the function given, by modified secant method.

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

$$(PV^2+a)(V-b) - RTV^2 = 0$$

$$PV^3 - PbV^2 + aV - ab - RTV^2 = 0$$

$$PV^3 - (Pb+RT)V^2 + aV - ab = 0 \quad \{\text{given P}\}$$

(we need V to satisfy this equation)

And by modified sec. method, we can calculate V at a given P.

~~AO~~

~~Matt~~

Modified Secant method

In secant method, we use two arbitrarily values to calculate the derivative and further calculate new closer values.

But in modified secant method, we guess one value initially and the other value is a value fractionally ~~not~~ very near the initial guess.

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

and

$$x_{i+1} = x_i - \left(\frac{f(x_i)}{f'(x_i)}\right) \quad \{\delta = \text{Small fraction}\}$$

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

And repeat till convergence.

- Pseudo Code

Let DELTA = 0.01
Let ERR = 0.001
X_0 is initial guess
P is pressure
~~$X_1 = X_0$~~
$F(V) = PV^3 - (Pb+RT)V^2 + aV - ab$
$X_1 = X_0 - (DELTA \times X_0)\, F(X_0) / (F(X_0 + DELTA X_0) - F(X_0))$

WHILE $X_1 - X_0$ NOT less than ERR
Change $X_0 = X_1$

$$X_1 = X_0 - (\delta X_0)\, F(X_0) / (F(X_0 + \delta X_0) - F(X_0))$$

END

RETURN X_1

~~END~~

- Iteration

$f(n) = PV^3 - (bP+RT)V^2 + aV - ab = 0$

$R = 0.082$; $a = 3.592$; $b = 0.04267$; $T = 345$;

let $P = 2.8$ atm
and $x_0 = V = 5\,l$
$\delta = 0.01$
$x_0 = 5$

$$x_1 = x_0 - \frac{\delta x_0 f(x_0)}{f(x_0 + \delta x_0) - f(x_0)}$$

$$x_1 = 5 - \frac{(0.01 \times 5) f(5)}{f(5.05) - f(5)}$$

$$x_1 = 5. \cdots - 4.8980$$

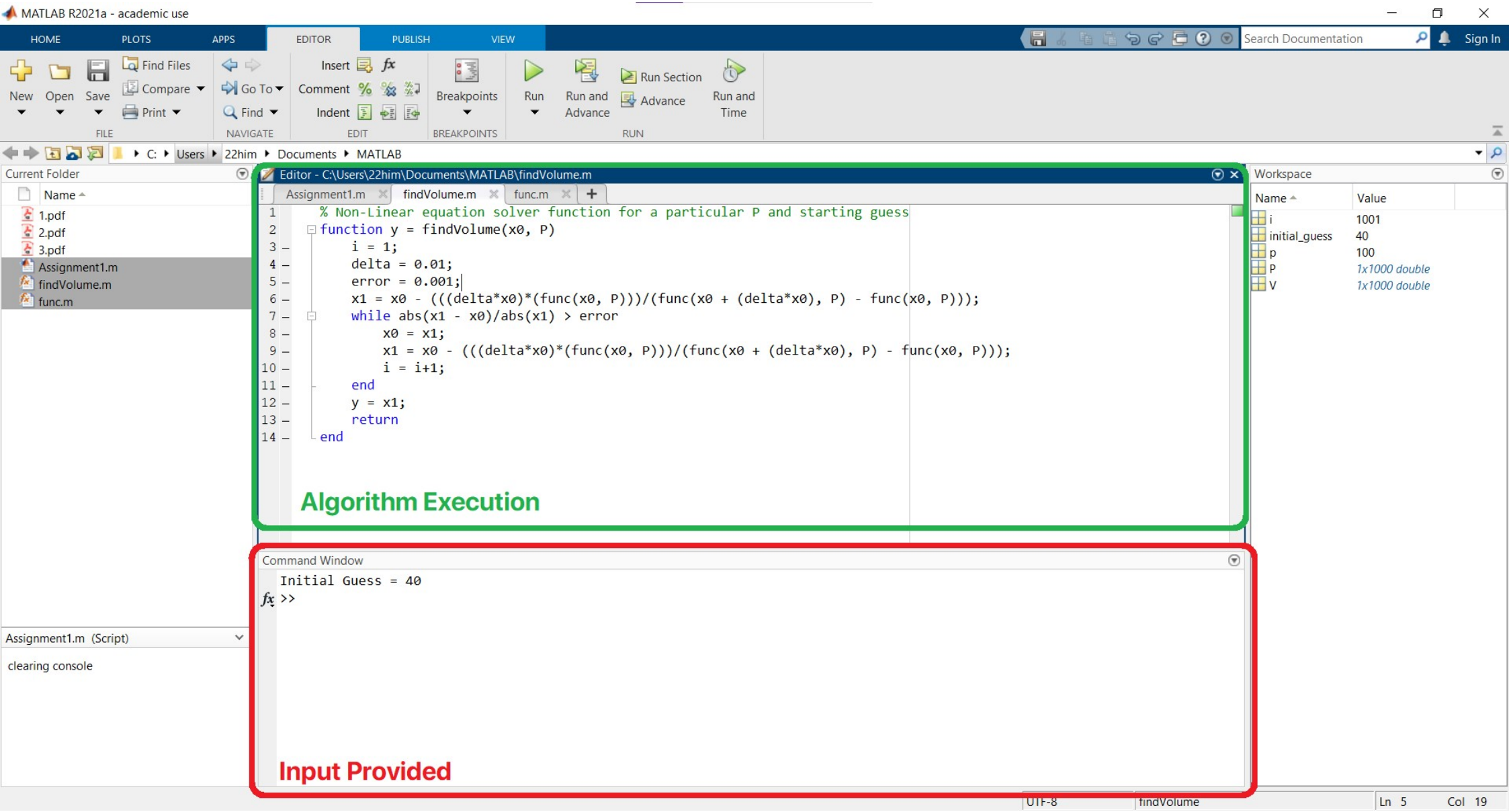
$$x_1 = 0.1020$$

1. $x_0 = 5$; $x_1 = 0.1020$
2. $x_0 = 0.1020$; $x_1 = 0.0649$

```
% clearing console
clear
clc

% Taking user input for initial guess for the modified secant method
initial_guess = input("Initial Guess = ");

% Array containing values for pressure from 1 atm to 100 atm
P = linspace(1, 100, 1000);

% Volume array (initially zero)
V = zeros(1, 1000);

i = 1;
% Calculating V for every value of P (find_V() is the function for find V at a given ↙
P)
for p = P
    V(i) = findVolume(initial_guess, p);
    i = i+1;
end

plot(P, V,'LineWidth', 1.5);
title("PV Isotherm (T = 345K)");
xlabel("Pressure (P)");
ylabel("Volume (V)");
```

```
% Non-Linear equation solver function for a particular P and starting guess
function y = findVolume(x0, P)
    i = 1;
    delta = 0.01;
    error = 0.001;
    x1 = x0 - (((delta*x0)*(func(x0, P)))/(func(x0 + (delta*x0), P) - func(x0, P)));
    while abs(x1 - x0)/abs(x1) > error
        x0 = x1;
        x1 = x0 - (((delta*x0)*(func(x0, P)))/(func(x0 + (delta*x0), P) - func(x0, ↙
P)));
        i = i+1;
    end
    y = x1;
    return
end
```

```
% Code of function f(V, P)
function y = func(V, P)
    a = 3.592;
    b = 0.04267;
    R = 0.082056;
    T = 345;

    % rearranged van der Waal's equation
    y = (P*(V^3)) - ((V^2)*((P*b) + (R*T))) +(a*V) - (a*b);
    return
end
```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Assignment1.m
findVolume.m
func.m
Editor - C:\Users\22him\Documents\MATLAB\findVolume.m
Assignment1.m
findVolume.m
func.m
1 % Non-Linear equation solver function for a particular P and starting guess
2 function y = findVolume(x0, P)
3 i = 1;
4 delta = 0.01;
5 error = 0.001;
6 x1 = x0 - (((delta*x0)*(func(x0, P)))/(func(x0 + (delta*x0), P) - func(x0, P)));
7 while abs(x1 - x0)/abs(x1) > error
8 x0 = x1;
9 x1 = x0 - (((delta*x0)*(func(x0, P)))/(func(x0 + (delta*x0), P) - func(x0, P)));
10 i = i+1;
11 end
12 y = x1;
13 return
14 end
Algorithm Execution
Workspace
Name
Value
i 1001
initial_guess 40
p 100
P 1x1000 double
V 1x1000 double
Command Window
Initial Guess = 40
>>
Input Provided
Assignment1.m (Script)
clearing console
UTF-8
findVolume
Ln 5
Col 19

Figure 1

File Edit View Insert Tools Desktop Window Help