LU Decomposition

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Transforming Numerical Methods Education for STEM Undergraduates

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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

How does LU Decomposition work?

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	$[L][Z] = [C] \quad (1)$
and	$[U][X] = [Z] \quad (2)$

LU Decomposition

How can this be used?

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

1. Decompose $[A]$ into $[L]$ and $[U]$
2. Solve $[L][Z] = [C]$ for $[Z]$
3. Solve $[U][X] = [Z]$ for $[X]$

When is LU Decomposition better than Gaussian Elimination?

To solve $[A][X]=[B]$

Table. Time taken by methods

Gaussian Elimination	LU Decomposition
$T\left(\frac{8n^3}{3}+12n^2+\frac{4n}{3}\right)$	$T\left(\frac{8n^3}{3}+12n^2+\frac{4n}{3}\right)$

where T = clock cycle time and n = size of the matrix

So both methods are equally efficient.

To find inverse of [A]

Time taken by Gaussian Elimination

$$= n\left(CT|_{FE} + CT|_{BS}\right)$$

$$= T\left(\frac{8n^4}{3} + 12n^3 + \frac{4n^2}{3}\right)$$

Time taken by LU Decomposition

$$= CT|_{LU} + n \times CT|_{FS} + n \times CT|_{BS}$$

$$= T\left(\frac{32n^3}{3} + 12n^2 + \frac{20n}{3}\right)$$

Table 1 Comparing computational times of finding inverse of a matrix using LU decomposition and Gaussian elimination.

n	10	100	1000	10000
$CT\|_{\text{inverse GE}} / CT\|_{\text{inverse LU}}$	3.28	25.83	250.8	2501

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

Finding the [U] matrix

Using the Forward Elimination Procedure of Gauss Elimination

$$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix}$$

Step 1: $\frac{64}{25} = 2.56; \quad Row2 - Row1(2.56) = \begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 144 & 12 & 1 \end{bmatrix}$

$\frac{144}{25} = 5.76; \quad Row3 - Row1(5.76) = \begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & -16.8 & -4.76 \end{bmatrix}$

Finding the [U] Matrix

Matrix after Step 1: $\begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & -16.8 & -4.76 \end{bmatrix}$

Step 2: $\dfrac{-16.8}{-4.8} = 3.5; \quad Row3 - Row2(3.5) = \begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & 0 & 0.7 \end{bmatrix}$

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

Finding the [*L*] matrix

$$\begin{bmatrix} 1 & 0 & 0 \\ \ell_{21} & 1 & 0 \\ \ell_{31} & \ell_{32} & 1 \end{bmatrix}$$

Using the multipliers used during the Forward Elimination Procedure

From the first step of forward elimination

$$\begin{bmatrix} 25 & 5 & 1 \\ 64 & 8 & 1 \\ 144 & 12 & 1 \end{bmatrix}$$

$$\ell_{21} = \frac{a_{21}}{a_{11}} = \frac{64}{25} = 2.56$$

$$\ell_{31} = \frac{a_{31}}{a_{11}} = \frac{144}{25} = 5.76$$

Finding the [L] Matrix

From the second step of forward elimination

$$\begin{bmatrix} 25 & 5 & 1 \\ 0 & -4.8 & -1.56 \\ 0 & -16.8 & -4.76 \end{bmatrix} \qquad \ell_{32} = \frac{a_{32}}{a_{22}} = \frac{-16.8}{-4.8} = 3.5$$

$$[L] = \begin{bmatrix} 1 & 0 & 0 \\ 2.56 & 1 & 0 \\ 5.76 & 3.5 & 1 \end{bmatrix}$$

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

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

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 set of experimental data from the laboratory is given below:

Ni aqueous phase, *a* (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:

$$g = x_1 a^2 + x_2 a + x_3,\ 2 \le a \le 3$$

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

Use Forward Elimination to find the [U] matrix

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

Step 1 $\quad \dfrac{6.25}{4} = 1.5625; \quad Row2 - Row1(1.5625) = \begin{bmatrix} 4 & 2 & 1 \\ 0 & -0.625 & -0.5625 \\ 9 & 3 & 1 \end{bmatrix}$

$$\frac{9}{4} = 2.25; \quad Row3 - Row1(2.25) = \begin{bmatrix} 4 & 2 & 1 \\ 0 & -0.625 & -0.5625 \\ 0 & -1.5 & -1.25 \end{bmatrix}$$

Example: Liquid-Liquid Extraction

The matrix after the 1st step:

$$\begin{bmatrix} 4 & 2 & 1 \\ 0 & -0.625 & -0.5625 \\ 0 & -1.5 & -1.25 \end{bmatrix}$$

Step 2

$$\frac{-1.5}{-0.625} = 2.4; \quad Row3 - Row2(2.4) = \begin{bmatrix} 4 & 2 & 1 \\ 0 & -0.625 & -0.5625 \\ 0 & 0 & 0.1 \end{bmatrix}$$

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

Example: Liquid-Liquid Extraction

Find the [*L*] matrix

$$\begin{bmatrix} 1 & 0 & 0 \\ \ell_{21} & 1 & 0 \\ \ell_{31} & \ell_{32} & 1 \end{bmatrix}$$

Use the multipliers from the Forward Elimination Procedure

From the first step of forward elimination

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

$$\ell_{21} = \frac{a_{21}}{a_{11}} = \frac{6.25}{4} = 1.5625$$

$$\ell_{31} = \frac{a_{31}}{a_{11}} = \frac{9}{4} = 2.25$$

From the second step of forward elimination

$$\begin{bmatrix} 4 & 2 & 1 \\ 0 & -0.625 & -0.5625 \\ 0 & -1.5 & -1.25 \end{bmatrix}$$

$$\ell_{32} = \frac{a_{32}}{a_{22}} = \frac{-1.5}{-0.625} = 2.4$$

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

Set [L][Z] = [C]

$$\begin{bmatrix} 1 & 0 & 0 \\ 1.5625 & 1 & 0 \\ 2.25 & 2.4 & 1 \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} = \begin{bmatrix} 8.57 \\ 10 \\ 12 \end{bmatrix}$$

Solve for [Z]

$$z_1 = 8.57$$

$$1.5625 z_1 + z_2 = 10$$

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

Example: Liquid-Liquid Extraction

Complete the forward substitution to solve for [Z]

$$z_1 = 8.57$$

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

$$\begin{aligned} z_3 &= 12 - 2.25 z_1 - 2.4 z_2 \\ &= 12 - 2.25 \times 8.57 - 2.4 \times (-3.3906) \\ &= 0.855 \end{aligned}$$

$$[Z] = \begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} = \begin{bmatrix} 8.57 \\ -3.3906 \\ 0.855 \end{bmatrix}$$

Example: Liquid-Liquid Extraction

Set [U][X] = [Z]

$$\begin{bmatrix} 4 & 2 & 1 \\ 0 & -0.625 & -0.5625 \\ 0 & 0 & 0.1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 8.57 \\ -3.3906 \\ 0.855 \end{bmatrix}$$

Solve for [X]

The 3 equations become

$$4x_1 + 2x_2 + x_3 = 8.57$$
$$-0.625x_2 + (-0.5625)x_3 = -3.3906$$
$$0.1x_3 = 0.855$$

Example: Liquid-Liquid Extraction

Solve for [X]

$$x_3 = \frac{0.855}{0.1}$$
$$= 8.55$$

$$x_2 = \frac{-3.3906 - (-0.5625)x_3}{-0.625}$$
$$= \frac{-3.3906 - (-0.5625) \times 8.55}{-0.625}$$
$$= -2.27$$

$$x_1 = \frac{8.57 - 2x_2 - x_3}{4}$$
$$= \frac{8.57 - 2 \times (-2.27) - 8.55}{4}$$
$$= 1.14$$

Example: Liquid-Liquid Extraction

The Solution Vector is:

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

Example: Liquid-Liquid Extraction

Solution

The polynomial that passes through the three data points is then

$$g(a) = x_1 a^2 + x_2 a + x_3$$
$$= 1.14a^2 + (-2.27)a + 8.55,\ 2 \le a \le 3$$

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 amount of nickel in the organic phase is

$$g(2.3) = 1.14 \times (2.3)^2 + (-2.27) \times (2.3) + 8.55$$
$$= 1.14 \times 5.29 + (-2.27) \times 2.3 + 8.55$$
$$g(2.3) = 9.3596 \text{ g/l}$$

Finding the inverse of a square matrix

The inverse [B] of a square matrix [*A*] is defined as

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

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

Example: Inverse of a Matrix

Find the inverse of a square matrix [*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

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

Example: Inverse of a Matrix

Solving for the each column of [*B*] requires two steps

1) Solve [*L*] [*Z*] = [*C*] for [*Z*]

2) Solve [*U*] [*X*] = [*Z*] for [*X*]

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:

$$z_1=1$$

$$2.56z_1+z_2=0$$

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

Example: Inverse of a Matrix

Solving for [Z]

$$z_1 = 1$$

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

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

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

Example: Inverse of a Matrix

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

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

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

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

$$0.7b_{31} = 3.2$$

Example: Inverse of a Matrix

Using Backward Substitution

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

$$b_{21} = \frac{-2.56 + 1.560 b_{31}}{-4.8}$$

$$= \frac{-2.56 + 1.560(4.571)}{-4.8} = -0.9524$$

$$b_{11} = \frac{1 - 5b_{21} - b_{31}}{25}$$

$$= \frac{1 - 5(-0.9524) - 4.571}{25} = 0.04762$$

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

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

Example: Inverse of a 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

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

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

Example: Inverse of a Matrix

The inverse of [A] is

$$[A]^{-1} = \begin{bmatrix} 0.04762 & -0.08333 & 0.03571 \\ -0.9524 & 1.417 & -0.4643 \\ 4.571 & -5.000 & 1.429 \end{bmatrix}$$

To check your work do the following operation

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

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/lu_decomposition.html

THE END

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