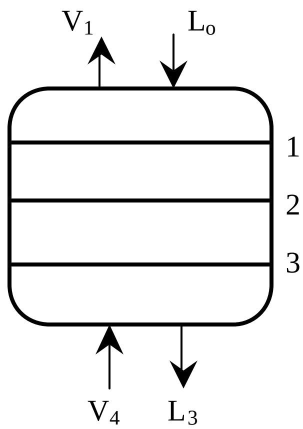
Problem Set # 3

(No need to submit)

1. Lean oil at the rate L_o = 1 gmol/s enters the top plate of a three-plate absorber. Rich gas at the rate V_4 = 2 gmole/s enter the absorber at the bottom of the column on plate 3 (see figure). If the reflux ratio, R_j, is given by $R_j = L_j/V_j = ½$ for j = 1, 2,3 find the corresponding flow rates V_1, V_2 and V_3 by Gauss elimination.



2. By using **LU** decomposition solve the systems

$$\mathbf{Ax}_1 = b_1 \text{ and } \mathbf{Ax}_2 = \mathbf{b}_2$$

where

$$A = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 1 & 4 & 9 & 16 \\ 1 & 8 & 27 & 64 \\ 1 & 16 & 81 & 256 \end{bmatrix} \qquad b_1 = \begin{bmatrix} 2 \\ 10 \\ 44 \\ 190 \end{bmatrix} \qquad b_2 = x_1 x_1^T \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

3. When a pure sample of a compound is bombarded by low energy electrons in a mass spectrometer the galvanometer shows peak heights that correspond to individual *m/e* (mass-to-electron) ratios for the resulting mixture of ions. For the i^{th} peak produced by a pure sample j, sensitivity, S_{ij}, can then be assigned. These coefficients are unique for each compound.

A distribution of peak heights may also be obtained for an n-component mixture that is to be analyzed for concentrations of each of the components. The height h_i of a certain (i^{th}) peak is a linear combination of the products of the individual sensitivities, S_{ij}, and component concentrations, C_j:

$$\sum_{j=1}^{m} S_{ij} C_j = h_i, \quad i = 1, 2, \ldots n.$$

In general, there may be more than n peaks, however, n most distinct ones are usually chosen so that individual concentrations are given by the solution of n simultaneous linear equations.

A typical mass spectra of an organic compound is shown below:

Peak #	Peak height	Component				
		CH_4	C_2H_4	C_2H_6	C_3H_6	C_3H_8
1	5.2	0.165	0.202	0.317	0.234	0.182
2	61.7	27.7	0.862	0.062	0.073	0.131
3	149.2	0	22.35	13.05	4.42	6.001
4	79.4	0	0	11.28	0	1.11
5	89.3	0	0	0	9.85	1.684
6	69.3	0	0	0	0	15.94

Find the concentration of individual components in the mixture. How do you solve above system when $m \neq n$?

4. The following series of $\mathbf{A}\,\mathbf{x} = \mathbf{b}$ problems need to be solved, where

$$\mathbf{A}\,\mathbf{x}_1 = \mathbf{x}_o$$

$$\mathbf{A}\,\mathbf{x}_2 = \mathbf{x}_1$$

•

•

$$\mathbf{A}\,\mathbf{x}_n = \mathbf{x}_{n-1}$$

where

$\mathbf{x}_o = [1 \;\; 1 \ldots\ldots \;\; 1]^T$ and matrix $\mathbf{A}$ is same for all the cases.

(a) How many total FLOPs (in terms of n) are required for all n solutions using full matrix Gauss elimination with partial pivoting for each of the above n problems? (Note that **A** is n x n matrix with n >> 1).

(b) Describe a better approach for computing the above n solutions and its total FLOP requirement.

Note that the above systems of equations need to be solved while finding eigenvalues and eigenvectors numerically using Inverse Power method.

5. It is necessary to solve $\mathbf{A}\ \mathbf{x}_i = i\ \mathbf{b}$, $i = 1, 100$ where **A** is tridiagonal with – 3 for all diagonal elements and 1 for all off-diagonal elements. Clearly state the most efficient strategy for solving above systems. Note that **A** and **b** are the same for each value of i.

6. Consider the system Ax = b, where

$$A = \begin{bmatrix} 3.01 & 6.03 & 1.99 \\ 1.27 & 4.16 & -1.23 \\ 0.987 & -4.81 & 9.34 \end{bmatrix}; \quad b = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

(a) Solve for x.

(b) Is the system ill-conditioned? What evidence is there to support your conclusion?

(c) Suppose that uncertainties of measurement give slight changes in some of the elements of A. Specifically, suppose a_{11} is 3.00 instead of 3.01 and a_{31} is 0.99 instead of 0.987. What changes does this cause in the solution vector?

(d) What is the condition number of the coefficient matrices in part (a)? Use 1-norm.

7. Consider the 2×2 linear system

$$\varepsilon X + (1/\varepsilon) Y = 1/\varepsilon \qquad \text{where } 0 < \varepsilon < 1$$

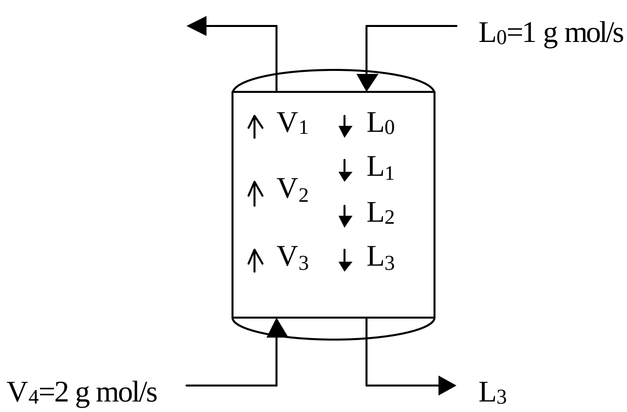
$$X + Y = 1$$

(a) Calculate the condition number using ∞-norm.

(b) State whether the above system is ill conditioned when $\varepsilon \approx 1$ and $\varepsilon \approx 0$.

Explain your answer using the values of determinant and the condition number.

Problem set #3



Flux ratio $R_j = \frac{L_j}{V_j} = \frac{1}{2}$, for j = 1,2,3 (given)

V_1, V_2, V_3 = ? (by G.E.)

Mass balance:

Plate (1): $L_0 + V_2 = L_1 + V_1$ (1)

Plate (2): $L_1 + V_3 = L_2 + V_2$ (2)

Plate (3): $L_2 + V_4 = L_3 + V_3$ (3)

Substituting $2L_j = V_j$ for j = 1,2,3

$$(1) \Rightarrow \quad 1 + V_2 = \frac{1}{2}V_1 + V_1$$

$$2 + 2V_2 = V_1 + 2V_1$$

$$3V_1 - 2V_2 = 2$$

$$(2) \Rightarrow \quad \frac{1}{2}V_1 + V_3 = \frac{1}{2}V_2 + V_2$$

$$V_1 + 2V_3 = V_2 + 2V_2$$

$$V_1 - 3V_2 + 2V_3 = 0$$

$$(3) \Rightarrow \quad \frac{1}{2}V_2 + 2 = \frac{1}{2}V_3 + V_3$$

$$V_2 + 4 = V_3 + 2V_3$$

$$V_2 - 3V_3 = -4$$

$$\text{or,} \quad \underset{A}{\begin{bmatrix} 3 & -2 & 0 \\ 1 & -3 & 2 \\ 0 & 1 & -3 \end{bmatrix}} \underset{x}{\begin{bmatrix} V_1 \\ V_2 \\ V_3 \end{bmatrix}} = \underset{b}{\begin{bmatrix} 2 \\ 0 \\ -4 \end{bmatrix}}$$

By Gauss elimination with partial pivoting

$$\left[A \middle| b\right] = \left[\begin{array}{ccc|c} 3 & -2 & 0 & 2 \\ 1 & -3 & 2 & 0 \\ 0 & 1 & -3 & -4 \end{array}\right]$$

$$\Downarrow$$

$$\left[\begin{array}{ccc|c} 3 & -2 & 0 & 2 \\ 0 & -7/3 & 2 & -2/3 \\ 0 & 1 & -3 & -4 \end{array}\right]$$

$$\Downarrow$$

$$\left[\begin{array}{ccc|c} 3 & -2 & 0 & 2 \\ 0 & -7/3 & 2 & -2/3 \\ 0 & 0 & -15/7 & -30/7 \end{array}\right]$$

U g

$$V_3 = \frac{g_3}{U_{33}} = \frac{-30/7}{-15/7} = 2$$

$$V_2 = \frac{1}{U_{22}}\left[g_2 - U_{23}\times V_3\right] = \frac{1}{-7/3}\left[\frac{-2}{3} - 2\times 2\right] = 2$$

$$V_1 = \frac{1}{U_{11}}\left[g_1 - U_{12}\times V_2 - U_{13}V_3\right] = \frac{1}{3}\left[2-(-2)2-0(2)\right] = \frac{6}{3} = 2 \quad \leftarrow$$

2. By using LU decomposition, solve the systems

$Ax_1 = b_1$ and $Ax_2 = b_2$

$$A = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 1 & 4 & 9 & 16 \\ 1 & 8 & 27 & 64 \\ 1 & 16 & 81 & 256 \end{bmatrix}, \quad b_1 = \begin{bmatrix} 2 \\ 10 \\ 44 \\ 190 \end{bmatrix}, \quad b_2 = x_1 x_1^T \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

$m_{21} = 1/1 = 1$

$m_{31} = 1/1 = 1$

$m_{41} = 1/1 = 1$

$$\begin{bmatrix} 1 & 2 & 3 & 4 \\ 0 & 2 & 6 & 12 \\ 0 & 6 & 24 & 60 \\ 0 & 14 & 78 & 252 \end{bmatrix}$$

$m_{32} = 6/2 = 3$

$m_{42} = 14/2 = 7$

$$\begin{bmatrix} 1 & 2 & 3 & 4 \\ 0 & 2 & 6 & 12 \\ 0 & 0 & 6 & 24 \\ 0 & 0 & 36 & 168 \end{bmatrix}$$

$m_{43} = 36/6 = 6$

$$\begin{bmatrix} 1 & 2 & 3 & 4 \\ 0 & 2 & 6 & 12 \\ 0 & 0 & 6 & 24 \\ 0 & 0 & 0 & 24 \end{bmatrix}$$

U

$$A = \underbrace{\begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 3 & 1 & 0 \\ 1 & 7 & 6 & 1 \end{bmatrix}}_{L} \underbrace{\begin{bmatrix} 1 & 2 & 3 & 4 \\ 0 & 2 & 6 & 12 \\ 0 & 0 & 6 & 24 \\ 0 & 0 & 0 & 24 \end{bmatrix}}_{U}$$

$Ly = b$

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 3 & 1 & 0 \\ 1 & 7 & 6 & 1 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix} = \begin{bmatrix} 2 \\ 10 \\ 44 \\ 190 \end{bmatrix}$$

$$y_1 = 2$$
$$y_1 + y_2 = 10 \quad \Rightarrow \quad y_2 = 10 - 2 = 8$$
$$y_1 + 3y_2 + y_3 = 44 \quad \Rightarrow \quad y_3 = 44 - 2 - 3\times 8 = 18$$
$$y_1 + 7y_2 + 6y_3 + 4y_4 = 190 \quad \Rightarrow \quad y_4 = 190 - 2 - 7\times 8 - 6\times 18 = 24$$

Ux = y

$$\begin{bmatrix} 1 & 2 & 3 & 4 \\ 0 & 2 & 6 & 12 \\ 0 & 0 & 6 & 24 \\ 0 & 0 & 0 & 24 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 2 \\ 8 \\ 18 \\ 24 \end{bmatrix}$$

$$x_4 = \frac{g_4}{U_{44}} = \frac{24}{24} = 1$$
$$x_3 = \frac{1}{U_{33}}\left[g_3 - U_{34}x_4\right] = \frac{1}{6}\left[18 - 24\times 1\right] = -1$$
$$x_2 = \frac{1}{U_{22}}\left[g_2 - U_{23}x_3 - U_{24}x_4\right] = \frac{1}{2}\left[8 - 6\times(-1) - 12\times 1\right] = 1$$
$$x_1 = \frac{1}{U_{11}}\left[g_1 - U_{12}x_2 - U_{13}x_3 - U_{14}x_4\right] = \frac{1}{1}\left[2 - 2\times 1 - 3\times(-1) - 4\times 1\right] = -1$$
$$x_1 = \begin{bmatrix} -1 \\ 1 \\ -1 \\ 1 \end{bmatrix} \quad \leftarrow$$

For $\quad Ax_2 = b_2$

$$b_2 = x_1 x_1^T \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} -1 \\ 1 \\ -1 \\ 1 \end{bmatrix} \begin{bmatrix} -1 & 1 & -1 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 2 & 3 & 4 \\ 1 & 4 & 9 & 16 \\ 1 & 8 & 27 & 64 \\ 1 & 16 & 81 & 256 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\therefore \text{solution of } \; Ax_2 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \; \text{ is } \; x_2 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

as A is non-singular and only possible solution for x_2 is 0.

3. We have 6 equations, but 5 unknown. However one equation must linearly dependent on the other 5 equations. This is because we have to satisfy the overall mass balance.

If we choose equations 2 to 6 ignoring equation number 1, we do not only have a upper triangular matrix but also a diagonally dominant system.

$$\begin{bmatrix} 27.7 & 0.862 & 0.062 & 0.073 & 0.131 \\ 0 & 22.35 & 13.05 & 4.42 & 6.001 \\ 0 & 0 & 11.28 & 0 & 1.11 \\ 0 & 0 & 0 & 9.85 & 1.684 \\ 0 & 0 & 0 & 0 & 15.94 \end{bmatrix} \begin{bmatrix} C_{CH_4} \\ C_{C_2H_4} \\ C_{C_2H_6} \\ C_{C_3H_6} \\ C_{C_3H_8} \end{bmatrix} = \begin{bmatrix} 61.7 \\ 149.2 \\ 79.4 \\ 89.3 \\ 69.3 \end{bmatrix}$$

$$C_{C_3H_8} = C_5 = \frac{69.3}{15.94} = 4.3476$$

$$C_{C_3H_6} = C_4 = \frac{1}{U_{44}}\left[g_4 - U_{45}C_5\right] = \frac{1}{9.85}\left[89.3 - 1.684 \times 4.3776\right] = 8.3227$$

$$C_{C_2H_6} = C_3 = \frac{1}{U_{33}}\left[g_3 - U_{34}C_4 - U_{35}C_5\right] = \frac{1}{11.28}\left[79.4 - 0 \times C_4 - 1.11 \times 4.3476\right] = 6.6111$$

$$C_{C_2H_4} = C_2 = \frac{1}{U_{22}}\left[g_2 - U_{23}C_3 - U_{24}C_4 - U_{25}C_5\right]$$

$$= \frac{1}{22.35}\left[149.2 - 13.05 \times 6.6111 - 4.42 \times 8.3227 - 6.001 \times 4.3476\right] = 0.0022$$

$$C_{CH_4} = C_1 = \frac{1}{U_{11}}\left[g_1 - U_{12}C_2 - U_{13}C_3 - U_{14}C_4 - U_{15}C_5\right]$$

$$= \frac{1}{27.7}\left[61.7 - 0.862 \times 0.0022 - 0.062 \times 6.6111 - 0.073 \times 8.3227 - 0.131 \times 4.3476\right]$$

$$= 2.17$$

4.

(a) A is n x n

\# of flops when using G.E for 1 problem

$$= \frac{n^3}{3}(\text{for F.E}) + \frac{n^2}{2}(\text{forB.S})$$

For n-equations

$$\#\text{of Flops} = n\left(\frac{n^3}{3} + \frac{n^2}{2}\right) = \frac{n^4}{3} + \frac{n^3}{2}$$

(b) Use LU decomposition

- compute LU of A once and solve the n-equations by B.S & F.S.

$$\#\text{of Flops} = \frac{n^3}{3} + n \times n^2 = \frac{n^3}{3} + n^3 = \frac{4}{3}n^3$$

(for LU)

\# of eqns:

(for F.S & B.S)

<u>OR</u>

Use Gauss-Jordon method

- compute A^{-1}, since all problem involve same A

$\frac{4n^3}{3} + n \times n^2$ (for multiplication)

(A^{-1} by G.J)

$= \frac{7}{3} n^3$ (total # of flops)

7.
Consider the 2 x 2 linear system,

$$\varepsilon x + \left(\frac{1}{\varepsilon}\right) y = \frac{1}{\varepsilon} \quad \text{where} 0 < \varepsilon < 1$$

$x + y = 1$

(a) Calculate the condition number using α_norm

(b) State whether the above system is ill conditioned when $\varepsilon \approx 1$ and $\varepsilon \approx 0$. Explain your answer using the values of determinant and the condition number.

$$\varepsilon x + \left(\frac{1}{\varepsilon}\right) y = \frac{1}{\varepsilon},\ 0 < \varepsilon < 1$$

$x + y = 1$

$$\begin{bmatrix} \varepsilon & 1/\varepsilon \\ 1 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 1/\varepsilon \\ 1 \end{bmatrix}$$

A x = b

$$\|A\|_\alpha = \text{max row sum} = \left\{\varepsilon + \frac{1}{\varepsilon}, 2\right\} = \varepsilon + \frac{1}{\varepsilon} = \frac{\varepsilon^2 + 1}{\varepsilon}$$

$$A^{-1} = \frac{1}{\det A} \begin{bmatrix} 1 & -1/\varepsilon \\ -1 & \varepsilon \end{bmatrix} = \frac{1}{\varepsilon - 1/\varepsilon} \begin{bmatrix} 1 & -1/\varepsilon \\ -1 & \varepsilon \end{bmatrix} = \frac{1}{\varepsilon^2 - 1/\varepsilon} \begin{bmatrix} 1 & -1/\varepsilon \\ -1 & \varepsilon \end{bmatrix} = \frac{\varepsilon}{\varepsilon^2 - 1} \begin{bmatrix} 1 & -1/\varepsilon \\ -1 & \varepsilon \end{bmatrix}$$

$$\left\|A_\alpha^{-1}\right\| = \text{maxrowsum} = \frac{\varepsilon}{\varepsilon^2 - 1} \text{max rowsum}$$

$$= \frac{\varepsilon}{\varepsilon - 1} \left\{1 + \frac{1}{\varepsilon}, 1 + \varepsilon\right\}$$

$$= \frac{e}{e^2 - 1} \left(1 + \frac{1}{e}\right) = \frac{e}{e^2 - 1} \frac{(e+1)}{e}$$

$$= \frac{(\varepsilon + 1)}{(\varepsilon + 1)(\varepsilon - 1)} = \frac{1}{(\varepsilon - 1)}$$

Condition number = $r_A = \|A\| \|A^{-1}\|$

$$= \frac{\varepsilon^2 + 1}{\varepsilon} \frac{1}{(\varepsilon - 1)} = \frac{\varepsilon^2 + 1}{\varepsilon^2 - \varepsilon}$$

If $\varepsilon \approx 1$

$$\det A = \frac{\varepsilon^2 - 1}{\varepsilon}, \quad \det A \approx 0$$

$$r_A = \frac{\varepsilon^2+1}{\varepsilon^2-1}, \quad r_A = \text{large}$$

$\therefore$ The matrix is ill condition.

If $\varepsilon \approx 0$

$$\det A = \frac{\varepsilon^2-1}{\varepsilon}, \quad \det A \;□\; \text{large}$$

$$r_A = \frac{\varepsilon^2+1}{\varepsilon^2-1}, \quad r_A = \text{large}$$

Since det. is large, matrix A is not ill conditioned. r is large because some of the element of the matrix is large when $\varepsilon = 0$, and it is reflected in r-valves.

$$\begin{bmatrix} \varepsilon & 1/\varepsilon \\ 1 & 1 \end{bmatrix} \Rightarrow \begin{bmatrix} \approx 0 & \text{large} \\ 1 & 1 \end{bmatrix}$$

When $\varepsilon = 0$, $r_A > 1$

$$\det A = \frac{\varepsilon}{\varepsilon^2-1} \approx 1$$

$\therefore$ The matrix is ill conditioned.