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.

Ni aqueous phase, $a\,(\text{g/l})$	2	2.5	3
Ni organic phase, $g\,(\text{g/l})$	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 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

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

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

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

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_i then is

$$\left|\in_a\right|_1 = \left|\frac{1.3925 - 1}{1.3925}\right| \times 100$$
$$= 28.187\%$$
$$\left|\in_a\right|_2 = \left|\frac{0.11875 - 1}{0.11875}\right| \times 100$$
$$= 742.11\%$$
$$\left|\in_a\right|_3 = \left|\frac{-0.88875 - 1}{-0.88875}\right| \times 100$$
$$= 212.52\%$$

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

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

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	$\|\in_a\|_1$ %	x_2	$\|\in_a\|_2$ %	x_3	$\|\in_a\|_3$ %
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	$\|\in_a\|_1$ %	x_2	$\|\in_a\|_2$ %	x_3	$\|\in_a\|_3$ %
32	2.1428×10^8	46.0703	-3.3920×10^8	46.0703	-9.1095×10^8	46.0703

The exact solution vector is

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

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.

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

<u>Iteration #1</u>

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

$$x_1 = \frac{12 - 3\times 1 - 1}{9}$$
$$= 0.88889$$
$$x_2 = \frac{10 - 6.25\times 0.88889 - 1}{2.5}$$
$$= 1.3778$$
$$x_3 = \frac{8.57 - 4\times 0.88889 - 2\times 1.3778}{1}$$
$$= 2.2589$$

The absolute relative approximate error for each x_i then is

$$\left|\in_a\right|_1 = \left|\frac{0.88889 - 1}{0.88889}\right|\times 100$$
$$= 12.5\%$$
$$\left|\in_a\right|_2 = \left|\frac{1.3778 - 1}{1.3778}\right|\times 100$$
$$= 27.419\%$$
$$\left|\in_a\right|_3 = \left|\frac{2.2589 - 1}{2.2589}\right|\times 100$$
$$= 55.730\%$$

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%.

<u>Iteration #2</u>

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

$$|\epsilon_a|_1 = \left|\frac{0.62309 - 0.88889}{0.62309}\right| \times 100$$
$$= 42.659\%$$
$$|\epsilon_a|_2 = \left|\frac{1.5387 - 1.3778}{1.5387}\right| \times 100$$
$$= 10.460\%$$
$$|\epsilon_a|_3 = \left|\frac{3.0002 - 2.2589}{3.0002}\right| \times 100$$
$$= 24.709\%$$

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	$\lvert\epsilon_a\rvert_1$ %	x_2	$\lvert\epsilon_a\rvert_2$ %	x_3	$\lvert\epsilon_a\rvert_3$ %
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	$\left\|\in_a\right\|_1 \%$	x_2	$\left\|\in_a\right\|_2 \%$	x_3	$\left\|\in_a\right\|_3 \%$
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

$$\begin{aligned} g(a) &= x_1(a)^2 + x_2(a) + x_3 \\ &= 1.1337(a)^2 + (-2.2397)(a) + 8.5148 \end{aligned}$$

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

$$\begin{aligned} g(2.3) &= 1.1337(2.3)^2 + (-2.2397)\times(2.3) + 8.5148 \\ &= 9.3608\,\mathrm{g/l} \end{aligned}$$

SIMULTANEOUS LINEAR EQUATIONS	
Topic	Gauss-Seidel Method – More Examples
Summary	Examples of the Gauss-Seidel method
Major	Chemical Engineering
Authors	Autar Kaw
Date	August 8, 2009
Web Site	http://numericalmethods.eng.usf.edu