Simultaneous Linear Equations

Topic: Gauss-Seidel Method

Major: Chemical Engineering

Gauss-Seidel Method

An *iterative* 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 prespecified tolerance.

Gauss-Seidel Method

Why?

The Gauss-Siedel 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]

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

Use rewritten equations to solve for each value of xi.

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

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

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.

Example: Liquid-Liquid Extraction

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 experimental data from the laboratory is given below:

Ni aqueous phase (g/l)	2	2.5	3
Ni organic phase (g/l)	8.57	10	12

Assuming *g* is the amount of Ni in organic phase and *a* is the amount of Ni in the aqueous phase, the quadratic interpolant that estimates *g* is given by

$$g = x_1 a^2 + x_2 a + x_3,\ 2 \le a \le 3.5$$

Example: Liquid-Liquid Extraction

The solution for the unknowns *x1, x2,* and *x3* 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 *x1, x2,*and *x3* using the Gauss Seidel method. Estimate the amount of nickel in organic phase when 2.3 g/l is in the aqueous phase using quadratic interpolation

Example: Liquid-Liquid Extraction

The system of equations is:

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

Initial Guess: Assume an initial guess of

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

Example: Liquid-Liquid Extraction

Rewriting each equation

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

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

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

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

Example: Liquid-Liquid Extraction

Applying the initial guess and solving for a_i

$$x_1 = \frac{8.57 - 2 \times 1 - 1}{4} = 1.3925$$

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

$$x_2 = \frac{10 - 6.25 \times 1.3925 - 1}{2.5} = 0.11875$$

$$x_3 = \frac{12 - 9 \times 1.3925 - 3 \times 0.11875}{1} = -0.88875$$

When solving for x_2, how many of the initial guess values were used?

Example: Liquid-Liquid Extraction

Finding the absolute relative approximate error

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

$$\left|\varepsilon_a\right|_1 = \left|\frac{1.3925 - 1}{1.3925}\right| x100 = 28.1867\%$$

$$\left|\varepsilon_a\right|_2 = \left|\frac{0.11875 - 1}{0.11875}\right| x100 = 742.1053\%$$

$$\left|\varepsilon_a\right|_3 = \left|\frac{-0.88875 - 1}{-0.88875}\right| x100 = 212.5176\%$$

At the end of the first iteration

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

The maximum absolute relative approximate error is 742.1053%

Example: Liquid-Liquid Extraction

Iteration #2

Using

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

from iteration #1

the values of x_i are found:

$$x_1 = \frac{8.57 - 2 \times 0.11875 - (-0.88875)}{4} = 2.30531$$

$$x_2 = \frac{10 - 6.25 \times 2.30531 - (-0.88875)}{2.5} = -1.40778$$

$$x_3 = \frac{12 - 9 \times 2.30531 - 3 \times (-1.407781)}{1} = -4.52447$$

Example: Liquid-Liquid Extraction

Finding the absolute relative approximate error

$$\left|\in_{\mathrm{a}}\right|_1 = \left|\frac{2.30531-1.3925}{2.30531}\right| \mathrm{x}100 = 39.5960\ \%$$

$$\left|\in_{\mathrm{a}}\right|_2 = \left|\frac{-1.40778-0.11875}{-1.40778}\right| \mathrm{x}100 = 108.43526\ \%$$

$$\left|\in_{\mathrm{a}}\right|_3 = \left|\frac{-4.52447-(-0.88875)}{-4.52447}\right| \mathrm{x}100 = 80.3568\ \%$$

At the end of the second iteration

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 2.30531 \\ -1.40778 \\ -4.52447 \end{bmatrix}$$

The maximum absolute relative approximate error is 108.43526%

Example: Liquid-Liquid Extraction

Repeating more iterations, the following values are obtained

Iteration	x_1	$\left\|\in_a\right\|_1 \%$	x_2	$\left\|\in_a\right\|_2 \%$	x_3	$\left\|\in_a\right\|_3 \%$
1	1.3925	28.1867	0.1186	742.1053	-0.8888	212.5176
2	2.3053	39.5960	-1.4078	108.4353	-4.5245	80.3568
3	3.9775	42.0413	-4.1340	65.9461	-11.3956	60.2964
4	7.0584	43.6486	-9.0878	54.5104	-24.2623	53.0316
5	12.7520	44.6485	-18.1750	49.9985	-48.2428	49.7078
6	23.2907	45.2486	-34.9296	47.9668	-92.8273	48.0296

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

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

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1.140 \\ -2.269 \\ 8.549 \end{bmatrix}$$

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-Seidel 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 $$\left|a_{ii}\right| \rangle \sum_{\substack{j=1 \\ j\neq i}}^{n} \left|a_{ij}\right|$$ for at least one ‘i’

Gauss-Siedel 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.

Original (Non-Diagonally dominant)

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

Rewritten (Diagonally dominant)

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

Example: Liquid-Liquid Extraction

With an initial guess of

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

Rewriting each equation

$$x_1 = \frac{12 - 3\times 1 - 1}{9} = 0.8889$$

$$x_2 = \frac{10 - 6.25\times 0.8889 - 1}{2.5} = 1.3778$$

$$x_3 = \frac{8.57 - 4\times 0.8889 - 2\times 1.3778}{1} = 2.2589$$

Example: Liquid-Liquid Extraction

The absolute relative approximate error

$$\left|\varepsilon_a\right|_1 = \left|\frac{0.8889-1}{0.8889}\right| \text{x}100 = 12.5\%$$

$$\left|\varepsilon_a\right|_2 = \left|\frac{1.3778-1}{1.3778}\right| \text{x}100 = 27.4194\%$$

$$\left|\varepsilon_a\right|_3 = \left|\frac{2.2589-1}{2.2589}\right| \text{x}100 = 55.7305\%$$

The maximum absolute relative error after the first iteration is 55.7305%

Example: Liquid-Liquid Extraction

After Iteration #1

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0.8889 \\ 1.3778 \\ 2.2589 \end{bmatrix}$$

Substituting the x values into the equations

$$x_1 = \frac{12 - 3 \times 1.3778 - 1 \times 2.2589}{9} = 0.6321$$

$$x_2 = \frac{10 - 6.25 \times 0.6231 - 1 \times 2.2589}{2.5} = 1.5387$$

$$x_3 = \frac{8.57 - 4 \times 0.6231 - 2 \times 1.5387}{1} 3.0002$$

After Iteration #2

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0.6231 \\ 1.5387 \\ 3.0002 \end{bmatrix}$$

Example: Liquid-Liquid Extraction

Iteration #2 absolute relative approximate error

$$\left|\in_a\right|_1 = \left|\frac{0.6231 - 0.8889}{0.6231}\right| \text{x}100 = 42.6590\%$$

$$\left|\in_a\right|_2 = \left|\frac{1.5387 - 1.3778}{1.5387}\right| \text{x}100 = 10.46\%$$

$$\left|\in_a\right|_3 = \left|\frac{3.0002 - 2.2589}{3.0002}\right| \text{x}100 = 24.7087\%$$

The maximum absolute relative error after the first iteration is 10.46%

Example: Liquid-Liquid Extraction

Repeating more iterations, the following values are obtained

Iteration	x_1	$\left\|\varepsilon_a\right\|_1$	x_2	$\left\|\varepsilon_a\right\|_2$	x_3	$\left\|\varepsilon_a\right\|_3$
1	0.8889	12.5	1.3778	27.4194	2.2589	55.7305
2	0.6231	42.6590	1.5387	10.4560	3.0002	24.7087
3	0.4871	27.9258	1.5822	2.7506	3.4572	13.2195
4	0.4218	15.4792	1.5627	1.2537	3.7576	7.9928
5	0.3950	6.7960	1.5096	3.5131	3.9710	5.3747
6	0.3889	1.5521	1.4393	4.8828	4.1357	3.9826

After six iterations, the absolute relative approximate error seems to be decreasing. Conducting more iterations allows the absolute relative approximate error to decrease to an acceptable level.

Example: Liquid-Liquid Extraction

Repeating more iterations, the following values are obtained

Iteration	x_1	$\left\|\varepsilon_a\right\|_1$	x_2	$\left\|\varepsilon_a\right\|_2$	x_3	$\left\|\varepsilon_a\right\|_3$
199	1.1335	0.01441	-2.2389	0.034871	8.5139	0.010666
200	1.1337	0.014056	-2.2397	0.034005	8.5148	0.010403

The value of closely approaches the true value of

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1.1337 \\ -2.2397 \\ 8.5148 \end{bmatrix}$$

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1.140 \\ -2.269 \\ 8.549 \end{bmatrix}$$

Example: Liquid-Liquid Extraction

The polynomial that passes through the three data points is then:

$$g(g/l) = x_1(g/l)^2 + x_2(g/l) + x_3 \qquad = 1.140(g/l)^2 + (-2.269)(g/l) + 8.549$$

Where g is grams of nickel in the organic phase and g/l is the grams/liter in the aqueous phase.

Solution:

Estimate the amount of nickel in the organic phase when 2.3g/l is in the aqueous phase using quadratic interpolation

$$g(2.3g/l) = 1.140 \times (2.3g/l)^2 + (-2.269) \times (2.3g/l) + 8.549$$

$$= 1.140 \times 5.29 + (-2.269) \times 2.3 + 8.549$$

$$g(2.3g/l) = 9.3609g/l$$

Gauss-Seidel Method

Summary

-Advantages of the Gauss-Seidel Methed

-Algorithm for the Gauss-Seidel Method

-Pitfalls of the Gauss-Seidel Method

Gauss-Siedel Method

Questions?