Chemical Engineering Example for the LU Decomposition Method
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Example 1

A liquid-liquid extraction process conducted in the Electrochemical Materials Laboratory involved the extraction of nickel from the aqueous phase into an organic phase. A typical set of experimental data from the laboratory is given below.

Ni aqueous phase, a (g/l)	2	2.5	3
Ni organic phase, g (g/l)	8.57	10	12

Assuming g is the amount of Ni in the organic phase and a is the amount of Ni in the aqueous phase, the quadratic interpolant that estimates g is given by

$$g = x_1 a^2 + x_2 a + x_3,\ 2 \le a \le 3$$

The solution for the unknowns x_1, x_2, and x_3 is given by

$$\begin{bmatrix} 4 & 2 & 1 \\ 6.25 & 2.5 & 1 \\ 9 & 3 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 8.57 \\ 10 \\ 12 \end{bmatrix}$$

Find the values of x_1, x_2, and x_3 using LU decomposition. Estimate the amount of nickel in the organic phase when $2.3\,\text{g/l}$ is in the aqueous phase using quadratic interpolation.

Solution

$$[A] = [L][U] = \begin{bmatrix} 1 & 0 & 0 \\ \ell_{21} & 1 & 0 \\ \ell_{31} & \ell_{32} & 1 \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}$$

The $[U]$ matrix is the same as the one found at the end of the forward elimination steps of the naïve Gauss elimination method.

Forward Elimination of Unknowns

Since there are three equations, there will be two steps of forward elimination of unknowns.

$$\begin{bmatrix} 4 & 2 & 1 \\ 6.25 & 2.5 & 1 \\ 9 & 3 & 1 \end{bmatrix}$$

First step

Divide Row 1 by 4 and multiply it by 6.25, that is, multiply it by $6.25/4 = 1.5625$. Then subtract the result from Row 2.

$$\text{Row 2} - (\text{Row 1} \times (1.5625)) = \begin{bmatrix} 4 & 2 & 1 \\ 0 & -0.625 & -0.5625 \\ 9 & 3 & 1 \end{bmatrix}$$

Divide Row 1 by 4 and multiply it by 9, that is, multiply it by $9/4 = 2.25$. Then subtract the result from Row 3.

$$\text{Row 3} - (\text{Row 1} \times (2.25)) = \begin{bmatrix} 4 & 2 & 1 \\ 0 & -0.625 & -0.5625 \\ 0 & -1.5 & 0.1 \end{bmatrix}$$

Second step

Now divide Row 2 by -0.625 and multiply it by -1.5, that is, multiply it by $-1.5/-0.625 = 2.4$. Then subtract the result from Row 3.

$$\text{Row 3} - (\text{Row 2} \times (2.4)) = \begin{bmatrix} 4 & 2 & 1 \\ 0 & -0.625 & -0.5625 \\ 0 & 0 & 0.1 \end{bmatrix}$$

$$[U] = \begin{bmatrix} 4 & 2 & 1 \\ 0 & -0.625 & -0.5625 \\ 0 & 0 & 0.1 \end{bmatrix}$$

Now find $[L]$.

$$[L]=\begin{bmatrix} 1 & 0 & 0 \\ \ell_{21} & 1 & 0 \\ \ell_{31} & \ell_{32} & 1 \end{bmatrix}$$

From Step 1 of the forward elimination process

$$\ell_{21}=\frac{6.25}{4}=1.5625$$

$$\ell_{31}=\frac{9}{4}=2.25$$

From Step 2 of the forward elimination process

$$\ell_{32}=\frac{-1.5}{-0.625}=2.4$$

$$[L]=\begin{bmatrix} 1 & 0 & 0 \\ 1.5625 & 1 & 0 \\ 2.25 & 2.4 & 1 \end{bmatrix}$$

Now that $[L]$ and $[U]$ are known, solve $[L][Z]=[C]$.

$$\begin{bmatrix} 1 & 0 & 0 \\ 1.5625 & 1 & 0 \\ 2.25 & 2.4 & 1 \end{bmatrix}\begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix}=\begin{bmatrix} 8.57 \\ 10 \\ 12 \end{bmatrix}$$

gives

$$z_1=8.57$$

$$1.5625z_1+z_2=10$$

$$2.25z_1+2.4z_2+z_3=12$$

Forward substitution starting from the first equation gives

$$z_1=8.57$$

$$z_2 = 10 - 1.5625 z_1$$

$$= 10 - 1.5625 \times 8.57$$

$$= -3.3906$$

$$z_3 = 12 - 2.25 z_1 - 2.4 z_2$$

$$= 12 - 2.25 \times 8.57 - 2.4 \times (-3.3906)$$

$$= 0.855$$

Hence

$$[Z] = \begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} = \begin{bmatrix} 8.57 \\ -3.3906 \\ 0.855 \end{bmatrix}$$

Now solve $[U][X] = [Z]$.

$$\begin{bmatrix} 4 & 2 & 1 \\ 0 & -0.625 & -0.5625 \\ 0 & 0 & 0.1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 8.57 \\ -3.3906 \\ 0.855 \end{bmatrix}$$

$$4x_1 + 2x_2 + x_3 = 8.57$$

$$-0.625 x_2 + (-0.5625) x_3 = -3.3906$$

$$0.1 x_3 = 0.855$$

From the third equation,

$$0.1 x_3 = 0.855$$

$$x_3 = \frac{0.855}{0.1}$$

$$= 8.55$$

Substituting the value of x_3 in the second equation,

$$-0.625x_2 + (-0.5625)x_3 = -3.3906$$

$$x_2 = \frac{-3.3906 - (-0.5625)x_3}{-0.625}$$

$$= \frac{-3.3906 - (-0.5625) \times 8.55}{-0.625}$$

$$= -2.27$$

Substituting the value of x_2 and x_3 in the first equation,

$$4x_1 + 2x_2 + x_3 = 8.57$$

$$x_1 = \frac{8.57 - 2x_2 - x_3}{4}$$

$$= \frac{8.57 - 2 \times (-2.27) - 8.55}{4}$$

$$= 1.14$$

The solution vector is

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1.14 \\ -2.27 \\ 8.55 \end{bmatrix}$$

The polynomial that passes through the three data points is then

$$g(a) = x_1 a^2 + x_2 a + x_3$$

$$= 1.14a^2 + (-2.27)a + 8.55, 2 \le a \le 3$$

where g is the amount of nickel in the organic phase and a is the amount of nickel in the aqueous phase.

When $2.3\,\mathrm{g/l}$ is in the aqueous phase, using quadratic interpolation, the estimated amount of nickel in the organic phase is

$$g(2.3) = 1.14 \times (2.3)^2 + (-2.27) \times (2.3) + 8.55$$

$$= 9.3596\,\mathrm{g/l}$$