Simultaneous Linear Equations

Topic: Gaussian Elimination

Major: Chemical Engineering

Gaussian Elimination

One of the most popular techniques for solving simultaneous linear equations of the form $[A][X]=[C]$

Consists of 2 steps

1. Forward Elimination of Unknowns.

2. Back Substitution

Forward Elimination

The goal of Forward Elimination is to transform the coefficient matrix into an Upper Triangular Matrix

$$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix} \rightarrow \begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & 0 & 0.7 \end{bmatrix}$$

Forward Elimination

Linear Equations

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

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

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

$$\begin{matrix} . & & . \\ . & & . \\ . & & . \end{matrix}$$

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

Forward Elimination

Transform to an Upper Triangular Matrix

Step 1: Eliminate x_1 in 2nd equation using equation 1 as the pivot equation

$$\left[\frac{Eqn1}{a_{11}}\right]\times(a_{21})$$

Which will yield

$$a_{21}x_1+\frac{a_{21}}{a_{11}}a_{12}x_2+...+\frac{a_{21}}{a_{11}}a_{1n}x_n=\frac{a_{21}}{a_{11}}b_1$$

Forward Elimination

Zeroing out the coefficient of x_1 in the 2^{nd} equation.

Subtract this equation from 2^{nd} equation

$$\left(a_{22} - \frac{a_{21}}{a_{11}} a_{12}\right) x_2 + \ldots + \left(a_{2n} - \frac{a_{21}}{a_{11}} a_{1n}\right) x_n = b_2 - \frac{a_{21}}{a_{11}} b_1$$

Or

$$a'_{22} x_2 + \ldots + a'_{2n} x_n = b'_2$$

Where

$$a'_{22} = a_{22} - \frac{a_{21}}{a_{11}} a_{12}$$

$$\vdots$$

$$a'_{2n} = a_{2n} - \frac{a_{21}}{a_{11}} a_{1n}$$

Forward Elimination

Repeat this procedure for the remaining equations to reduce the set of equations as

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

$$a'_{22}x_2 + a'_{23}x_3 + \ldots + a'_{2n}x_n = b'_2$$

$$a'_{32}x_2 + a'_{33}x_3 + \ldots + a'_{3n}x_n = b'_3$$

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

$$a'_{n2}x_2 + a'_{n3}x_3 + \ldots + a'_{nn}x_n = b'_n$$

Forward Elimination

Step 2: Eliminate x_2 in the 3rd equation.

Equivalent to eliminating x_1 in the 2nd equation using equation 2 as the pivot equation.

$$Eqn3 - \left[\frac{Eqn2}{a_{22}} \right] \times (a_{32})$$

Forward Elimination

This procedure is repeated for the remaining equations to reduce the set of equations as

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

$$a'_{22}x_2 + a'_{23}x_3 + \ldots + a'_{2n}x_n = b'_2$$

$$a''_{33}x_3 + \ldots + a''_{3n}x_n = b''_3$$

$$\vdots \qquad \vdots$$

$$a''_{n3}x_3 + \ldots + a''_{nn}x_n = b''_n$$

Forward Elimination

Continue this procedure by using the third equation as the pivot equation and so on.

At the end of (n-1) Forward Elimination steps, the system of equations will look like:

$$
\begin{aligned}
a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \ldots + a_{1n}x_n &= b_1 \\
a'_{22}x_2 + a'_{23}x_3 + \ldots + a'_{2n}x_n &= b'_2 \\
a''_{33}x_3 + \ldots + a''_{n}x_n &= b''_3 \\
\vdots \qquad & \quad \vdots \\
a_{nn}^{(n-1)}x_n &= b_n^{(n-1\ \ )}
\end{aligned}
$$

Forward Elimination

At the end of the Forward Elimination steps

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1n} \\ & a'_{22} & a'_{23} & \cdots & a'_{2n} \\ & & a''_{33} & \cdots & a''_{3n} \\ & & & \vdots & \vdots \\ & & & & a_{nn}^{(n-1)} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b'_2 \\ b''_3 \\ \vdots \\ b_n^{(n-1)} \end{bmatrix}$$

Back Substitution

The goal of Back Substitution is to solve each of the equations using the upper triangular matrix.

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 0 & a_{22} & a_{23} \\ 0 & 0 & a_{33} \end{bmatrix} \begin{bmatrix} \mathrm{x}_1 \\ \mathrm{x}_2 \\ \mathrm{x}_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$$

Example of a system of 3 equations

Back Substitution

Start with the last equation because it has only one unknown

$$x_n = \frac{b_n^{(n-1)}}{a_{nn}^{(n-1)}}$$

Solve the second from last equation $(n-1)^{th}$ using x_n solved for previously.

This solves for x_{n-1}.

Back Substitution

Representing Back Substitution for all equations by formula

$$x_i = \frac{b_i^{(i-1)} - \sum_{j=i+1}^{n} a_{ij}^{(i-1)} x_j}{a_{ii}^{(i-1)}}$$

For $i=n-1, n-2, \ldots, 1$

and

$$x_n = \frac{b_n^{(n-1)}}{a_{nn}^{(n-1)}}$$

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 Naïve Guass Elimination.
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

Forward Elimination: Step 1

$$Row2 - \left[\frac{Row1}{4}\right] \times (6.25) =$$

Yields

$$\begin{bmatrix} 4 & 2 & 1 \\ 0 & -0.625 & -0.5625 \\ 9 & 3 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 8.57 \\ -3.3906 \\ 12 \end{bmatrix}$$

Example: Liquid-Liquid Extraction

Forward Elimination: Step 1

$$Row3 - \left[\frac{Row1}{4}\right] \times (9) =$$

Yields

$$\begin{bmatrix} 4 & 2 & 1 \\ 0 & -0.625 & -0.5625 \\ 0 & -1.5 & -1.25 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 8.57 \\ -3.3906 \\ -7.2825 \end{bmatrix}$$

Example: Liquid-Liquid Extraction

Forward Elimination: Step 2

$$Row3 - \left[\frac{Row2}{-0.625} \right] \times (-1.5) =$$

Yields

$$\begin{bmatrix} 4 & 2 & 1 \\ 0 & -0.625 & -0.5625 \\ 0 & 0 & 0.1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 8.57 \\ -3.3906 \\ 0.8549 \end{bmatrix}$$

This is now ready for Back Substitution

Example: Liquid-Liquid Extraction

Back Substitution: Solve for x_3 using the third equation

$$0.1x_3 = 0.8549$$

$$x_3 = \frac{0.8549}{0.1}$$

$$= 8.549$$

Example: Liquid-Liquid Extraction

Back Substitution: Solve for x_2 using the second equation

$$(-0.625)x_2 + (-0.5625)x_3 = -3.3906$$

$$x_2 = \frac{-3.3906 - (-0.5625)x_3}{-0.625}$$

$$= \frac{-3.3906 - (-0.5625)\times 8.549}{-0.625}$$

$$= -2.269$$

Example: Liquid-Liquid Extraction

Back Substitution: Solve for x_1 using the first equation

$$4x_1 + 2x_2 + x_3 = 8.57$$

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

$$= \frac{8.57 - 2 \times (-2.269) - 8.549}{4}$$

$$= 1.140$$

Example: Liquid-Liquid Extraction

Solution:

The solution vector is

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

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

$$g\left(g/l\right) = x_1 (g/l)^2 + x_2 (g/l) + x_3$$

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

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

Example: Liquid-Liquid Extraction

Solution:

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

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

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

$$g\left(2.3g/l\right) = 9.3609g/l$$

Pitfalls

Two Potential Pitfalls

-Division by zero: May occur in the forward elimination steps. Consider the set of equations:

$$10x_2 - 7x_3 = 7$$

$$6x_1 + 2.099x_2 + 3x_3 = 3.901$$

$$5x_1 - x_2 + 5x_3 = 6$$

- Round-off error: Prone to round-off errors.

Pitfalls: Example

Consider the system of equations:

Use five significant figures with chopping

$$\begin{bmatrix} 10 & -7 & 0 \\ -3 & 2.099 & 6 \\ 5 & -1 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 7 \\ 3.901 \\ 6 \end{bmatrix}$$

At the end of Forward Elimination

$$\begin{bmatrix} 10 & -7 & 0 \\ 0 & -0.001 & 6 \\ 0 & 0 & 15005 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 7 \\ 6.001 \\ 15004 \end{bmatrix}$$

Pitfalls: Example

Back Substitution

$$\begin{bmatrix} 10 & -7 & 0 \\ 0 & -0.001 & 6 \\ 0 & 0 & 15005 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 7 \\ 6.001 \\ 15004 \end{bmatrix}$$

$$x_3 = \frac{15004}{15005} = 0.99993$$

$$x_2 = \frac{6.001 - 6x_3}{-0.001} = -1.5$$

$$x_1 = \frac{7 + 7x_2 - 0x_3}{10} = -0.3500$$

Pitfalls: Example

Compare the calculated values with the exact solution

$$[X]_{exact} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 \\ -1 \\ 1 \end{bmatrix}$$

$$[X]_{calculated} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} -0.35 \\ -1.5 \\ 0.99993 \end{bmatrix}$$

Improvements

Increase the number of significant digits

- Decreases round off error
- Does not avoid division by zero

Gaussian Elimination with Partial Pivoting

- Avoids division by zero
- Reduces round off error

Partial Pivoting

Gaussian Elimination with partial pivoting applies row switching to normal Gaussian Elimination.

How?

At the beginning of the k^{th} step of forward elimination, find the maximum of

$$\left|a_{kk}\right|, \left|a_{k+1,k}\right|, \ldots\ldots\ldots\ldots\ldots\ldots, \left|a_{nk}\right|$$

If the maximum of the values is $\left|a_{pk}\right|$ In the p^{th} row, $k \leq p \leq n,$

then switch rows p and k.

Partial Pivoting

What does it Mean?

Gaussian Elimination with Partial Pivoting ensures that each step of Forward Elimination is performed with the pivoting element $|a_{kk}|$ having the largest absolute value.

Partial Pivoting: Example

Consider the system of equations

$$10x_1 - 7x_2 = 7$$
$$-3x_1 + 2.099x_2 + 3x_3 = 3.901$$
$$5x_1 - x_2 + 5x_3 = 6$$

In matrix form

$$\begin{bmatrix} 10 & 7 & 0 \\ -3 & 2.099 & 6 \\ 5 & -1 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 7 \\ 3.901 \\ 6 \end{bmatrix}$$

Solve using Gaussian Elimination with Partial Pivoting using five significant digits with chopping

Partial Pivoting: Example

Forward Elimination: Step 1

Examining the values of the first column

|10|, |-3|, and |5| or 10, 3, and 5

The largest absolute value is 10, which means, to follow the rules of Partial Pivoting, we switch row1 with row1.

Performing Forward Elimination

$$\begin{bmatrix} 10 & 7 & 0 \\ -3 & 2.099 & 6 \\ 5 & -1 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 7 \\ 3.901 \\ 6 \end{bmatrix} \Rightarrow \begin{bmatrix} 10 & -7 & 0 \\ 0 & -0.001 & 6 \\ 0 & 2.5 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 7 \\ 6.001 \\ 2.5 \end{bmatrix}$$

Partial Pivoting: Example

Forward Elimination: Step 2

Examining the values of the first column

|-0.001| and |2.5| or 0.0001 and 2.5

The largest absolute value is 2.5, so row 2 is switched with row 3

Performing the row swap

$$\begin{bmatrix} 10 & -7 & 0 \\ 0 & -0.001 & 6 \\ 0 & 2.5 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 7 \\ 6.001 \\ 2.5 \end{bmatrix} \Rightarrow \begin{bmatrix} 10 & -7 & 0 \\ 0 & 2.5 & 5 \\ 0 & -0.001 & 6 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 7 \\ 2.5 \\ 6.001 \end{bmatrix}$$

Partial Pivoting: Example

Forward Elimination: Step 2

Performing the Forward Elimination results in:

$$\begin{bmatrix} 10 & -7 & 0 \\ 0 & 2.5 & 5 \\ 0 & 0 & 6.002 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 7 \\ 2.5 \\ 6.002 \end{bmatrix}$$

Partial Pivoting: Example

Back Substitution

Solving the equations through back substitution

$$\begin{bmatrix} 10 & -7 & 0 \\ 0 & 2.5 & 5 \\ 0 & 0 & 6.002 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 7 \\ 2.5 \\ 6.002 \end{bmatrix}$$

$$x_3 = \frac{6.002}{6.002} = 1$$

$$x_2 = \frac{2.5 - 5x_2}{2.5} = 1$$

$$x_1 = \frac{7 + 7x_2 - 0x_3}{10} = 0$$

Partial Pivoting: Example

Compare the calculated and exact solution

The fact that they are equal is coincidence, but it does illustrate the advantage of Partial Pivoting

$$[X]_{calculated} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 \\ -1 \\ 1 \end{bmatrix} \qquad [X]_{exact} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 0 \\ -1 \\ 1 \end{bmatrix}$$

Summary

-Forward Elimination

-Back Substitution

-Pitfalls

-Improvements

-Partial Pivoting