# Chapter 04.07
# LU Decomposition – More Examples
# Chemical Engineering

**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, $a\ (\mathrm{g/l})$ | 2 | 2.5 | 3 |
| Ni organic phase, $g\ (\mathrm{g/l})$ | 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 $2.3\,\mathrm{g/l}$ 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

$$z_1 = 8.57$$
$$\begin{aligned} z_2 &= 10 - 1.5625z_1 \\ &= 10 - 1.5625 \times 8.57 \\ &= -3.3906 \end{aligned}$$
$$\begin{aligned} z_3 &= 12 - 2.25z_1 - 2.4z_2 \\ &= 12 - 2.25 \times 8.57 - 2.4 \times (-3.3906) \\ &= 0.855 \end{aligned}$$

Hence

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

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

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

$$4x_1 + 2x_2 + x_3 = 8.57$$
$$-0.625x_2 + (-0.5625)x_3 = -3.3906$$
$$0.1x_3 = 0.855$$

From the third equation,

$$0.1x_3 = 0.855$$
$$\begin{aligned} x_3 &= \frac{0.855}{0.1} \\ &= 8.55 \end{aligned}$$

Substituting the value of $x_3$ in the second equation,

$$-0.625x_2 + (-0.5625)x_3 = -3.3906$$
$$\begin{aligned} x_2 &= \frac{-3.3906 - (-0.5625)x_3}{-0.625} \\ &= \frac{-3.3906 - (-0.5625) \times 8.55}{-0.625} \\ &= -2.27 \end{aligned}$$

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

$$g(2.3) = 1.14\times(2.3)^2 + (-2.27)\times(2.3) + 8.55$$
$$= 9.3596\,\text{g/l}$$

| SIMULTANEOUS LINEAR EQUATIONS | |
|---|---|
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