Chapter 04.06
Gaussian Elimination – 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 naïve Gauss elimination. Estimate the amount of nickel in the organic phase when $2.3\,\mathrm{g/l}$ is in the aqueous phase using quadratic interpolation.

Solution

Forward Elimination of Unknowns

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

First step

Divide Row 1 by 4 and then multiply it by 6.25, that is, multiply Row 1 by $6.25/4 = 1.5625$.

$$\text{Row } 1 \times (1.5625) = \begin{bmatrix} 6.25 & 3.125 & 1.5625 \end{bmatrix} \quad \begin{bmatrix} 13.391 \end{bmatrix}$$

Subtract the result from Row 2 to get

$$\begin{bmatrix} 4 & 2 & 1 \\ 0 & -0.625 & -0.5625 \\ 9 & 3 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 8.57 \\ -3.3906 \\ 12 \end{bmatrix}$$

Divide Row 1 by 4 and then multiply it by 9, that is, multiply Row 1 by $9/4 = 2.25$.

$$\text{Row } 1 \times (2.25) = \begin{bmatrix} 9 & 4.5 & 2.25 \end{bmatrix} \quad \begin{bmatrix} 19.283 \end{bmatrix}$$

Subtract the result from Row 3 to get

$$\begin{bmatrix} 4 & 2 & 1 \\ 0 & -0.625 & -0.5625 \\ 0 & -1.5 & -1.25 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 8.57 \\ -3.3906 \\ -7.2825 \end{bmatrix}$$

Second step

We now divide Row 2 by -0.625 and then multiply it by -1.5, that is, multiply Row 2 by $-1.5/-0.625 = 2.4$.

$$\text{Row } 2 \times (2.4) = \begin{bmatrix} 0 & -1.5 & -1.35 \end{bmatrix} \quad \begin{bmatrix} -8.1375 \end{bmatrix}$$

Subtract the result from Row 3 to get

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

Back Substitution

From the third equation,

$$0.1x_3 = 0.855$$

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

$$= 8.55$$

Substituting the value of x_3 in the second equation,

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

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

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

$$= -2.27$$

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

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

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

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

$$= 1.14$$

Hence 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

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

$$= 1.14a^2 + (-2.27)a + 8.55$$

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

When 2.3g/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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