# Homework#2 Solutions

## Problem 1: Iterative Methods (Gauss-Seidel Method)

### Given System of Equations

$$
\begin{aligned}
10x_1 + 2x_2 - x_3 &= 27 \\
-3x_1 - 6x_2 + 2x_3 &= -61.5 \\
x_1 + x_2 + 5x_3 &= -21.5
\end{aligned}
$$

### (a) Perform 1 iteration of the Gauss-Seidel method analytically

Rearrange the equations to solve for each variable:

$$
\begin{aligned}
x_1 &= \frac{27 - 2x_2 + x_3}{10} \\
x_2 &= \frac{-61.5 + 3x_1 - 2x_3}{-6} \\
x_3 &= \frac{-21.5 - x_1 - x_2}{5}
\end{aligned}
$$

Assume initial guesses: $x_1 = 0, x_2 = 0, x_3 = 0$.
1st iteration:

$$
\begin{aligned}
x_1^{(1)} &= \frac{27 - 2(0) + 0}{10} = 2.7 \\
x_2^{(1)} &= \frac{-61.5 + 3(2.7) - 2(0)}{-6} = 8.9 \\
x_3^{(1)} &= \frac{-21.5 - 2.7 - 8.9}{5} = -6.62
\end{aligned}
$$

## Problem 2: Newton-Raphson Method for Nonlinear Equations

### Given Equations

$$
\begin{aligned}
y &= -x^2 + x + 0.75 \\
y + 1 &= x^2
\end{aligned}
$$

Initial guesses: $x = 1.2, y = 1.2$.
Rewrite as:

$$
\begin{aligned}
f_1(x, y) &= y + x^2 - x - 0.75 = 0 \\
f_2(x, y) &= x^2 - y - 1 = 0
\end{aligned}
$$

1. Evaluate Jacobian and functions:

$$
J = \begin{bmatrix} \frac{\partial f_1}{\partial x} & \frac{\partial f_1}{\partial y} \\ \frac{\partial f_2}{\partial x} & \frac{\partial f_2}{\partial y} \end{bmatrix} = \begin{bmatrix} 2x - 1 & 1 \\ 2x & -1 \end{bmatrix}
$$

2. Use Newton-Raphson update:

$$\begin{bmatrix} x_{k+1} \\ y_{k+1} \end{bmatrix} = \begin{bmatrix} x_k \\ y_k \end{bmatrix} - J^{-1} \begin{bmatrix} f_1(x_k, y_k) \\ f_2(x_k, y_k) \end{bmatrix}$$

1st iteration:

$$J(1.2, 1.2) = \begin{bmatrix} 1.4 & 1 \\ 2.4 & -1 \end{bmatrix}$$

$$f_1(1.2, 1.2) = 1.2 + 1.44 - 1.2 - 0.75 = 0.69$$

$$f_2(1.2, 1.2) = 1.44 - 1.2 - 1 = -0.76$$

Solve for $\Delta x, \Delta y$:

$$J^{-1} = \frac{1}{-1.4 - 2.4} \begin{bmatrix} -1 & -1 \\ -2.4 & 1.4 \end{bmatrix}$$

$$J^{-1} = \begin{bmatrix} 0.2631 & 0.2631 \\ 0.6315 & -0.3684 \end{bmatrix}$$

$$\Delta = J^{-1} \begin{bmatrix} 0.69 \\ -0.76 \end{bmatrix} = \begin{bmatrix} -0.018417 \\ 0.715719 \end{bmatrix}$$

$$\begin{bmatrix} x_{k+1} \\ y_{k+1} \end{bmatrix} = \begin{bmatrix} 1.2 \\ 1.2 \end{bmatrix} - \begin{bmatrix} -0.018417 \\ 0.715719 \end{bmatrix} = \begin{bmatrix} 1.218417 \\ 0.484281 \end{bmatrix}$$

2nnd iteration:

$$J(1.218417, 0.484281) = \begin{bmatrix} 1.436834 & 1 \\ 2.436834 & -1 \end{bmatrix}$$

$$f_1(1.218417, 0.484281) = 0.000402985889000022914$$

$$f_2(1.218417, 0.484281) = 0.0002599858890002249$$

Solve for $\Delta x, \Delta y$:

$$J^{-1} = \begin{bmatrix} 0.258153242 & 0.258153242 \\ 0.6290766271 & -0.3709233729 \end{bmatrix}$$

$$\Delta = J^{-1} \begin{bmatrix} 0.000402985889000022914 \\ 0.0002599858890002249 \end{bmatrix} = \begin{bmatrix} 0.000171148313845321487 89 \\ 0.00015707416096679070974 \end{bmatrix}$$

$$\begin{bmatrix} x_{k+1} \\ y_{k+1} \end{bmatrix} = \begin{bmatrix} 1.218417 \\ 0.484281 \end{bmatrix} - \begin{bmatrix} 0.00017114831384532148789 \\ 0.00015707416096679070974 \end{bmatrix} = \begin{bmatrix} 1.218399885 \\ 0.48271025839 \end{bmatrix}$$

3rd iteration:

$$J(1.218399885, 0.48271025839) = \begin{bmatrix} 1.467997 & 1 \\ 2.4367997 & -1 \end{bmatrix}$$

$$f_1(1.21839988, 0.48271025839) = -0.0011913540259855804$$

$$f_2(1.21839988, 0.48271025839) = 0.0017880091940143394$$

Solve for $\Delta x, \Delta y$:

$$J^{-1} = \begin{bmatrix} 0.258157826 & 0.258157826 \\ 0.629078913 & -0.370921087 \end{bmatrix}$$

$$\Delta = J^{-1} \begin{bmatrix} -0.0011913540259855804 \\ 0.0017880091940143394 \end{bmatrix} = \begin{bmatrix} 0.00015403120104996912892 \\ -0.00141266660094749753355 \end{bmatrix}$$

$$\begin{bmatrix} x_{k+1} \\ y_{k+1} \end{bmatrix} = \begin{bmatrix} 1.218399885 \\ 0.48271025839 \end{bmatrix} - \begin{bmatrix} 0.00015403120104996912892 \\ -0.00141266660094749753355 \end{bmatrix} = \begin{bmatrix} 1.2182458537989500308 \\ 0.4841229243994749754 \end{bmatrix}$$

# Problem 3: LU Factorization and Matrix Inverse

## (a) Mass Balances for Reactors 2 and 3

For reactor 2:

$$-Q_{21}c_2 + Q_{12}c_1 - Q_{23}c_2 + Q_{32}c_3 - kV_2c_2 = 0$$

For reactor 3:

$$-Q_{31}c_3 + Q_{13}c_1 - Q_{32}c_3 + Q_{23}c_2 - kV_3c_3 = 0$$

## (b) Mass Balances for All Reactors

Combine the equations for all reactors:

$$\begin{aligned} Q_{in}c_{in} - (Q_{12} + Q_{13} + kV_1)c_1 + Q_{21}c_2 + Q_{31}c_3 &= 0 \\ Q_{12}c_1 - (Q_{21} + Q_{23} + kV_2)c_2 + Q_{32}c_3 &= 0 \\ Q_{13}c_1 + Q_{23}c_2 - (Q_{31} + Q_{32} + kV_3)c_3 &= 0 \end{aligned}$$

## (c) LU Factorization

The system in matrix form is $A\mathbf{c} = \mathbf{b}$.

$$A = \begin{bmatrix} -(Q_{12} + Q_{13} + kV_1) & Q_{21} & Q_{31} \\ Q_{12} & -(Q_{21} + Q_{23} + kV_2) & Q_{32} \\ Q_{13} & Q_{23} & -(Q_{31} + Q_{32} + kV_3) \end{bmatrix}$$

$$\mathbf{b} = \begin{bmatrix} -Q_{in}c_{in} \\ 0 \\ 0 \end{bmatrix}$$

Factorization is done in the python file script.py

## (d) Answer Questions Using Matrix Inverse

Values belowar are respective to reactor 1, 2, and 3.
(i) Steady-state concentrations:
73.62497731 62.00762389 67.4532583

(ii) If the inflow in the second reactor is set to zero:
73.62497731 62.00762389 67.4532583

(iii) If the inflow concentration to reactor 1 is doubled and reactor 2 is halved:
147.24995462 124.01524778 134.90651661

# Problem 4: Gauss Elimination

Given system:

$$-3x_2 + 7x_3 = 4$$

$$x_2 + 2x_2 - x_3 = 0$$

$$5x_1 - 2x_2 = 3$$

### (a) Compute the determinant analytically.

The matrix would be:

$$\begin{pmatrix} 0 & -3 & 7 \\ 1 & 2 & -1 \\ 5 & -2 & 0 \end{pmatrix}$$

$$\det(A) = 0 \cdot \begin{vmatrix} 2 & -1 \\ -2 & 0 \end{vmatrix} - (-3) \cdot \begin{vmatrix} 1 & -1 \\ 5 & 0 \end{vmatrix} + 7 \cdot \begin{vmatrix} 1 & 2 \\ 5 & -2 \end{vmatrix} = -69$$

### (b) Solve using Cramer's rule.

we replace the first column with to get the matrix $A_1$ for $x_1$:

$$\begin{pmatrix} 4 & -3 & 7 \\ 0 & 2 & -1 \\ 3 & -2 & 0 \end{pmatrix}$$

$$x_1 = \frac{\det(A_1)}{\det(A)} = 0.59420$$

we replace the second column with to get the matrix $A_2$ for $x_2$:

$$\begin{pmatrix} 0 & 4 & 7 \\ 1 & 0 & -1 \\ 5 & 3 & 0 \end{pmatrix}$$

$$x_2 = \frac{\det(A_2)}{\det(A)} = -0.14493$$

we replace the third column with to get the matrix $A_3$ for $x_3$:

$$\begin{pmatrix} 0 & -3 & 4 \\ 1 & 2 & 0 \\ 5 & -2 & 3 \end{pmatrix}$$

$$x_3 = \frac{\det(A_3)}{\det(A)} = 0.56521$$

## 0.1 Gaussian Elimination using Partial Pivoting:

$$\begin{pmatrix} 0 & -3 & 7 & \|4 \\ 1 & 2 & -1 & \|0 \\ 5 & -2 & 0 & \|3 \end{pmatrix}$$

We look at the first column and realize 5 is the largest and do row-swaps to make it the pivot element, which results in the matrix: switch the rows 1 and 3 to make the pivot element 5:

$$\begin{pmatrix} 5 & -2 & 0 & \|3 \\ 1 & 2 & -1 & \|0 \\ 0 & -3 & 7 & \|4 \end{pmatrix}$$

now, we need the transformation

$$r_2 = r_2 - \frac{1}{5} r_1$$

$$\begin{pmatrix} 5 & -2 & 0 & \|3 \\ 0 & -2.4 & -1 & \| - 0.6 \\ 0 & -3 & 7 & \|4 \end{pmatrix}$$

Next, we need the transformation

$$r_3 = r_3 - \frac{1}{3} r_2 \times 2.4$$

$$\begin{pmatrix} 5 & -2 & 0 & \|3 \\ 0 & -3 & 7 & \|4 \\ 0 & 0 & 4.6 & \|2.6 \end{pmatrix}$$

Now, we can back-substitute to get the values of $x_1, x_2, x_3$:

$$x_3 = \frac{2.6}{4.6} = 0.5652178913$$

$$x_2 = \frac{4 - 7 \times 0.5652178913}{-3} = -0.1449275362$$

$$x_1 = \frac{3 + 2 \times 0.1449275362}{5} = 0.5942028986$$

Finding the determinant: A=

$$\begin{pmatrix} 5 & -2 & 0 \\ 0 & -3 & 7 \\ 0 & 0 & 4.6 \end{pmatrix}$$

$$\det(A) = 5 \times -3 \times 4.6 = -69$$

which is equal to the derminant found in part (a).

(d) Substitute your results back into the original equations to check your solution:

$$-3 \times -0.1449275362 + 7 \times 0.5652178913 \approx 4$$

# Problem 5: Eigenvalues

Given matrix:

$$\begin{pmatrix} 20 & 3 & 2 \\ 3 & 9 & 4 \\ 2 & 4 & 12 \end{pmatrix}$$

## (a) Determine eigenvalues from characteristic polynomial

we can get the characteristic polynomial of a 3×3 matrix by expanding the below equation:

$$\lambda^3 - s_1\lambda^2 + s_2\lambda - \det A$$

Where S1 and S2 are the sum of the diagonal elements and sum of principal minors.
Here,

$$s_1 = 41$$

$$s_2 = 108 - 16 + 240 - 4 + 180 - 9 = 499$$

$$\det A = 1744$$

The equationw would then become:

$$\lambda^3 - 41\lambda^2 + 499\lambda - 1744 = 0$$

Obtained Eingenvalues are 21.72915618 13.18232626 6.08851756

## (b) Use the power method to find the largest eigenvalue and compare this with the result from (a)

The power method is used to find the largest eigenvalue of a matrix. Perform 3 iterations analytically:

1. **Choose an initial vector $x_0$:**

$$x_0 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

2. **Iteration 1:**

$$y_1 = Ax_0 = \begin{pmatrix} 20 & 3 & 2 \\ 3 & 9 & 4 \\ 2 & 4 & 12 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 25 \\ 16 \\ 18 \end{pmatrix}$$

$$\text{Normalize } y_1 :$$

$$25 \times \begin{pmatrix} 1 \\ 0.64 \\ 0.73 \end{pmatrix}$$

3. **Iteration 2:**

$$y_2 = Ax_1 = \begin{pmatrix} 20 & 3 & 2 \\ 3 & 9 & 4 \\ 2 & 4 & 12 \end{pmatrix} \begin{pmatrix} 1 \\ 0.64 \\ 0.73 \end{pmatrix} = \begin{pmatrix} 23.36 \\ 11.64 \\ 13.2 \end{pmatrix}$$

$$\text{Normalize } y_2 :$$

$$23.36 \times \begin{pmatrix} 1 \\ 0.4982876712 \\ 0.5650684932 \end{pmatrix}$$

4. **Iteration 3:**

$$y_3 = Ax_2 = \begin{pmatrix} 20 & 3 & 2 \\ 3 & 9 & 4 \\ 2 & 4 & 12 \end{pmatrix} \begin{pmatrix} 1 \\ 0.4982876712 \\ 0.5650684932 \end{pmatrix} = \begin{pmatrix} 22.625 \\ 9.744863014 \\ 10.7738726 \end{pmatrix}$$

The largest eigenvalue found using the power method is approximately 22.625, which is close to the exact eigenvalue of 22.251 found using the characteristic polynomial.

## (c) Use the inverse power method to find the smallest eigenvalue and compare this with the result from (a)

The python script gave the smallest eigen value as 6.088517562501856, which is close to the exact eigenvalue of 6.08852 found using the characteristic polynomial.