Gauss-Seidel Method

Computational Physics

Gauss-Seidel Method

An <u>*iterative*</u> method.

Basic Procedure:

-Algebraically solve each linear equation for x_i

-Assume an initial guess solution array

-Solve for each x_i and repeat

-Use absolute relative approximate error after each iteration to check if error is within a pre-specified tolerance.

Gauss-Seidel Method

Why?

The Gauss-Seidel Method allows the user to control round-off error.

Elimination methods such as Gaussian Elimination and LU Decomposition are prone to prone to round-off error.

Also: If the physics of the problem are understood, a close initial guess can be made, decreasing the number of iterations needed.

Gauss-Seidel Method

Algorithm

A set of *n* equations and *n* unknowns:

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \ldots + a_{1n}x_n = b_1$$

$$a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \ldots + a_{2n}x_n = b_2$$

$$\vdots \qquad \vdots$$

$$a_{n1}x_1 + a_{n2}x_2 + a_{n3}x_3 + \ldots + a_{nn}x_n = b_n$$

If: the diagonal elements are non-zero

Rewrite each equation solving for the corresponding unknown

ex:

First equation, solve for x_1

Second equation, solve for x_2

Gauss-Seidel Method

Algorithm

Rewriting each equation

$$x_1 = \frac{c_1 - a_{12}x_2 - a_{13}x_3 \ldots\ldots - a_{1n}x_n}{a_{11}}$$ ← From Equation 1

$$x_2 = \frac{c_2 - a_{21}x_1 - a_{23}x_3 \ldots\ldots - a_{2n}x_n}{a_{22}}$$ ← From equation 2

$$\vdots \qquad \vdots \qquad \vdots$$

$$x_{n-1} = \frac{c_{n-1} - a_{n-1,1}x_1 - a_{n-1,2}x_2 \ldots\ldots - a_{n-1,n-2}x_{n-2} - a_{n-1,n}x_n}{a_{n-1,n-1}}$$ ← From equation n-1

$$x_n = \frac{c_n - a_{n1}x_1 - a_{n2}x_2 - \ldots\ldots - a_{n,n-1}x_{n-1}}{a_{nn}}$$ ← From equation n

Gauss-Seidel Method

Algorithm

General Form of each equation

$$x_1 = \frac{c_1 - \sum\limits_{\substack{j=1 \\ j \neq 1}}^{n} a_{1j} x_j}{a_{11}}$$

$$x_{n-1} = \frac{c_{n-1} - \sum\limits_{\substack{j=1 \\ j \neq n-1}}^{n} a_{n-1,j} x_j}{a_{n-1,n-1}}$$

$$x_2 = \frac{c_2 - \sum\limits_{\substack{j=1 \\ j \neq 2}}^{n} a_{2j} x_j}{a_{22}}$$

$$x_n = \frac{c_n - \sum\limits_{\substack{j=1 \\ j \neq n}}^{n} a_{nj} x_j}{a_{nn}}$$

Gauss-Seidel Method

Algorithm

General Form for any row 'i'

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

How or where can this equation be used?

Gauss-Seidel Method

Solve for the unknowns

Assume an initial guess for [X]

$$\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_{n\text{-}1} \\ x_n \end{bmatrix}$$

Use rewritten equations to solve for each value of x_i.

Important: Remember to use the most recent value of x_i. Which means to apply values calculated to the calculations remaining in the **current** iteration.

Gauss-Seidel Method

Calculate the Absolute Relative Approximate Error

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

So when has the answer been found?

The iterations are stopped when the absolute relative approximate error is less than a prespecified tolerance for all unknowns.

Gauss-Seidel Method: Example 1

The upward velocity of a rocket is given at three different times

Table 1 Velocity vs. Time data.

Time, t (s)	**Velocity** v (m/s)
5	106.8
8	177.2
12	279.2

The velocity data is approximated by a polynomial as:

$$v(t) = a_1 t^2 + a_2 t + a_3 \, , 5 \le \mathrm{t} \le 12.$$

Gauss-Seidel Method: Example 1

Using a Matrix template of the form

$$\begin{bmatrix} t_1^2 & t_1 & 1 \\ t_2^2 & t_2 & 1 \\ t_3^2 & t_3 & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix}$$

The system of equations becomes

$$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ 177.2 \\ 279.2 \end{bmatrix}$$

Initial Guess: Assume an initial guess of

$$\begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \\ 5 \end{bmatrix}$$

Gauss-Seidel Method: Example 1

Rewriting each equation

$$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 106.8 \\ 177.2 \\ 279.2 \end{bmatrix}$$

$$a_1 = \frac{106.8 - 5a_2 - a_3}{25}$$

$$a_2 = \frac{177.2 - 64a_1 - a_3}{8}$$

$$a_3 = \frac{279.2 - 144a_1 - 12a_2}{1}$$

Gauss-Seidel Method: Example 1

Applying the initial guess and solving for a_i

$$\begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \\ 5 \end{bmatrix}$$

Initial Guess

$$a_1 = \frac{106.8 - 5(2) - (5)}{25} = 3.6720$$

$$a_2 = \frac{177.2 - 64(3.6720) - (5)}{8} = -7.8510$$

$$a_3 = \frac{279.2 - 144(3.6720) - 12(-7.8510)}{1} = -155.36$$

When solving for a_2, how many of the initial guess values were used?

Gauss-Seidel Method: Example 1

Finding the absolute relative approximate error

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

$$\left|\in_a\right|_1 = \left|\frac{3.6720 - 1.0000}{3.6720}\right| x100 = 72.76\%$$

$$\left|\in_a\right|_2 = \left|\frac{-7.8510 - 2.0000}{-7.8510}\right| x100 = 125.47\%$$

$$\left|\in_a\right|_3 = \left|\frac{-155.36 - 5.0000}{-155.36}\right| x100 = 103.22\%$$

At the end of the first iteration

$$\begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 3.6720 \\ -7.8510 \\ -155.36 \end{bmatrix}$$

The maximum absolute relative approximate error is 125.47%

Gauss-Seidel Method: Example 1

Iteration #2

Using

$$\begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 3.6720 \\ -7.8510 \\ -155.36 \end{bmatrix}$$

from iteration #1

the values of a_i are found:

$$a_1 = \frac{106.8 - 5(-7.8510) - 155.36}{25} = 12.056$$

$$a_2 = \frac{177.2 - 64(12.056) - 155.36}{8} = -54.882$$

$$a_3 = \frac{279.2 - 144(12.056) - 12(-54.882)}{1} = -798.34$$

Gauss-Seidel Method: Example 1

Finding the absolute relative approximate error

$$\left|\in_a\right|_1 = \left|\frac{12.056 - 3.6720}{12.056}\right| x100 = 69.543\%$$

$$\left|\in_a\right|_2 = \left|\frac{-54.882 - (-7.8510)}{-54.882}\right| x100 = 85.695\%$$

$$\left|\in_a\right|_3 = \left|\frac{-798.34 - (-155.36)}{-798.34}\right| x100 = 80.540\%$$

At the end of the second iteration

$$\begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 12.056 \\ -54.882 \\ -798.54 \end{bmatrix}$$

The maximum absolute relative approximate error is 85.695%

Gauss-Seidel Method: Example 1

Repeating more iterations, the following values are obtained

Iteration	a_1	$\left|\in_a\right|_1 \%$	a_2	$\left|\in_a\right|_2 \%$	a_3	$\left|\in_a\right|_3 \%$
1	3.6720	72.767	−7.8510	125.47	−155.36	103.22
2	12.056	69.543	−54.882	85.695	−798.34	80.540
3	47.182	74.447	−255.51	78.521	−3448.9	76.852
4	193.33	75.595	−1093.4	76.632	−14440	76.116
5	800.53	75.850	−4577.2	76.112	−60072	75.963
6	3322.6	75.906	−19049	75.972	−249580	75.931

Notice – The relative errors are not decreasing at any significant rate

Also, the solution is not converging to the true solution of

$$\begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 0.29048 \\ 19.690 \\ 1.0857 \end{bmatrix}$$

Gauss-Seidel Method: Pitfall

What went wrong?

Even though done correctly, the answer is not converging to the correct answer

This example illustrates a pitfall of the Gauss-Siedel method: not all systems of equations will converge.

Is there a fix?

One class of system of equations always converges: One with a *diagonally dominant* coefficient matrix.

Diagonally dominant: [A] in [A] [X] = [C] is diagonally dominant if:

$$\left|a_{\mathrm{ii}}\right| \geq \sum_{\substack{j=1 \\ j \neq \mathrm{i}}}^{n} \left|a_{ij}\right|$$ for all 'i' and $$\left|a_{ii}\right| > \sum_{\substack{j=1 \\ j \neq i}}^{n} \left|a_{ij}\right|$$ for at least one 'i'

Gauss-Seidel Method: Pitfall

Diagonally dominant: The coefficient on the diagonal must be at least equal to the sum of the other coefficients in that row and at least one row with a diagonal coefficient greater than the sum of the other coefficients in that row.

Which coefficient matrix is diagonally dominant?

$$[A]=\begin{bmatrix} 2 & 5.81 & 34 \\ 45 & 43 & 1 \\ 123 & 16 & 1 \end{bmatrix}$$

$$[B]=\begin{bmatrix} 124 & 34 & 56 \\ 23 & 53 & 5 \\ 96 & 34 & 129 \end{bmatrix}$$

Most physical systems do result in simultaneous linear equations that have diagonally dominant coefficient matrices.

Gauss-Seidel Method: Example 2

Given the system of equations

$$12x_1 + 3x_2 - 5x_3 = 1$$
$$x_1 + 5x_2 + 3x_3 = 28$$
$$3x_1 + 7x_2 + 13x_3 = 76$$

The coefficient matrix is:

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

With an initial guess of

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

Will the solution converge using the Gauss-Siedel method?

Gauss-Seidel Method: Example 2

Checking if the coefficient matrix is diagonally dominant

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

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

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

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

The inequalities are all true and at least one row is *strictly* greater than:

Therefore: The solution should converge using the Gauss-Siedel Method

Gauss-Seidel Method: Example 2

Rewriting each equation

$$\begin{bmatrix} 12 & 3 & -5 \\ 1 & 5 & 3 \\ 3 & 7 & 13 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 28 \\ 76 \end{bmatrix}$$

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

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

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

With an initial guess of

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

$$x_1 = \frac{1 - 3(0) + 5(1)}{12} = 0.50000$$

$$x_2 = \frac{28 - (0.5) - 3(1)}{5} = 4.9000$$

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

Gauss-Seidel Method: Example 2

The absolute relative approximate error

$$\left|\in_a\right|_1 = \left|\frac{0.50000 - 1.0000}{0.50000}\right| \times 100 = 100.00\%$$

$$\left|\in_a\right|_2 = \left|\frac{4.9000 - 0}{4.9000}\right| \times 100 = 100.00\%$$

$$\left|\in_a\right|_3 = \left|\frac{3.0923 - 1.0000}{3.0923}\right| \times 100 = 67.662\%$$

The maximum absolute relative error after the first iteration is 100%

Gauss-Seidel Method: Example 2

After Iteration #1

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0.5000 \\ 4.9000 \\ 3.0923 \end{bmatrix}$$

Substituting the x values into the equations

$$x_1 = \frac{1-3(4.9000)+5(3.0923)}{12} = 0.14679$$

$$x_2 = \frac{28-(0.14679)-3(3.0923)}{5} = 3.7153$$

$$x_3 = \frac{76-3(0.14679)-7(4.900)}{13} = 3.8118$$

After Iteration #2

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0.14679 \\ 3.7153 \\ 3.8118 \end{bmatrix}$$

Gauss-Seidel Method: Example 2

Iteration #2 absolute relative approximate error

$$\left|\in_a\right|_1 = \left|\frac{0.14679 - 0.50000}{0.14679}\right| \times 100 = 240.61\%$$

$$\left|\in_a\right|_2 = \left|\frac{3.7153 - 4.9000}{3.7153}\right| \times 100 = 31.889\%$$

$$\left|\in_a\right|_3 = \left|\frac{3.8118 - 3.0923}{3.8118}\right| \times 100 = 18.874\%$$

The maximum absolute relative error after the first iteration is 240.61%

This is much larger than the maximum absolute relative error obtained in iteration #1. Is this a problem?

Gauss-Seidel Method: Example 2

Repeating more iterations, the following values are obtained

Iteration	a_1	$\left|\in_a\right|_1 \%$	a_2	$\left|\in_a\right|_2 \%$	a_3	$\left|\in_a\right|_3 \%$
1	0.50000	100.00	4.9000	100.00	3.0923	67.662
2	0.14679	240.61	3.7153	31.889	3.8118	18.876
3	0.74275	80.236	3.1644	17.408	3.9708	4.0042
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

The solution obtained $\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0.99919 \\ 3.0001 \\ 4.0001 \end{bmatrix}$ is close to the exact solution of $\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 3 \\ 4 \end{bmatrix}$.

Gauss-Seidel Method: Example 3

Given the system of equations

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

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

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

With an initial guess of

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

Rewriting the equations

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

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

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

Gauss-Seidel Method: Example 3

Conducting six iterations, the following values are obtained

Iteration	a_1	$\left\|\in_a\right\|_1 \%$	A_2	$\left\|\in_a\right\|_2 \%$	a_3	$\left\|\in_a\right\|_3 \%$
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	-2.0579×10^5	109.89	1.2272×10^5	109.89	-4.8653×10^6	109.89

The values are not converging.

Does this mean that the Gauss-Seidel method cannot be used?

Gauss-Seidel Method

The Gauss-Seidel Method can still be used

The coefficient matrix is not diagonally dominant

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

But this is the same set of equations used in example #2, which did converge.

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

If a system of linear equations is not diagonally dominant, check to see if rearranging the equations can form a diagonally dominant matrix.

Gauss-Seidel Method

Not every system of equations can be rearranged to have a diagonally dominant coefficient matrix.

Observe the set of equations

$$x_1 + x_2 + x_3 = 3$$

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

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

Which equation(s) prevents this set of equation from having a diagonally dominant coefficient matrix?

Gauss-Seidel Method

Summary

-Advantages of the Gauss-Seidel Method

-Algorithm for the Gauss-Seidel Method

-Pitfalls of the Gauss-Seidel Method

Gauss-Seidel Method

Questions?

THE END

Computational Physics