

2. Consider the following four methods for calculating $2^{1/4}$, the fourth root of 2.

(a) Rank them for speed of convergence, from fastest to slowest. Be sure to give reasons for your ranking.

(A) Bisection Method applied to $f(x) = x^4 - 2$

(B) Secant Method applied to $f(x) = x^4 - 2$

(C) Fixed-Point Iteration applied to $g(x) = \frac{x}{2} + \frac{1}{x^3}$

(D) Fixed-Point Iteration applied to $g(x) = \frac{2x}{3} + \frac{2}{3x^3}$

The rank will be (B), (D), (A), and (C). All methods converge to $root \approx 1.1892$. (B) is going to be the fastest, since it converges Super linearly. The other three methods all converge linearly, and are dependent on parameters. Considering the convergence to be 10^{-7} difference from iteration i and $i + 1$, Bisection is going to be a little slower than (D), since it is going to have some trouble inside the small intervals, but still faster than (C), since $S = 0.5$. The difference between (C) and (D) is quite big, since the derivative of (C) at the root is $S = -0.3333$, while the derivative of (D) at the root is $S = -0.9975$.

(b) Are there any methods that will converge faster than all above suggestions?

Yes, Newton's Method is going to converge faster than all the previous suggestions. Since it is quadratically convergent.

3. i) Computer problem 1.4.11. The ideal gas law for a gas at low temperature and pressure is $PV = nRT$, where P is pressure (in atm), V is volume (in L), T is temperature (in K), n is the number of moles of gas, and $R = 0.0820578$ is the molar gas constant. The van der Waals equation

$$\left(P + \frac{n^2a}{V^2}\right)(V - nb) = nRT$$

covers the non ideal case where these assumptions do not hold. Use the ideal gas law to compute an initial guess, followed by Newton's Method applied to the van der Waals equation to find the volume of one mole of oxygen at 320 K and a pressure of 15 atm. For oxygen, $a = 1.36L^2\text{-atm}/\text{mole}^2$ and $b = 0.003183L/\text{mole}$. State your initial guess and solution with three significant digits.

In MATLAB

```
clear all;
close all;

f = @(P,V,n,a,b,R,T) P*V+n^2*a*n*b/V^2+n^2*a*V/V^2-P*n*b
    -n*R*T;
df = @(P,a,n,b,V) P-2*b*n^3*a/V^3-a*n^2/V^2;

R = 0.0820575;
T = 320;
P = 15;
n = 1;
a = 1.36;
b = 0.003183;
V(1) = n*R*T/P;
tol = 1e-7;
deltax = inf;
i = 1;
while deltax > tol
    V(i+1) = V(i)-f(P,V(i),n,a,b,R,T)/df(P,a,n,b,V(i));
    deltax = abs(V(i+1)-V(i));
    i = i+1;
end
fprintf(['Algorithm converged after %d ' ...
        'iterations. \n V(final) = %.8f ' ...
        '\n f(root) = %.8f' ...
        '\n Initial guess: %.8f\n'] ...
        ,i,V(i),f(P,V(i),n,a,b,R,T),V(1))
% Output:
%Algorithm converged after 4 iterations.
```

```
% V(final) = 1.70031988
% f(root) = 0.00000000
% Initial guess: 1.75056000
```

- ii) Computer problem 1.4.12. Use the data from Computer Problem 11 to find the volume of 1 mole of benzene vapor at 700 K under a pressure of 20 atm. For benzene, $a = 18.0L^2 - atm/mole^2$ and $b = 0.1154L/mole$

```
clear all;
close all;

f = @(P,V,n,a,b,R,T) P*V+n^2*a*n*b/V^2+n^2*a*V/V^2-P*n*b
    -n*R*T;
df = @(P,a,n,b,V) P-2*b*n^3*a/V^3-a*n^2/V^2;

R = 0.0820575;
T = 700;
P = 20;
n = 1;
a = 18;
b = 0.1154;
V(1) = n*R*T/P;
tol = 1e-7;
deltax = inf;
i = 1;
while deltax > tol
    V(i+1) = V(i)-f(P,V(i),n,a,b,R,T)/df(P,a,n,b,V(i));
    deltax = abs(V(i+1)-V(i));
    i = i+1;
end
fprintf(['Algorithm converged after %d ' ...
        'iterations. \n V(final) = %.8f ' ...
        '\n f(root) = %.8f' ...
        '\n Initial guess: %.8f\n'] ...
        ,i,V(i),f(P,V(i),n,a,b,R,T),V(1))
% Output:
% Algorithm converged after 5 iterations.
% V(final) = 2.63022340
% f(root) = 0.00000000
% Initial guess: 2.87201250
```