Chemical Engineering Majors

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Transforming Numerical Methods Education for STEM Undergraduates

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 pre-specified tolerance.

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:

$$a_{11}x_{1} + a_{12}x_{2} + a_{13}x_{3} + \dots + a_{1n}x_{n} = b_{1}$$

$$a_{21}x_{1} + a_{22}x_{2} + a_{23}x_{3} + \dots + a_{2n}x_{n} = b_{2}$$

$$\vdots$$

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

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





Algorithm

General Form for any row 'i'

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

How or where can this equation be used?

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 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.

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.

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, <i>a</i> (g/l)	2	2.5	3
Ni organic phase, g (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

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

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 organic phase when 2.3 g/l is in the aqueous phase using quadratic interpolation.

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

Conduct two iterations.

Rewriting each equation

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

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

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

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

Iteration 1

Applying the initial guess and solving for each x_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?

Finding the absolute relative approximate error for Iteration 1.

$$\left| \in_{a} \right|_{i} = \left| \frac{x_{i}^{new} - x_{i}^{old}}{x_{i}^{new}} \right| \times 100$$
$$\left| \in_{a} \right|_{1} = \left| \frac{1.3925 - 1}{1.3925} \right| \times 100 = 28.187\%$$

$$\left|\epsilon_{a}\right|_{2} = \left|\frac{0.11875 - 1}{0.11875}\right| \times 100 = 742.11\%$$

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

The maximum absolute relative approximate error is 742.11%.

$$\left|\epsilon_{a}\right|_{3} = \left|\frac{-0.88875 - 1}{-0.88875}\right| \times 100 = 212.52\%$$

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.

$$x_{1} = \frac{8.57 - 2 \times 0.11875 - (-0.88875)}{4} = 2.3053$$
$$x_{2} = \frac{10 - 6.25 \times 2.3053 - (-0.88875)}{2.5} = -1.4078$$
$$x_{3} = \frac{12 - 9 \times 2.3053 - 3 \times (-1.4078)}{1} = -4.5245$$

Finding the absolute relative approximate error for Iteration 2.

$$\begin{split} \left| \in_{a} \right|_{1} &= \left| \frac{2.3053 - 1.3925}{2.3053} \right| \times 100 \\ &= 39.596 \% \\ \left| \in_{a} \right|_{2} &= \left| \frac{-1.40778 - 0.11875}{-1.4078} \right| \times 100 \\ &= 108.44 \% \\ \left| \in_{a} \right|_{3} &= \left| \frac{-4.5245 - (-0.88875)}{-4.5245} \right| \times 100 \\ &= 80.357 \% \end{split}$$

At the end of the Iteration 1

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

The maximum absolute relative approximate error is 108.44%

Repeating more iterations, the following values are obtained

Iteration	<i>x</i> ₁	$\left \in_{a} \right _{1} \%$	<i>x</i> ₂	$\left \epsilon_{a}\right _{2}\%$	<i>x</i> ₃	$\left \epsilon_{a}\right _{3}\%$
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

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

Also, the solution is not converging to the true solution of
$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1.14 \\ -2.27 \\ 8.55 \end{bmatrix}$$

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:

$$|a_{\mathrm{ii}}| \ge \sum_{\substack{j=1\\j\neq\mathrm{i}}}^{n} |a_{ij}| \quad \text{for all 'i'} \qquad \text{and } |a_{ii}| > \sum_{\substack{j=1\\j\neq\mathrm{i}}}^{n} |a_{ij}| \qquad \text{for at least one 'i'}$$

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)

Rewritten (Diagonally dominant)

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

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

<u>Iteration 1</u> 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

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

Example: Liquid-Liquid Extraction The absolute relative approximate error for Iteration 1 is

$$\begin{split} \left| \in_{a} \right|_{1} &= \left| \frac{0.88889 - 1}{0.88889} \right| \times 100 = 12.5\% \\ \left| \in_{a} \right|_{2} &= \left| \frac{1.3778 - 1}{1.3778} \right| \times 100 = 27.419\% \\ \left| \in_{a} \right|_{3} &= \left| \frac{2.2589 - 1}{2.2589} \right| \times 100 = 55.730\% \end{split}$$

At the end of Iteration 1

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

The maximum absolute relative error after the first iteration is 55.730%

Example: Liquid-Liquid Extraction <u>Iteration 2</u>

Using $\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0.8889 \\ 1.3778 \\ 2.2589 \end{bmatrix}$ from Iteration 1

the values for x_i are found

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

The absolute relative approximate error for Iteration 2

$$\begin{aligned} \left| \in_{a} \right|_{1} &= \left| \frac{0.62309 - 0.88889}{0.62309} \right| \times 100 = 42.659\% \end{aligned}$$
At the end of Iteration
$$\left| \in_{a} \right|_{2} &= \left| \frac{1.5387 - 1.3778}{1.5387} \right| \times 100 = 10.460\% \qquad \begin{bmatrix} x_{1} \\ x_{2} \\ x_{3} \end{bmatrix} = \begin{bmatrix} 0.62309 \\ 1.5387 \\ 3.0002 \end{bmatrix}$$
$$\left| \in_{a} \right|_{3} &= \left| \frac{3.0002 - 2.2589}{3.0002} \right| \times 100 = 24.709\% \qquad \begin{bmatrix} x_{1} \\ x_{2} \\ x_{3} \end{bmatrix} = \begin{bmatrix} 0.62309 \\ 1.5387 \\ 3.0002 \end{bmatrix}$$

The maximum absolute relative error after the first iteration is 42.659%

Repeating more iterations, the following values are obtained

Iteration	<i>x</i> ₁	$\left \epsilon_{a}\right _{1}\%$	<i>x</i> ₂	$\left \in_{a} \right _{2} \%$	<i>x</i> ₃	$\left \epsilon_{a}\right _{3}\%$
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 error seems to be decreasing. Conducting more iterations allows the absolute relative approximate error to decrease to an acceptable level.

Repeating more iterations, the following values are obtained

Iteration	<i>x</i> ₁	$\left \in_{a} \right _{1} \%$	<i>x</i> ₂	$\left \in_{a} \right _{2} \%$	<i>x</i> 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

The value of

closely approaches the true value of

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

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

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 grams of nickel in the organic phase and *a* is the grams/liter in the aqueous phase.

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

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

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	<i>a</i> ₁	$\left\ \in_{a} \right\ _{1} \%$	A ₂	$\left \epsilon_{a}\right _{2}\%$	<i>a</i> ₃	$\left \epsilon_{a}\right _{3}\%$
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?

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 same set of equations will converge.

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

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

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

Questions?

Additional Resources

For all resources on this topic such as digital audiovisual lectures, primers, textbook chapters, multiple-choice tests, worksheets in MATLAB, MATHEMATICA, MathCad and MAPLE, blogs, related physical problems, please visit

http://numericalmethods.eng.usf.edu/topics/gauss_seid el.html

THE END