Fall, 2023 **06-606**

Nonlinear Optimization in Process Systems Engineering

Due 9/7/23

1. Construct the L/U algorithm using the Crout decomposition, using the same notation as in class.

2. For the following system of linear equations
   a) Solve using Gauss elimination
   b) Develop the LU factors and calculate the determinant
   c) Resolve using L and U for the RHS provided

$$2x_1 + 4x_2 - x_4 = b_1$$

$$- x_3 + x_4 = b_2$$

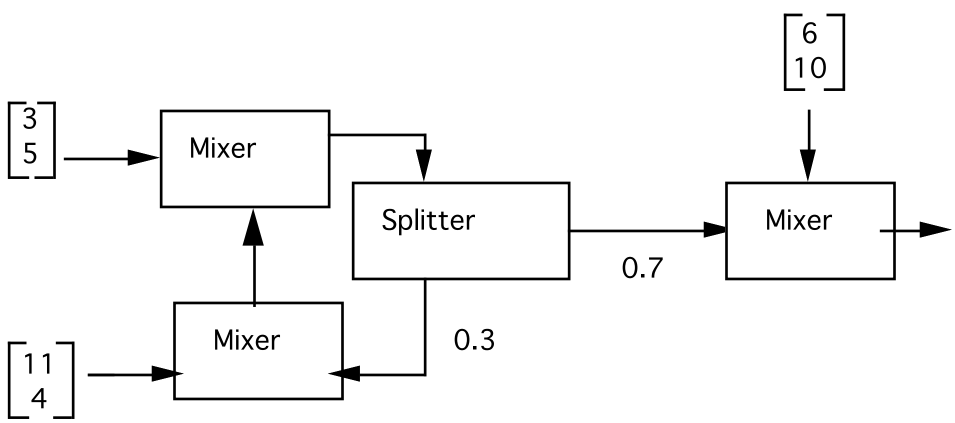
$$x_1 + 6x_2 + 7x_3 = b_3$$

$$x_1 + x_4 = b_4$$

$$\underline{b}^T = (3,2,5,4)$$

3. Retrieve the LU and QR decomposition programs from LINPACK in NETLIB and solve problem 2 again using both procedures. Alternately, MathCAD or MATLAB may be used.

4. Derive the linear balance equations for the problem



   a) Develop pivot sequences using the Markowitz criterion. Indicate the number of new non-zero elements created in developing L and U.

   b) For this case calculate L and U and solve the material balance equations.

1. Crout decomposition

1) let $r = 1$
2) let $u_{rr} = 1$
3) Generate column r for L

$$l_{ir} = a_{ir} - \sum_{k=1}^{r-1} l_{ik} u_{kr} \qquad i \geq r$$

4) Generate row r for U

$$u_{rj} = \left(a_{rj} - \sum_{k=1}^{r-1} l_{rk} u_{kj}\right) / l_{rr} \qquad j \geq r$$

5) Solve
$Ly = b \qquad y_i = \left(b_i - \sum_{j=1}^{i-1} l_{ij} y_j\right) / l_{ii} \quad i = 1, n$
$Ux = y \qquad x_i = \left(y_i - \sum_{j=i+1}^{n} u_{ij} x_j\right) \quad i = n \to 1$

3 a) *Gaussian elimination*

$$2x_1 + 4x_2 - x_4 = 3$$

$$x_1 + 6x_2 + 7x_3 = 5$$

$$-x_3 + x_4 \quad 2$$

$$x_1 + x_4 = 4$$

$$\begin{bmatrix} 2 & 4 & 0 & -1 & 3 \\ 1 & 6 & 7 & 0 & 5 \\ 0 & 0 & -1 & 1 & 2 \\ 1 & 0 & 0 & 1 & 4 \end{bmatrix} \longrightarrow \begin{bmatrix} 2 & 4 & 0 & -1 & 3 \\ 0 & 4 & 7 & 1/2 & 7/2 \\ 0 & 0 & -1 & 1 & 2 \\ 0 & -2 & 0 & 3/2 & 5/2 \end{bmatrix}$$

$$\begin{bmatrix} 2 & 4 & 0 & -1 & 3 \\ 0 & 4 & 7 & 1/2 & 7/2 \\ 0 & 0 & -1 & 1 & 2 \\ 0 & 0 & 7/2 & 7/4 & 17/4 \end{bmatrix} \longrightarrow \begin{bmatrix} 2 & 4 & 0 & -1 & 3 \\ 0 & 4 & 7 & 1/2 & 7/2 \\ 0 & 0 & -1 & 1 & 2 \\ 0 & 0 & 0 & 21/4 & 45/4 \end{bmatrix}$$

$$x_1 = 1.8571$$

$$x_2 = 0.3571$$

$$x_3 = 0.1428$$

$$x_4 = 2.1429$$

b) *L/U decomposition*

$$\begin{bmatrix} 2 & 4 & 0 & -1 \\ 1 & 6 & 7 & 0 \\ 0 & 0 & -1 & 1 \\ 1 & 0 & 0 & 1 \end{bmatrix} = \overset{L}{\begin{bmatrix} 1 & 0 & 0 & 0 \\ 1/2 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1/2 & -1/2 & -7/2 & 1 \end{bmatrix}} \times$$

$$\det(A) = \det(L)\det(U) \quad \underset{U}{\begin{bmatrix} 2 & 4 & 0 & -1 \\ 0 & 4 & 7 & 1/2 \\ 0 & 0 & -1 & 1 \\ 0 & 0 & 0 & 21/4 \end{bmatrix}}$$

$$= (-42)(-1)$$

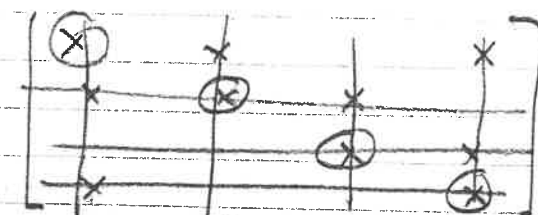
one row exchange $= 42$

c.) alternate right hand side:

$$LU = \begin{bmatrix} 1 \\ 6 \\ 7 \\ 3 \end{bmatrix} \qquad Ly = b \qquad y = \begin{bmatrix} 1 \\ 5.5 \\ 7 \\ 29.75 \end{bmatrix}$$

$$Ux = y \qquad x = \begin{bmatrix} -2.667 \\ 3.0 \\ -1.333 \\ 5.667 \end{bmatrix}$$

d.)



This sequence is not unique!

3 4 1 2

$$\begin{array}{c|c} & \begin{array}{ccccc} 3 & 4 & 1 & 2 & \end{array} \\ \begin{array}{c} 3 \\ 4 \\ 1 \\ 2 \end{array} & \begin{bmatrix} -1 & 1 & 0 & 0 & 2 \\ 0 & 1 & 1 & 0 & 4 \\ 0 & -1 & 2 & 4 & 3 \\ 7 & 0 & 1 & 6 & 5 \end{bmatrix} \end{array}$$

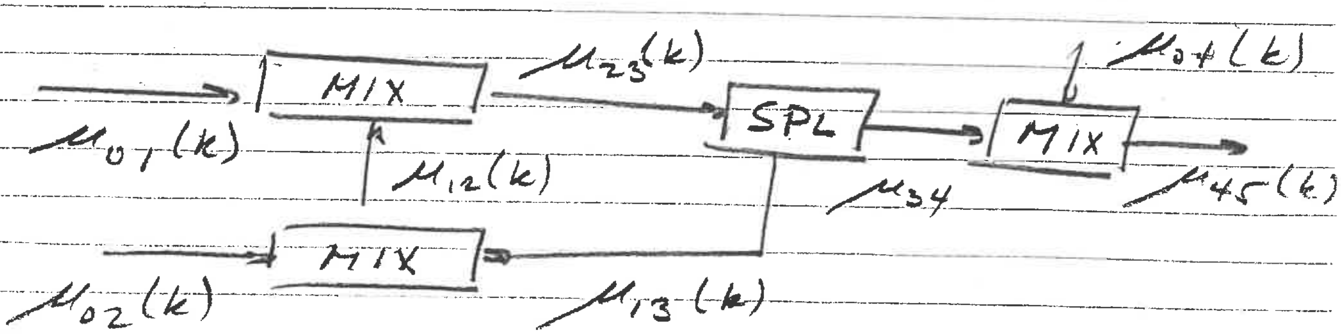
$$\longrightarrow \begin{bmatrix} -1 & 1 & 0 & 0 & 2 \\ 0 & 1 & 1 & 0 & 4 \\ 0 & -1 & 2 & 4 & 3 \\ 0 & 7 & 1 & 6 & 19 \end{bmatrix} \longrightarrow \begin{bmatrix} -1 & 1 & 0 & 0 & 2 \\ 0 & 1 & 1 & 0 & 4 \\ 0 & 0 & 3 & 4 & 7 \\ 0 & 0 & -6 & 6 & -9 \end{bmatrix}$$

$$\begin{bmatrix} -1 & 1 & 0 & 0 & 2 \\ 0 & 1 & 1 & 0 & 4 \\ 0 & 0 & 3 & 4 & 7 \\ 0 & 0 & 0 & 14 & 5 \end{bmatrix}$$

$x_1 = 1.8571$
$x_2 = 0.3571$
$x_3 = 0.14286$
$x_4 = 2.14286$

3. Verify solutions for #2 with QR + LU.

4)



$$\mu_{23}(k) = \mu_{01}(k) + \mu_{12}(k)$$
$$\mu_{12}(k) = \mu_{13}(k) + \mu_{02}(k)$$
$$\mu_{13}(k) = 0.3\,\mu_{23}(k)$$
$$\mu_{34}(k) = 0.7\,\mu_{23}(k)$$
$$\mu_{45}(k) = \mu_{04}(k) + \mu_{34}(k)$$

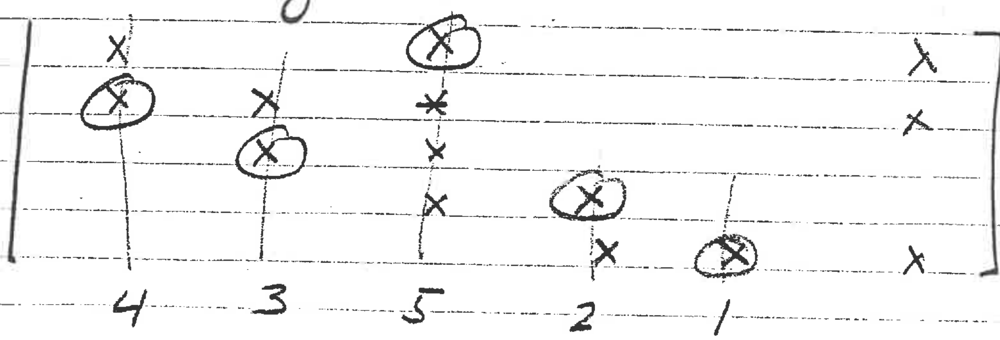
a) min row / min col. Since system is decoupled, can deal with a 5x5 system and get similar results since A and B do not interact.

$$\begin{array}{cccccc}
\mu_{12} & \mu_{13} & \mu_{23} & \mu_{34} & \mu_{45} & RHS \\
\hline
\times & & \times & & & \times \\
\times & \times & * & & & \times \\
 & \times & \times & & & \\
 & & \times & \times & & \\
 & & & \times & \times & \times \\
\hline
4 & 3 & 5 & 2 & 1 &
\end{array}$$

fillin due to 3.

1 (2) fill-ins.

Markowitz



Markowitz criterion (min $(\rho_i - 1)(\gamma_i - 1)$) can yield same sequence as min row / min col. for this problem.

b) solution to mass balance problem.

$$\mu_{12} = \begin{bmatrix} 17 \\ 7.86 \end{bmatrix} \qquad \mu_{13} = \begin{bmatrix} 6 \\ 3.86 \end{bmatrix}$$

$$\mu_{23} = \begin{bmatrix} 20 \\ 12.86 \end{bmatrix} \qquad \mu_{34} = \begin{bmatrix} 14.0 \\ 9 \end{bmatrix}$$

$$\mu_{45} = \begin{bmatrix} 20 \\ 19 \end{bmatrix}$$