Chapter 04.08  
Gauss-Seidel Method – 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.

<table>
<thead>
<tr>
<th>Ni aqueous phase, $a$ (g/l)</th>
<th>2</th>
<th>2.5</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ni organic phase, $g$ (g/l)</td>
<td>8.57</td>
<td>10</td>
<td>12</td>
</tr>
</tbody>
</table>

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

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

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 the Gauss-Seidel method. Estimate the amount of nickel in the organic phase when 2.3 g/l is in the aqueous phase using quadratic interpolation. Use

$$
\begin{bmatrix}
x_1 \\
x_2 \\
x_3
\end{bmatrix} =
\begin{bmatrix}
1 \\
1 \\
1
\end{bmatrix}
$$

as the initial guess and conduct two iterations.

Solution

Rewriting the equations gives

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

$$
x_2 = \frac{10 - 6.25x_1 - x_3}{2.5}
$$

$$
x_3 = \frac{12 - 9x_1 - 3x_2}{1}
$$

04.08.1
Iteration #1

Given the initial guess of the solution vector as

\[
\begin{bmatrix}
  x_1 \\
  x_2 \\
  x_3 
\end{bmatrix}
= \begin{bmatrix}
  1 \\
  1 \\
  1 
\end{bmatrix}
\]

we get

\[
x_1 = \frac{8.57 - 2 \times 1 - 1}{4} = 1.3925
\]
\[
x_2 = \frac{10 - 6.25 \times 1.3925 - 1}{2.5} = 0.11875
\]
\[
x_3 = \frac{12 - 9 \times 1.3925 - 3 \times 0.11875}{1} = -0.88875
\]

The absolute relative approximate error for each \(x\), then is

\[
|\varepsilon_x_1| = \left|\frac{1.3925 - 1}{1.3925}\right| \times 100 = 28.187\%
\]
\[
|\varepsilon_x_2| = \left|\frac{0.11875 - 1}{0.11875}\right| \times 100 = 742.11\%
\]
\[
|\varepsilon_x_3| = \left|\frac{-0.88875 - 1}{-0.88875}\right| \times 100 = 212.52\%
\]

At the end of the first iteration, the estimate of the solution vector is

\[
\begin{bmatrix}
  x_1 \\
  x_2 \\
  x_3 
\end{bmatrix}
= \begin{bmatrix}
  1.3925 \\
  0.11875 \\
  -0.88875 
\end{bmatrix}
\]

and the maximum absolute relative approximate error is 742.11\%.

Iteration #2

The estimate of the solution vector at the end of Iteration #1 is

\[
\begin{bmatrix}
  x_1 \\
  x_2 \\
  x_3 
\end{bmatrix}
= \begin{bmatrix}
  1.3925 \\
  0.11875 \\
  -0.88875 
\end{bmatrix}
\]

Now we get

\[
x_1 = \frac{8.57 - 2 \times 0.11875 - (-0.88875)}{4}
= 2.3053
\]
\[ x_2 = \frac{10 - 6.25 \times 2.3053 - (-0.88875)}{2.5} = -1.4078 \]
\[ x_3 = \frac{12 - 9 \times 2.3053 - 3 \times (-1.4078)}{1} = -4.5245 \]

The absolute relative approximate error for each \( x_i \) then is

\[ |\varepsilon_a|_1 = \left| \frac{2.3053 - 1.3925}{2.3053} \right| \times 100 = 39.596\% \]
\[ |\varepsilon_a|_2 = \left| \frac{-1.4078 - 0.11875}{-1.4078} \right| \times 100 = 108.44\% \]
\[ |\varepsilon_a|_3 = \left| \frac{-4.5245 - (-0.88875)}{-4.5245} \right| \times 100 = 80.357\% \]

At the end of the second iteration, the estimate of the solution vector is

\[
\begin{bmatrix}
  x_1 \\
  x_2 \\
  x_3
\end{bmatrix} = \begin{bmatrix}
  2.3053 \\
  -1.4078 \\
  -4.5245
\end{bmatrix}
\]

and the maximum absolute relative approximate error is 108.44\%.

Conducting more iterations gives the following values for the solution vector and the corresponding absolute relative approximate errors.

| Iteration | \( x_1 \) | \( |\varepsilon_a|_1 \) \% | \( x_2 \) | \( |\varepsilon_a|_2 \) \% | \( x_3 \) | \( |\varepsilon_a|_3 \) \% |
|-----------|----------|----------------|----------|----------------|----------|----------------|
| 1         | 1.3925   | 28.1867        | 0.11875  | 742.1053       | -0.88875 | 212.52         |
| 2         | 2.3053   | 39.5960        | -1.4078  | 108.4353       | -4.5245  | 80.357         |
| 3         | 3.9775   | 42.041         | -4.1340  | 65.946         | -11.396  | 60.296         |
| 4         | 7.0584   | 43.649         | -9.0877  | 54.510         | -24.262  | 53.032         |
| 5         | 12.752   | 44.649         | -18.175  | 49.999         | -48.243  | 49.708         |
| 6         | 23.291   | 45.249         | -34.930  | 47.967         | -92.827  | 48.030         |

After six iterations, the absolute relative approximate errors are not decreasing much. In fact, conducting more iterations reveals that the absolute relative approximate error converges to a value of 46.070\% for all three values with the solution vector diverging from the exact solution drastically.

| Iteration | \( x_1 \) | \( |\varepsilon_a|_1 \) \% | \( x_2 \) | \( |\varepsilon_a|_2 \) \% | \( x_3 \) | \( |\varepsilon_a|_3 \) \% |
|-----------|----------|----------------|----------|----------------|----------|----------------|
| 32        | \( 2.1428 \times 10^8 \) | 46.0703       | \( -3.3920 \times 10^8 \) | 46.0703    | \( -9.1095 \times 10^8 \) | 46.0703       |

The exact solution vector is
To correct this, the coefficient matrix needs to be more diagonally dominant. To achieve a more diagonally dominant coefficient matrix, rearrange the system of equations by exchanging equations one and three.

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

Iteration #1
Given the initial guess of the solution vector as
\[
\begin{bmatrix}
x_1 \\
x_2 \\
x_3 \\
\end{bmatrix}
=
\begin{bmatrix}
1 \\
1 \\
1 \\
\end{bmatrix}
\]
we get
\[
x_1 = \frac{12 - 3 \times 1 - 1}{9} = 0.88889
\]
\[
x_2 = \frac{10 - 6.25 \times 0.8889 - 1}{2.5} = 1.3778
\]
\[
x_3 = \frac{8.57 - 4 \times 0.8889 - 2 \times 1.3778}{1} = 2.2589
\]
The absolute relative approximate error for each \(x_i\) then is
\[
|\varepsilon_{a1}| = \left| \frac{0.88889 - 1}{0.8889} \right| \times 100 = 12.5\%
\]
\[
|\varepsilon_{a2}| = \left| \frac{1.3778 - 1}{1.3778} \right| \times 100 = 27.419\%
\]
\[
|\varepsilon_{a3}| = \left| \frac{2.2589 - 1}{2.2589} \right| \times 100 = 55.730\%
\]
At the end of the first iteration, the estimate of the solution vector is
\[
\begin{bmatrix}
x_1 \\
x_2 \\
x_3 \\
\end{bmatrix}
=
\begin{bmatrix}
0.88889 \\
1.3778 \\
2.2589 \\
\end{bmatrix}
\]
and the maximum absolute relative approximate error is 55.730\%.
Iteration #2
The estimate of the solution vector at the end of Iteration #1 is
\[
\begin{bmatrix}
  x_1 \\
  x_2 \\
  x_3
\end{bmatrix} = \begin{bmatrix}
  0.88889 \\
  1.3778 \\
  2.2589
\end{bmatrix}
\]
Now we get
\[
x_1 = \frac{12 - 3 \times 1.3778 - 1 \times 2.2589}{9} = 0.62309
\]
\[
x_2 = \frac{10 - 6.25 \times 0.62309 - 1 \times 2.2589}{2.5} = 1.5387
\]
\[
x_3 = \frac{8.57 - 4 \times 0.62309 - 2 \times 1.5387}{1} = 3.0002
\]
The absolute relative approximate error for each \( x_i \) then is
\[
|\varepsilon_{a,i}| = \left| \frac{0.62309 - 0.88889}{0.62309} \right| \times 100
\]
\[
= 42.659\%
\]
\[
|\varepsilon_{a,2}| = \left| \frac{1.5387 - 1.3778}{1.5387} \right| \times 100
\]
\[
= 10.460\%
\]
\[
|\varepsilon_{a,3}| = \left| \frac{3.0002 - 2.2589}{3.0002} \right| \times 100
\]
\[
= 24.709\%
\]
At the end of the second iteration, the estimate of the solution is
\[
\begin{bmatrix}
  x_1 \\
  x_2 \\
  x_3
\end{bmatrix} = \begin{bmatrix}
  0.62309 \\
  1.5387 \\
  3.0002
\end{bmatrix}
\]
and the maximum absolute relative approximate error is 42.659%.
Conducting more iterations gives the following values for the solution vector and the corresponding absolute relative approximate errors.

| Iteration | \( x_1 \) | \( |\varepsilon_{a,1}|\) % | \( x_2 \) | \( |\varepsilon_{a,2}|\) % | \( x_3 \) | \( |\varepsilon_{a,3}|\) % |
|-----------|--------|----------------|--------|----------------|--------|----------------|
| 1         | 0.88889| 12.5           | 1.3778 | 27.419         | 2.2589 | 55.730         |
| 2         | 0.62309| 42.659         | 1.5387 | 10.456         | 3.0002 | 24.709         |
| 3         | 0.48707| 27.926         | 1.5822 | 2.7506         | 3.4572 | 13.220         |
| 4         | 0.42178| 15.479         | 1.5627 | 1.2537         | 3.7576 | 7.9928         |
| 5         | 0.39494| 6.7960         | 1.5096 | 3.5131         | 3.9710 | 5.3747         |
| 6         | 0.38890| 1.5521         | 1.4393 | 4.8828         | 4.1357 | 3.9826         |
After six iterations, the absolute relative approximate errors seem to be decreasing. Conducting more iterations allows the absolute relative approximate error decrease to an acceptable level.

| Iteration | $x_1$ | $|e_{x_1}|\%$ | $x_2$ | $|e_{x_2}|\%$ | $x_3$ | $|e_{x_3}|\%$ |
|-----------|------|------------|------|------------|------|------------|
| 199       | 1.1335 | 0.014412 | −2.2389 | 0.034871 | 8.5139 | 0.010666 |
| 200       | 1.1337 | 0.014056 | −2.2397 | 0.034005 | 8.5148 | 0.010403 |

This is close to the exact solution vector of

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

The polynomial that passes through the three data points is then

$$g(a) = x_1(a)^2 + x_2(a) + x_3$$
$$= 1.1337(a)^2 + (−2.2397)(a) + 8.5148$$

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

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

$$g(2.3) = 1.1337(2.3)^2 + (−2.2397)(2.3) + 8.5148$$
$$= 9.3608 \, g/l$$