



Simultaneous Linear Equations



Topic: LU Decomposition
Major: Chemical Engineering



LU Decomposition

LU Decomposition is another method to solve a set of simultaneous linear equations

Which is better, Gauss Elimination or LU Decomposition?

To answer this, a closer look at LU decomposition is needed.



LU Decomposition

Method

For most non-singular matrix $[A]$ that one could conduct Naïve Gauss Elimination forward elimination steps, one can always write it as

$$[A] = [L][U]$$

Where

$[L]$ = lower triangular matrix

$[U]$ = upper triangular matrix



LU Decomposition

Proof

If solving a set of linear equations $[A][X] = [C]$

If $[A] = [L][U]$ Then $[L][U][X] = [C]$

Multiply by $[L]^{-1}$

Which gives $[L]^{-1}[L][U][X] = [L]^{-1}[C]$

Remember $[L]^{-1}[L] = [I]$ which leads to $[I][U][X] = [L]^{-1}[C]$

Now, if $[I][U] = [U]$ then $[U][X] = [L]^{-1}[C]$

Now, let $[L]^{-1}[C] = [Z]$

Which ends with $[L][Z] = [C]$ (1)

and $[U][X] = [Z]$ (2)



LU Decomposition

How can this be used?

Given $[A][X]=[C]$

Decompose $[A]$ into $[L]$ and $[U]$

Then solve $[L][Z]=[C]$ for $[Z]$

And then solve $[U][X]=[Z]$ for $[X]$



LU Decomposition

How is this better or faster than Gauss Elimination?

Let's look at computational time.

n = number of equations

To decompose $[A]$, time is proportional to $\frac{n^3}{3}$

To solve $[U][X] = [C]$ and $[L][Z] = [C]$

time proportional to $\frac{n^2}{2}$



LU Decomposition

Therefore, total computational time for LU Decomposition is proportional to

$$\frac{n^3}{3} + 2\left(\frac{n^2}{2}\right) \quad \text{or} \quad \frac{n^3}{3} + n^2$$

Gauss Elimination computation time is proportional to

$$\frac{n^3}{3} + \frac{n^2}{2}$$

How is this better?



LU Decomposition

What about a situation where the [C] vector changes?

In LU Decomposition, LU decomposition of [A] is independent of the [C] vector, therefore it only needs to be done once.

Let m = the number of times the [C] vector changes

The computational times are proportional to

$$\text{LU decomposition} = m\left(\frac{n^3}{3} + \frac{n^2}{2}\right) \quad \text{Gauss Elimination} = \frac{n^3}{3} + m(n^2)$$

Consider a 100 equation set with 50 right hand side vectors

$$\text{LU Decomposition} = 8.33 \times 10^5 \quad \text{Gauss Elimination} = 1.69 \times 10^7$$



LU Decomposition

Another Advantage

Finding the Inverse of a Matrix

LU Decomposition

$$\frac{n^3}{3} + n(n^2) = \frac{4n^3}{3}$$

Gauss Elimination

$$n \left(\frac{n^3}{3} + \frac{n^2}{2} \right) = \frac{n^4}{3} + \frac{n^3}{2}$$

For large values of n

$$\frac{n^4}{3} + \frac{n^3}{2} \gg \frac{4n^3}{3}$$



LU Decomposition

Method: [A] Decompose to [L] and [U]

$$[A] = [L][U] = \begin{bmatrix} 1 & 0 & 0 \\ \ell_{21} & 1 & 0 \\ \ell_{31} & \ell_{32} & 1 \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}$$

[U] is the same as the coefficient matrix at the end of the forward elimination step.

[L] is obtained using the *multipliers* that were used in the forward elimination process

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

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

Example: Liquid-Liquid Extraction

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 LU Decomposition.

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

Finding the $[U]$ matrix

Using the Forward Elimination Procedure of Gauss Elimination

$$\begin{bmatrix} 4 & 2 & 1 \\ 6.25 & 2.5 & 1 \\ 9 & 3 & 1 \end{bmatrix}$$

$$\text{Row2} - \left[\frac{\text{Row1}}{4} \right] \times (6.25) = \begin{bmatrix} 4 & 2 & 1 \\ 0 & -0.625 & -0.5625 \\ 9 & 3 & 1 \end{bmatrix}$$

$$\text{Row3} - \left[\frac{\text{Row1}}{4} \right] \times (9) = \begin{bmatrix} 4 & 2 & 1 \\ 0 & -0.625 & -0.5625 \\ 0 & -1.5 & -1.25 \end{bmatrix}$$

Example: Liquid-Liquid Extraction

Finding the $[U]$ matrix

Using the Forward Elimination Procedure of Gauss Elimination

$$\begin{bmatrix} 4 & 2 & 1 \\ 0 & -0.625 & -0.5625 \\ 0 & -1.5 & -1.25 \end{bmatrix} \quad \text{Row3} - \left[\frac{\text{Row2}}{-0.625} \right] \times (-1.5) = \begin{bmatrix} 4 & 2 & 1 \\ 0 & -0.625 & -0.5625 \\ 0 & 0 & 0.1 \end{bmatrix}$$

$$[U] = \begin{bmatrix} 4 & 2 & 1 \\ 0 & -0.625 & -0.5625 \\ 0 & 0 & 0.1 \end{bmatrix}$$

Example: Liquid-Liquid Extraction

Finding the $[L]$ matrix

Using the multipliers used during the Forward Elimination Procedure

From the first step
of forward
elimination

$$\begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{bmatrix}$$
$$l_{21} = \frac{a_{21}}{a_{11}} = \frac{6.25}{4} = 1.5625$$
$$l_{31} = \frac{a_{31}}{a_{11}} = \frac{9}{4} = 2.25$$

From the second
step of forward
elimination

$$\begin{bmatrix} 4 & 2 & 1 \\ 0 & -0.625 & -0.5625 \\ 0 & -1.5 & -1.25 \end{bmatrix}$$
$$l_{32} = \frac{a_{32}}{a_{22}} = \frac{-1.5}{-0.625} = 2.4$$

Example: Liquid-Liquid Extraction

$$[L] = \begin{bmatrix} 1 & 0 & 0 \\ 1.5625 & 1 & 0 \\ 2.25 & 2.4 & 1 \end{bmatrix}$$

Does $[L][U] = [A]$?

$$[L][U] = \begin{bmatrix} 1 & 0 & 0 \\ 1.5625 & 1 & 0 \\ 2.25 & 2.4 & 1 \end{bmatrix} \begin{bmatrix} 4 & 2 & 1 \\ 0 & -0.625 & -0.5625 \\ 0 & 0 & 0.1 \end{bmatrix}$$

Example: Liquid-Liquid Extraction

Example: Solving simultaneous linear equations using LU Decomposition

$$\text{Set } [L][Z] = [C] \quad \begin{bmatrix} 1 & 0 & 0 \\ 1.5625 & 1 & 0 \\ 2.25 & 2.4 & 1 \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} = \begin{bmatrix} 8.57 \\ 10 \\ 12 \end{bmatrix}$$

$$z_1 = 8.57$$

Solve for $[Z]$

$$1.5625z_1 + z_2 = 10$$

$$2.25z_1 + 2.4z_2 + z_3 = 12$$

Example: Liquid-Liquid Extraction

Example: Solving simultaneous linear equations using LU Decomposition

Complete the forward substitution to solve for $[Z]$

$$z_1 = 8.57$$

$$\begin{aligned} z_2 &= 10 - 1.5625z_1 \\ &= 10 - 1.5625 \times 8.57 \\ &= -3.3906 \end{aligned}$$

$$\begin{aligned} z_3 &= 12 - 2.25z_1 - 2.4z_2 \\ &= 12 - 2.25 \times 8.57 - 2.4 \times (-3.3906) \\ &= 0.8549 \end{aligned}$$

$$[Z] = \begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} = \begin{bmatrix} 8.57 \\ -3.3906 \\ 0.8549 \end{bmatrix}$$

Example: Liquid-Liquid Extraction

Example: Solving simultaneous linear equations using LU Decomposition

$$\text{Set } [U][X] = [Z] \quad \begin{bmatrix} 4 & 2 & 1 \\ 0 & -0.625 & -0.5625 \\ 0 & 0 & 0.1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 8.57 \\ -3.3906 \\ 0.8549 \end{bmatrix}$$

Solve for $[X]$

The 3 equations become

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

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

$$0.1x_3 = 0.8549$$

Example: Liquid-Liquid Extraction

Example: Solving simultaneous linear equations using LU Decomposition

From the 3rd equation

$$\begin{aligned}0.1x_3 &= 0.8549 \\ &= \frac{0.8549}{0.1} \\ &= 8.549\end{aligned}$$

Substituting in x_3 and using the second equation

$$\begin{aligned}-0.625x_2 + (-0.5625)x_3 &= -3.3906 \\ x_2 &= \frac{-3.3906 - (-0.5625)x_3}{-0.625} \\ &= \frac{-3.3906 - (-0.5625) \times 8.549}{-0.625} \\ &= -2.269\end{aligned}$$

Example: Liquid-Liquid Extraction

Example: Solving simultaneous linear equations using LU Decomposition

Substituting in x_3 and x_2
using the first equation

$$\begin{aligned}4x_1 + 2x_2 + x_3 &= 8.57 \\x_1 &= \frac{8.57 - 2x_2 - x_3}{4} \\&= \frac{8.57 - 2 \times (-2.269) - 8.549}{4} \\&= 1.140\end{aligned}$$

Hence the Solution Vector is:

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

Example: Liquid-Liquid Extraction

Solution:

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

$$\begin{aligned}g(g/l) &= x_1(g/l)^2 + x_2(g/l) + x_3 \\ &= 1.140(g/l)^2 + (-2.269)(g/l) + 8.549\end{aligned}$$

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

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

$$\begin{aligned}g(2.3g/l) &= 1.140 \times (2.3g/l)^2 + (-2.269) \times (2.3g/l) + 8.549 \\ &= 1.140 \times 5.29 + (-2.269) \times 2.3 + 8.549\end{aligned}$$

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



LU Decomposition

Finding the inverse of a square matrix

Remember, the relative computational time comparison of LU decomposition and Gauss elimination is:

$$\frac{n^4}{3} + \frac{n^3}{2} \gg \frac{4n^3}{3}$$

Review: The inverse $[B]$ of a square matrix $[A]$ is defined as

$$[A][B] = [I] = [B][A]$$



LU Decomposition

Finding the inverse of a square matrix

How can LU Decomposition be used to find the inverse?

Assume the first column of $[B]$ to be $[b_{11} \ b_{12} \ \dots \ b_{n1}]^T$

Using this and the definition of matrix multiplication

First column of $[B]$

$$[A] \begin{bmatrix} b_{11} \\ b_{21} \\ \vdots \\ b_{n1} \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

Second column of $[B]$

$$[A] \begin{bmatrix} b_{12} \\ b_{22} \\ \vdots \\ b_{n2} \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ \vdots \\ 0 \end{bmatrix}$$

The remaining columns in $[B]$ can be found in the same manner



LU Decomposition

Example: Finding the inverse of a square matrix

Find the inverse of $[A]$

$$[A] = \begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix}$$

Using the Decomposition procedure, the $[L]$ and $[U]$ matrices are found to be

$$[A] = [L][U] = \begin{bmatrix} 1 & 0 & 0 \\ 2.56 & 1 & 0 \\ 5.76 & 3.5 & 1 \end{bmatrix} \begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & 0 & 0.7 \end{bmatrix}$$



LU Decomposition

Example: Finding the inverse of a square matrix

Solving for the each column of $[B]$ requires to steps

1) Solve $[L][Z] = [C]$ for $[Z]$ and 2) Solve $[U][X] = [Z]$ for $[X]$

$$\text{Step 1: } [L][Z] = [C] \rightarrow \begin{bmatrix} 1 & 0 & 0 \\ 2.56 & 1 & 0 \\ 5.76 & 3.5 & 1 \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

This generates the equations:

$$z_1 = 1$$

$$2.56z_1 + z_2 = 0$$

$$5.76z_1 + 3.5z_2 + z_3 = 0$$



LU Decomposition

Example: Finding the inverse of a square matrix

Solving for $[Z]$

$$z_1 = 1$$

$$\begin{aligned} z_2 &= 0 - 2.56z_1 \\ &= 0 - 2.56(1) \\ &= -2.56 \end{aligned}$$

$$\begin{aligned} z_3 &= 0 - 5.76z_1 - 3.5z_2 \\ &= 0 - 5.76(1) - 3.5(-2.56) \\ &= 3.2 \end{aligned}$$

$$[Z] = \begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} = \begin{bmatrix} 1 \\ -2.56 \\ 3.2 \end{bmatrix}$$

LU Decomposition

Example: Finding the inverse of a square matrix

Solving for $[U] [X] = [Z]$ for $[X]$

$$\begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & 0 & 0.7 \end{bmatrix} \begin{bmatrix} b_{11} \\ b_{21} \\ b_{31} \end{bmatrix} = \begin{bmatrix} 1 \\ -2.56 \\ 3.2 \end{bmatrix}$$

$$25b_{11} + 5b_{21} + b_{31} = 1$$

$$-4.8b_{21} - 1.56b_{31} = -2.56$$

$$0.7b_{31} = 3.2$$



LU Decomposition

Example: Finding the inverse of a square matrix

Using Backward Substitution

$$b_{31} = \frac{3.2}{0.7} = 4.571$$

$$\begin{aligned} b_{21} &= \frac{-2.56 + 1.560b_{31}}{-4.8} \\ &= \frac{-2.56 + 1.560(4.571)}{-4.8} = -0.9524 \end{aligned}$$

$$\begin{aligned} b_{11} &= \frac{1 - 5b_{21} - b_{31}}{25} \\ &= \frac{1 - 5(-0.9524) - 4.571}{25} = 0.04762 \end{aligned}$$

So the first column of the inverse of $[A]$ is:

$$\begin{bmatrix} b_{11} \\ b_{21} \\ b_{31} \end{bmatrix} = \begin{bmatrix} 0.04762 \\ -0.9524 \\ 4.571 \end{bmatrix}$$

LU Decomposition

Example: Finding the inverse of a square matrix

Repeating for the second and third columns of the inverse

Second Column

$$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix} \begin{bmatrix} b_{12} \\ b_{22} \\ b_{32} \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} b_{12} \\ b_{22} \\ b_{32} \end{bmatrix} = \begin{bmatrix} -0.08333 \\ 1.417 \\ -5.000 \end{bmatrix}$$

Third Column

$$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix} \begin{bmatrix} b_{13} \\ b_{23} \\ b_{33} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

$$\begin{bmatrix} b_{13} \\ b_{23} \\ b_{33} \end{bmatrix} = \begin{bmatrix} 0.03571 \\ -0.4643 \\ 1.429 \end{bmatrix}$$



LU Decomposition

Example: Finding the inverse of a square matrix

The inverse of $[A]$ is

$$[A]^{-1} = \begin{bmatrix} 0.4762 & 0.08333 & 0.0357 \\ -0.9524 & 1.417 & -0.4643 \\ 4.571 & -5.050 & 1.429 \end{bmatrix}$$

To check your work do the following operation

$$[A][A]^{-1} = [I] = [A]^{-1}[A]$$