Problem 1 Three continuous stirred-tank reactors operating in series are used to produce ethanol. In each reactor the concentration of *EtOH*, $\mathcal{C}_i$ $\big($with $i \in \{1,2,3\}$ and $g/cm^3\big)$, is determined at the inlet of each reactor and can be expressed as,

$$\begin{cases} 17C_1 - 2C_2 - 3C_3 = 500 \\ -5C_1 + 21C_2 - 2C_3 = 200 \\ -5C_1 - 5C_2 + 22C_3 = 30 \end{cases}$$

(a) Assess the convergence of the resulting linear system;

(b) Calculate C_i after 2 iterations via Gauss-Seidel and Jacobi methods using $(34.0\ \ 19.0\ \ 13.0)^T$ as initial estimation;

(c) Design your own code (Matlab, Python, C, Fortran, etc) to solve this linear system using Gauss-Seidel, Jacobi and SOR ($\omega = 0.8$ and $\omega = 1.2$) iterative methods. Use $(0.0\ \ 1.0\ \ 1.0)^T$ as initial guess and

$$\frac{\left|\left|\boldsymbol{x}^{(k+1)} - \boldsymbol{x}^{(k)}\right|\right|}{\left|\left|\boldsymbol{x}^{(k)}\right|\right|} \leqslant 10^{-4}$$

as stoppage criteria. How many iterations will each method use to converge to the solution?

Problem 2 Solve the following system of equations via Gaussian elimination:

$$\begin{pmatrix} 7 & 1 & 3 & 2 \\ 3 & 12 & 1 & 5 \\ 0 & 0 & 8 & 1 \\ 1 & 3 & 2 & 9 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} 2 \\ 4 \\ 1 \\ 15 \end{pmatrix}$$

Problem 3 Calculate using Gauss-Jordan method:

(a) $\boldsymbol{A}^{-1}$ where $\boldsymbol{A} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 2 & 1 & 0 \\ 1 & 3 & 3 & 1 \end{pmatrix}$

(b) Solve $\boldsymbol{A}x = b$ using the inverse of $\boldsymbol{A}$ where $\boldsymbol{A} = \begin{pmatrix} 0 & 0 & 0 & 2 \\ 0 & 0 & 3 & 0 \\ 0 & 4 & 0 & 0 \\ 5 & 0 & 0 & 0 \end{pmatrix}$ and $b = (12\ \ 15\ \ 8\ \ 5)^T$.

P1

$$\begin{pmatrix} 17 & -2 & -3 \\ -5 & 21 & -2 \\ -5 & -5 & 22 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \begin{pmatrix} 500 \\ 200 \\ 30 \end{pmatrix}$$

(a) ~~[illegible]~~ A matrix $\underline{\underline{A}}$ fulfill the conditions for convergence in any iterative method if any of the conditions bellow is true:

- Strictly diagonal dominant, i.e.,

$$|a_{ii}| > \sum_{\substack{j=1 \\ j \neq i}}^{n} |a_{ij}| \quad , \; i = 1, 2, \ldots, n$$

row 1: $|17| > |-2| + |-3| \Leftrightarrow (T.)$

row 2: $|21| > |-5| + |-2| \Leftrightarrow (T)$

row 3. $|22| > |-5| + |-5| \Leftrightarrow (T)$

- symmetric and positive definite, i.e.,

$A^T = A$ (symmetric) $\Leftrightarrow (F)$

$z^T A z > 0$ for any matrix-column $\underline{\underline{z}}$

(b) Iterative methods with initial guess of

$$x^{(1)} = (34 \quad 19 \quad 13)^T$$

(b.1) Jacobi Method

$$x_i^{(k+1)} = \frac{1}{a_{ii}} \left[b_i - \sum_{\substack{i=1 \\ i \neq j}}^{n} a_{ij} x_j^{(k)} \right]$$

• 1st iteration ($k = 1$)

column 2 column 3

row 1
$\hookrightarrow$ * $x_1^{(2)} = \frac{1}{17} \left[500 - \left[(-2) \times 19 + (-3) \times 13 \right] \right]$
$i = 1$

$$x_1^{(2)} = 33.9412$$

column 1 column 3

row 2
$\hookrightarrow$ * $x_2^{(2)} = \frac{1}{21} \left[200 - \left[(-5) \times 34 + (-2) \times 13 \right] \right]$
$i = 2$

$$x_2^{(2)} = 18.8571$$

column 1 column 2

row 3
$\hookrightarrow$ * $x_3^{(2)} = \frac{1}{22} \left[30 - \left[(-5) \times 34 + (-5) \times 19 \right] \right]$
$i = 3$

$$x_3^{(2)} = 13.4091$$

$$\Longrightarrow x^{(2)} = (33.9412 \quad 18.8571 \quad 13.4091)^T$$

- 2^{nd} iteration $(K=2)$

* $x_1^{(3)} = \frac{1}{17}\left[500 - \left[(-2)\times \overset{18.8571}{\cancel{30}} + (-3)\times(13.4091)\right]\right]$

$x_1^{(3)} = 33.9966$

* $x_2^{(3)} = \frac{1}{21}\left[200 - \left[(-5)\times 33.9412 + (-2)\times 13.4091\right]\right]$

$x_2^{(3)} = 18.8821$

* $x_3^{(3)} = \frac{1}{22}\left[30 - \left[(-5)\times 33.9412 + (-5)\times 18.8571\right]\right]$

$x_3^{(3)} = 13.3632$

$$\underset{\sim}{x}^{(3)} = (33.9966 \quad 18.8821 \quad 13.3632)^T$$

(b.2) Gauss-Seidel Method

$$x_i^{(K+1)} = \frac{1}{a_{ii}} * \left(b_i - \sum_{j=1}^{i-1} a_{ij} x_j^{(K+1)} - \sum_{j=i+1}^{n} a_{ij} x_j^{(K)} \right)$$

- **1st iteration ($k=1$)**

$i=1$ $\quad * \; x_1^{(2)} = \frac{1}{17}\left\{500 - [0] - [(-2)\times 19 + (-3)\times 13]\right\}$

$x_1^{(2)} = 33.9412$

$i=2$ $\quad * \; x_2^{(2)} = \frac{1}{21}\left[200 - [(-5)\times 33.9412] - [(-2)\times 13]\right\}$

$x_2^{(2)} = 18.8431$

$i=3$ $\quad * \; x_3^{(2)} = \frac{1}{22}\left\{30 - [(-5)\times 33.9412 + (-5)\times 18.8431] - [0]\right\}$

$x_3^{(2)} = 13.3601$

- **2nd iteration ($k=2$)**

$i=1$ $\quad * \; x_1^{(3)} = \frac{1}{17}\left\{500 - [0] - [(-2)\times 18.8431 + (-3)\times 13.3601]\right\}$

$x_1^{(3)} = 33.9862$

$i=2$ $\quad * \; x_2^{(3)} = \frac{1}{21}\left\{200 - [(-5)\times 33.9862] - [(-2)\times 13.3601]\right\}$

$x_2^{(3)} = 18.8882$

$$* \; x_3^{(3)} = \frac{1}{22}\left\{30 - \left[(-5)\times 33.9862 + (-5)\times 18.8882\right] - [0]\right\}$$

$$x_3^{(3)} = 13.3805$$

$$\underset{\sim}{x}^{3} = (33.9862 \quad 18.8882 \quad 13.3805)^T$$

Note 1: Using a tolerance $\varepsilon = 10^{-4}$ such that the norm of two consecutive iterations is

$$IK = \frac{\|\underset{\sim}{x}^{(k+1)} - \underset{\sim}{x}^{(k)}\|}{\|\underset{\sim}{x}^{(k)}\|} \leqslant \varepsilon = 10^{-4}$$

This is used as a stoppage criteria during the iterative calculation.

(b.1) Jacobi method converged after 5 iterations to $\underset{\sim}{x} = (33.99588 \quad 18.89257 \quad 13.38342)^T$

With $IK = 3.78\times10^{-5}$

(b.2) Gauss-Seidel Method converged after $\underline{4}$ 6 iterations to $\underset{\sim}{x} = (33.996178 \quad 18.892757 \quad 13.3850)^T$ with $IK = 2.87 \times 10^{-5}$

(b.3) SOR Method converged after $\underline{5}$ iterations with $\omega = 0.80$ to $\underset{\sim}{x} = (33.994991 \quad 18.891865 \quad 13.382950)^T$ with $IK = 7.82 \times 10^{-5}$

(b.4) SOR Method converged after $\underline{5}$ iterations with $\omega = 1.20$ to $\underset{\sim}{x} = (33.996586 \quad 18.892868 \quad 13.383976)^T$ with $IK = 3.52 \times 10^{-5}$

Note 2: Using the same stoppage criteria – $\varepsilon = 10^{-4}$

(c) but using $\underset{\sim}{x}^{(1)} = (0 \quad 1 \quad 1)^T$:

- Jacobi: 10 iterations ($IK = 5.29 \times 10^{-5}$)
- GS: 6 iterations ($IK = 2.27 \times 10^{-5}$)
- SOR ($\omega = 0.80$): 10 iterations ($IK = 6.33 \times 10^{-5}$)
- SOR ($\omega = 1.20$): 7 iterations ($IK = 6.28 \times 10^{-5}$)

P2: Solving this system with Gaussian Elimination

$$\left(\begin{array}{cccc|c} 7 & 1 & 3 & 2 & 2 \\ 3 & 12 & 1 & 5 & 4 \\ 0 & 0 & 8 & 1 & 1 \\ 1 & 3 & 2 & 9 & 15 \end{array}\right) \xrightarrow[\times -\frac{R1}{7} + R4]{\times 1/7,\ \times -\frac{3R1}{7} + R2} \left(\begin{array}{cccc|c} 1 & 1/7 & 3/7 & 2/7 & 2/7 \\ 0 & 83/7 & 4/7 & 33/7 & 26/7 \\ 0 & 0 & 8 & 1 & 1 \\ 0 & 20/7 & 11/7 & 62/7 & 103/7 \end{array}\right) \quad \times -\frac{20}{83} R2 + R4$$

$$\rightarrow \left(\begin{array}{cccc|c} 1 & 1/7 & 3/7 & 2/7 & 2/7 \\ 0 & 83/7 & 4/7 & 33/7 & 26/7 \\ 0 & 0 & 8 & 1 & 1 \\ 0 & 0 & 833/581 & 4486/581 & 8029/581 \end{array}\right) \xrightarrow[\times 581]{(\times 7)} \left(\begin{array}{cccc|c} 1 & 1/7 & 3/7 & 2/7 & 2/7 \\ 0 & 83 & 4 & 33 & 26 \\ 0 & 0 & 8 & 1 & 1 \\ 0 & 0 & 833 & 4486 & 8029 \end{array}\right)$$

We still need to "zero" this!

Thus $R4 = -833/8\ R3 + R4$:

$$\left(\begin{array}{cccc|c} 1 & 1/7 & 3/7 & 2/7 & 2/7 \\ 0 & 83 & 4 & 33 & 26 \\ 0 & 0 & 8 & 1 & 1 \\ 0 & 0 & 0 & 35055/8 & 63399/8 \end{array}\right)$$

Now solving with backward elimination:

$$\begin{cases} x_1 + x_2/7 + 3x_3/7 + 2x_4/7 = 2/7 \\ 83x_2 + 4x_3 + 33x_4 = 26 \\ 8x_3 + x_4 = 1 \\ 35055/8\, x_4 = 63399 \end{cases}$$

$$\boxed{x_4 = 63399/35055} \cong 1.8086$$

$$8x_3 + \cancel{350550}\ \frac{63399}{35055} = 1$$

$$\boxed{x_3 = -\frac{28344}{280440}} \cong -0.1011$$

$$83x_2 + \cancel{4}\left(-\frac{28344}{\cancel{280440}_{70110}}\right) + 33 \times \frac{63399}{35055} = 26$$

$$\boxed{x_2 = -\frac{2333130}{5819130}} \cong -0.4009$$

$$\boxed{x_1 = \frac{2}{7} - \frac{1}{7}\left(-\frac{2333130}{5819130}\right) - \frac{3}{7}\left(-\frac{28344}{280440}\right) - \frac{2}{7}\ \frac{63399}{35055}}$$

$\cong 0.3851$

(b)

$$Ax = b \quad \times (A^{-1})$$

$$\underbrace{A^{-1}A}\, x = A^{-1}b$$

$$Ix = A^{-1}b$$

Swaping rows

$$\left(\begin{array}{cccc|cccc} 0 & 0 & 0 & 2 & 1 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 & 1 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 & 0 & 1 & 0 \\ 5 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{array}\right) \sim$$

$$\begin{array}{c} \left(\begin{array}{cccc|cccc} 5 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 4 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 3 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 2 & 1 & 0 & 0 & 0 \end{array}\right) \end{array} \begin{array}{l} \leftarrow \times 1/5 \\ \leftarrow \times 1/4 \\ \leftarrow \times 1/3 \\ \leftarrow \times 1/2 \end{array} \sim$$

$$\left(\begin{array}{cccc|cccc} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1/5 \\ 0 & 1 & 0 & 0 & 0 & 0 & 1/4 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1/3 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1/2 & 0 & 0 & 0 \end{array}\right)$$

$$\underbrace{\qquad\qquad}_{I} \qquad \underbrace{\qquad\qquad}_{A^{-1}}$$

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$$Ix = A^{-1}b$$

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 1/5 \\ 0 & 0 & 1/4 & 0 \\ 0 & 1/3 & 0 & 0 \\ 1/2 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 12 \\ 15 \\ 8 \\ 5 \end{pmatrix}$$

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \\ 5 \\ 6 \end{pmatrix}$$

P3

(a)

$$\begin{array}{c} A \quad\quad\quad I \\ \left(\begin{array}{cccc|cccc} 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 2 & 1 & 2 & 0 & 0 & 1 & 0 \\ 1 & 3 & 3 & 1 & 0 & 0 & 0 & 1 \end{array}\right) \end{array} \begin{array}{l} \\ -R1+R2 \\ -R1+R3 \\ -R1+R4 \end{array} \sim$$

$$\left(\begin{array}{cccc|cccc} 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 2 & 1 & 2 & -1 & 0 & 1 & 0 \\ 0 & 3 & 3 & 1 & -1 & 0 & 0 & 0 \end{array}\right) \begin{array}{l} \\ -2R2+R3 \\ -3R2+R4 \\ \end{array} \sim$$

$$\left(\begin{array}{cccc|cccc} 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 2 & 1 & -2 & 1 & 0 \\ 0 & 0 & 3 & 1 & 2 & -3 & 0 & 0 \end{array}\right) \begin{array}{l} \\ \\ -3R3+R4 \\ \end{array} \sim$$

$$\left(\begin{array}{cccc|cccc} 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 2 & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 5 & -1 & 3 & -3 & 0 \end{array}\right) \begin{array}{l} \\ \\ \\ \leftarrow \times 1/5 \end{array} \sim$$

[illegible]/10

$$\left(\begin{array}{cccc|cccc} 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 2 & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 1 & -1/5 & 3/5 & -3/5 & 0 \end{array}\right) \sim \quad -2R4 + R3$$

$$\left(\begin{array}{cccc|cccc} 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 7/5 & -16/5 & -1/5 & 0 \\ 0 & 0 & 0 & 1 & -1/5 & 3/5 & -3/5 & 0 \end{array}\right)$$

$$\underbrace{}_{I} \qquad \underbrace{}_{A^{-1}}$$