

Chapter 04.08

Gauss-Seidel Method

After reading this chapter, you should be able to:

1. *solve a set of equations using the Gauss-Seidel method,*
2. *recognize the advantages and pitfalls of the Gauss-Seidel method, and*
3. *determine under what conditions the Gauss-Seidel method always converges.*

Why do we need another method to solve a set of simultaneous linear equations?

In certain cases, such as when a system of equations is large, iterative methods of solving equations are more advantageous. Elimination methods, such as Gaussian elimination, are prone to large round-off errors for a large set of equations. Iterative methods, such as the Gauss-Seidel method, give the user control of the round-off error. Also, if the physics of the problem are well known, initial guesses needed in iterative methods can be made more judiciously leading to faster convergence.

What is the algorithm for the Gauss-Seidel method? Given a general set of n equations and n unknowns, we have

$$\begin{aligned}a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \dots + a_{1n}x_n &= c_1 \\a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \dots + a_{2n}x_n &= c_2 \\&\vdots \\&\vdots \\&\vdots \\a_{n1}x_1 + a_{n2}x_2 + a_{n3}x_3 + \dots + a_{nn}x_n &= c_n\end{aligned}$$

If the diagonal elements are non-zero, each equation is rewritten for the corresponding unknown, that is, the first equation is rewritten with x_1 on the left hand side, the second equation is rewritten with x_2 on the left hand side and so on as follows

$$\begin{aligned}
x_1 &= \frac{c_1 - a_{12}x_2 - a_{13}x_3 \dots - a_{1n}x_n}{a_{11}} \\
x_2 &= \frac{c_2 - a_{21}x_1 - a_{23}x_3 \dots - a_{2n}x_n}{a_{22}} \\
&\vdots \\
&\vdots \\
x_{n-1} &= \frac{c_{n-1} - a_{n-1,1}x_1 - a_{n-1,2}x_2 \dots - a_{n-1,n-2}x_{n-2} - a_{n-1,n}x_n}{a_{n-1,n-1}} \\
x_n &= \frac{c_n - a_{n1}x_1 - a_{n2}x_2 - \dots - a_{nn}x_{n-1}}{a_{nn}}
\end{aligned}$$

These equations can be rewritten in a summation form as

$$\begin{aligned}
x_1 &= \frac{c_1 - \sum_{\substack{j=1 \\ j \neq 1}}^n a_{1j}x_j}{a_{11}} \\
x_2 &= \frac{c_2 - \sum_{\substack{j=1 \\ j \neq 2}}^n a_{2j}x_j}{a_{22}} \\
&\vdots \\
&\vdots \\
x_{n-1} &= \frac{c_{n-1} - \sum_{\substack{j=1 \\ j \neq n-1}}^n a_{n-1,j}x_j}{a_{n-1,n-1}} \\
x_n &= \frac{c_n - \sum_{\substack{j=1 \\ j \neq n}}^n a_{nj}x_j}{a_{nn}}
\end{aligned}$$

Hence for any row i ,

$$x_i = \frac{c_i - \sum_{\substack{j=1 \\ j \neq i}}^n a_{ij}x_j}{a_{ii}}, i = 1, 2, \dots, n.$$

Now to find x_i 's, one assumes an initial guess for the x_i 's and then uses the rewritten equations to calculate the new estimates. Remember, one always uses the most recent estimates to calculate the next estimates, x_i . At the end of each iteration, one calculates the absolute relative approximate error for each x_i as

$$\left| \epsilon_a \right|_i = \left| \frac{x_i^{\text{new}} - x_i^{\text{old}}}{x_i^{\text{new}}} \right| \times 100$$

where x_i^{new} is the recently obtained value of x_i , and x_i^{old} is the previous value of x_i .

When the absolute relative approximate error for each x_i is less than the pre-specified tolerance, the iterations are stopped.

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

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

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

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

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

$$\begin{aligned} x_1 &= \frac{8.57 - 2 \times 1 - 1}{4} \\ &= 1.3925 \\ x_2 &= \frac{10 - 6.25 \times 1.3925 - 1}{2.5} \\ &= 0.11875 \\ x_3 &= \frac{12 - 9 \times 1.3925 - 3 \times 0.11875}{1} \\ &= -0.88875 \end{aligned}$$

The absolute relative approximate error for each x_i then is

$$\begin{aligned} |\epsilon_a|_1 &= \left| \frac{1.3925 - 1}{1.3925} \right| \times 100 \\ &= 28.187\% \\ |\epsilon_a|_2 &= \left| \frac{0.11875 - 1}{0.11875} \right| \times 100 \\ &= 742.11\% \\ |\epsilon_a|_3 &= \left| \frac{-0.88875 - 1}{-0.88875} \right| \times 100 \\ &= 212.52\% \end{aligned}$$

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

$$\begin{aligned} x_1 &= \frac{8.57 - 2 \times 0.11875 - (-0.88875)}{4} \\ &= 2.3053 \\ x_2 &= \frac{10 - 6.25 \times 2.3053 - (-0.88875)}{2.5} \end{aligned}$$

$$\begin{aligned}
 &= -1.4078 \\
 x_3 &= \frac{12 - 9 \times 2.3053 - 3 \times (-1.4078)}{1} \\
 &= -4.5245
 \end{aligned}$$

The absolute relative approximate error for each x_i then is

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

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	$ \epsilon_a _1 \%$	x_2	$ \epsilon_a _2 \%$	x_3	$ \epsilon_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	$ \epsilon_a _1 \%$	x_2	$ \epsilon_a _2 \%$	x_3	$ \epsilon_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.

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

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

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

The absolute relative approximate error for each x_i then is

$$\begin{aligned} |\epsilon_a|_1 &= \left| \frac{0.88889 - 1}{0.88889} \right| \times 100 \\ &= 12.5\% \\ |\epsilon_a|_2 &= \left| \frac{1.3778 - 1}{1.3778} \right| \times 100 \\ &= 27.419\% \\ |\epsilon_a|_3 &= \left| \frac{2.2589 - 1}{2.2589} \right| \times 100 \\ &= 55.730\% \end{aligned}$$

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

$$\begin{aligned} x_1 &= \frac{12 - 3 \times 1.3778 - 1 \times 2.2589}{9} \\ &= 0.62309 \\ x_2 &= \frac{10 - 6.25 \times 0.62309 - 1 \times 2.2589}{2.5} \\ &= 1.5387 \\ x_3 &= \frac{8.57 - 4 \times 0.62309 - 2 \times 1.5387}{1} \\ &= 3.0002 \end{aligned}$$

The absolute relative approximate error for each x_i then is

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

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	$ \epsilon_a _1\%$	x_2	$ \epsilon_a _2\%$	x_3	$ \epsilon_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	$ \epsilon_a _1\%$	x_2	$ \epsilon_a _2\%$	x_3	$ \epsilon_a _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

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

The above system of equations does not seem to converge. Why?

Well, a pitfall of most iterative methods is that they may or may not converge. However, the solution to a certain classes of systems of simultaneous equations does always converge using the Gauss-Seidel method. This class of system of equations is where the coefficient matrix $[A]$ in $[A][X] = [C]$ is diagonally dominant, that is

$$\begin{aligned} |a_{ii}| &\geq \sum_{\substack{j=1 \\ j \neq i}}^n |a_{ij}| \text{ for all } i \\ |a_{ii}| &> \sum_{\substack{j=1 \\ j \neq i}}^n |a_{ij}| \text{ for at least one } i \end{aligned}$$

If a system of equations has a coefficient matrix that is not diagonally dominant, it may or may not converge. Fortunately, many physical systems that result in simultaneous linear equations have a diagonally dominant coefficient matrix, which then assures convergence for iterative methods such as the Gauss-Seidel method of solving simultaneous linear equations.

Example 2

Find the solution to the following system of equations using the Gauss-Seidel method.

$$12x_1 + 3x_2 - 5x_3 = 1$$

$$x_1 + 5x_2 + 3x_3 = 28$$

$$3x_1 + 7x_2 + 13x_3 = 76$$

Use

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}$$

as the initial guess and conduct two iterations.

Solution

The coefficient matrix

$$[A] = \begin{bmatrix} 12 & 3 & -5 \\ 1 & 5 & 3 \\ 3 & 7 & 13 \end{bmatrix}$$

is diagonally dominant as

$$|a_{11}| = |12| = 12 \geq |a_{12}| + |a_{13}| = |3| + |-5| = 8$$

$$|a_{22}| = |5| = 5 \geq |a_{21}| + |a_{23}| = |1| + |3| = 4$$

$$|a_{33}| = |13| = 13 \geq |a_{31}| + |a_{32}| = |3| + |7| = 10$$

and the inequality is strictly greater than for at least one row. Hence, the solution should converge using the Gauss-Seidel method.

Rewriting the equations, we get

$$x_1 = \frac{1 - 3x_2 + 5x_3}{12}$$

$$x_2 = \frac{28 - x_1 - 3x_3}{5}$$

$$x_3 = \frac{76 - 3x_1 - 7x_2}{13}$$

Assuming an initial guess of

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}$$

Iteration #1

$$x_1 = \frac{1 - 3(0) + 5(1)}{12}$$

$$= 0.50000$$

$$x_2 = \frac{28 - (0.50000) - 3(1)}{5}$$

$$\begin{aligned}
 &= 4.9000 \\
 x_3 &= \frac{76 - 3(0.50000) - 7(4.9000)}{13} \\
 &= 3.0923
 \end{aligned}$$

The absolute relative approximate error at the end of the first iteration is

$$\begin{aligned}
 |\epsilon_a|_1 &= \left| \frac{0.50000 - 1}{0.50000} \right| \times 100 \\
 &= 100.00\% \\
 |\epsilon_a|_2 &= \left| \frac{4.9000 - 0}{4.9000} \right| \times 100 \\
 &= 100.00\% \\
 |\epsilon_a|_3 &= \left| \frac{3.0923 - 1}{3.0923} \right| \times 100 \\
 &= 67.662\%
 \end{aligned}$$

The maximum absolute relative approximate error is 100.00%

Iteration #2

$$\begin{aligned}
 x_1 &= \frac{1 - 3(4.9000) + 5(3.0923)}{12} \\
 &= 0.14679 \\
 x_2 &= \frac{28 - (0.14679) - 3(3.0923)}{5} \\
 &= 3.7153 \\
 x_3 &= \frac{76 - 3(0.14679) - 7(3.7153)}{13} \\
 &= 3.8118
 \end{aligned}$$

At the end of second iteration, the absolute relative approximate error is

$$\begin{aligned}
 |\epsilon_a|_1 &= \left| \frac{0.14679 - 0.50000}{0.14679} \right| \times 100 \\
 &= 240.61\% \\
 |\epsilon_a|_2 &= \left| \frac{3.7153 - 4.9000}{3.7153} \right| \times 100 \\
 &= 31.889\% \\
 |\epsilon_a|_3 &= \left| \frac{3.8118 - 3.0923}{3.8118} \right| \times 100 \\
 &= 18.874\%
 \end{aligned}$$

The maximum absolute relative approximate error is 240.61%. This is greater than the value of 100.00% we obtained in the first iteration. Is the solution diverging? No, as you conduct more iterations, the solution converges as follows.

Iteration	x_1	$ \epsilon_a _1$ %	x_2	$ \epsilon_a _2$ %	x_3	$ \epsilon_a _3$ %
1	0.50000	100.00	4.9000	100.00	3.0923	67.662
2	0.14679	240.61	3.7153	31.889	3.8118	18.874

3	0.74275	80.236	3.1644	17.408	3.9708	4.0064
4	0.94675	21.546	3.0281	4.4996	3.9971	0.65772
5	0.99177	4.5391	3.0034	0.82499	4.0001	0.074383
6	0.99919	0.74307	3.0001	0.10856	4.0001	0.00101

This is close to the exact solution vector of

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 3 \\ 4 \end{bmatrix}$$

Example 3

Given the system of equations

$$3x_1 + 7x_2 + 13x_3 = 76$$

$$x_1 + 5x_2 + 3x_3 = 28$$

$$12x_1 + 3x_2 - 5x_3 = 1$$

find the solution using the Gauss-Seidel method. Use

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}$$

as the initial guess.

Solution

Rewriting the equations, we get

$$x_1 = \frac{76 - 7x_2 - 13x_3}{3}$$

$$x_2 = \frac{28 - x_1 - 3x_3}{5}$$

$$x_3 = \frac{1 - 12x_1 - 3x_2}{-5}$$

Assuming an initial guess of

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}$$

the next six iterative values are given in the table below.

Iteration	x_1	$ \epsilon_a _1 \%$	x_2	$ \epsilon_a _2 \%$	x_3	$ \epsilon_a _3 \%$
1	21.000	95.238	0.80000	100.00	50.680	98.027
2	-196.15	110.71	14.421	94.453	-462.30	110.96
3	1995.0	109.83	-116.02	112.43	4718.1	109.80
4	-20149	109.90	1204.6	109.63	-47636	109.90
5	2.0364×10^5	109.89	-12140	109.92	4.8144×10^5	109.89

6	-2.0579×10^6	109.89	1.2272×10^5	109.89	-4.8653×10^6	109.89
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You can see that this solution is not converging and the coefficient matrix is not diagonally dominant. The coefficient matrix

$$[A] = \begin{bmatrix} 3 & 7 & 13 \\ 1 & 5 & 3 \\ 12 & 3 & -5 \end{bmatrix}$$

is not diagonally dominant as

$$|a_{11}| = |3| = 3 \leq |a_{12}| + |a_{13}| = |7| + |13| = 20$$

Hence, the Gauss-Seidel method may or may not converge.

However, it is the same set of equations as the previous example and that converged. The only difference is that we exchanged first and the third equation with each other and that made the coefficient matrix not diagonally dominant.

Therefore, it is possible that a system of equations can be made diagonally dominant if one exchanges the equations with each other. However, it is not possible for all cases. For example, the following set of equations

$$x_1 + x_2 + x_3 = 3$$

$$2x_1 + 3x_2 + 4x_3 = 9$$

$$x_1 + 7x_2 + x_3 = 9$$

cannot be rewritten to make the coefficient matrix diagonally dominant.

Key Terms:

Gauss-Seidel method

Convergence of Gauss-Seidel method

Diagonally dominant matrix

SIMULTANEOUS LINEAR EQUATIONS	
Topic	Gauss-Seidel Method – More Examples
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