

Foundation of Computational Fluid Dynamics
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Lecture – 35

It is my pleasure to welcome you again to this course. Last two classes, we have seen in detail about Gauss elimination procedure, special form of Gauss elimination procedure, what is known as a tridiagonal matrix algorithm. In this class, we are going to see one more direct method what is known as LU decomposition.


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LU Decomposition

LU Decomposition: A is a full matrix, i.e. no zero value element.
 In LU Decomposition, the matrix A is decomposed into two matrices.
 L – Lower Triangular and U – Upper Triangular, matrices.

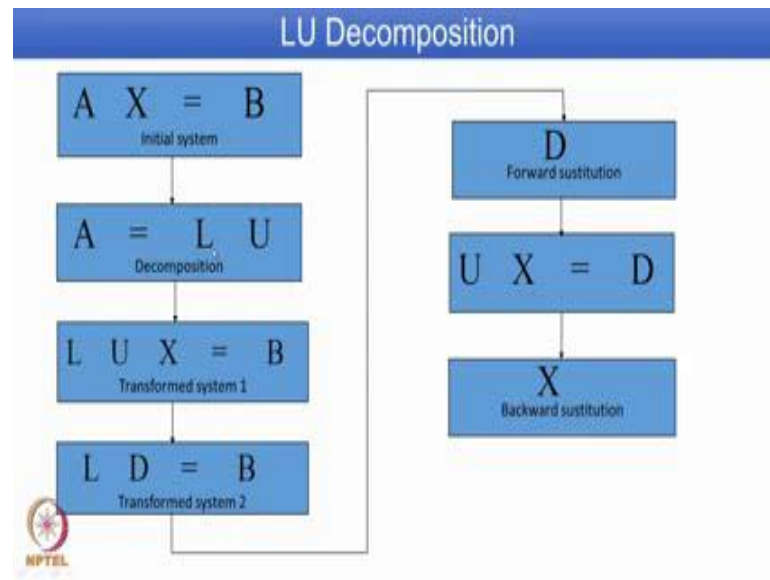
$$A = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \dots & \dots & \dots & \dots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix} \quad L = \begin{bmatrix} 1 & 0 & \dots & 0 \\ l_{21} & 1 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ l_{n1} & l_{n2} & \dots & 1 \end{bmatrix} \quad U = \begin{bmatrix} u_{11} & u_{12} & \dots & u_{1n} \\ 0 & u_{22} & \dots & u_{2n} \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & u_{nn} \end{bmatrix}$$

$A = LU$



LU decomposition, so A coefficient matrix, say for example, has no zero value element it is full matrix. In LU decomposition, matrix A decomposed into two matrices; such as L and U, where L refers to lower triangular matrix and U referred to upper triangular matrix. And it is shown here, A is equal to LU. And in the form of a matrix notation, it is shown here a coefficient matrix a 1 1 to a n n. It is now decomposed into L matrix and U matrix and structure of L matrix given, it has diagonal element value as 1, and it has elements on the lower side of the diagonals has shown here from 1 to 1 and all the way up to last row. Values on the upper part of this L matrix are zero. The lower part of the diagonal element of the U matrix are zero and it has values from the diagonal, and all the way up to the upper part. So this in case U 1 1 U 2 2 U n n are values along the diagonal and other upper side it is fill with values.

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So, procedure of the LU decomposition and solution is given in this flowchart. So, given coefficient matrix equation $A X = B$, such a initial system. Now coefficient matrix A is decomposed L and U product of L and U . Now, we rewrite equation is $A = B$ has $L U x = B$. Now in this, we substitute $U x = D$. So, we write now in $L U X = B$ as $L D = B$. When we solve this equation, we get the D known and that is by forward substitution. Initially we defined $U X = D$, we rewrite here now in this is D is known because we got it from the previous set $L D = B$. Now X is the unknown variable column vector and U upper triangular matrix. So, then we do the product and that should be equal to the column matrix. Now when you solve this, we get finally X . So, in $L U$ decomposition, there are additional steps in terms of decomposing the given matrix A in the form of L and U . And as you can observe it has steps overlapping with steps involved in gauss elimination procedure that is forward elimination and backward substitution.

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LU Decomposition

Calculation of elements in L and U matrix:

$$l_{ij} = a_{ij} - \sum_{k=1}^{j-1} l_{ik} \cdot u_{kj} \quad j \leq i, \quad i = 1, \dots, n$$
$$u_{ij} = \frac{(a_{ij} - \sum_{k=1}^{i-1} l_{ik} \cdot u_{kj})}{l_{ii}}$$

for $j=1$, the rule reduces to $l_{i1} = a_{i1}$

for $i=1$, the rule reduces to $u_{1j} = \frac{a_{1j}}{l_{11}} = \frac{a_{1j}}{a_{11}}$




Now, the question is how to find or how to decompose given coefficient matrix A into L and U. In other words, how to find element values in coefficient in coefficient matrix L and U. The mathematics is already given there is recursive procedure and what is shown here is the final steps in the recursive procedure. So calculation of elements in L and U matrix and l_{ij} equal to a_{ij} that is original value that is value in the original coefficient matrix minus summation $k=1$ to $j-1$ l_{ik} into u_{kj} where j is less than or equal to i and i going from 1 to n . Similarly, for upper diagonal matrix u_{ij} , there is another recursive relationship that is what is also displayed here. This recursive relation gets reduced for the first j is equal to 1, the rule gets reduced to l_{i1} is equal to a_{i1} . And for i equal to 1, the upper triangular matrix u_{ij} get reduced to u_{1j} is equal to a_{1j} by l_{11} . Now this sets first row element for a case of u , and first column elements for a case of l .

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LU Decomposition – Sample code listing

do for i = 1, n
  L(i,1) = A(i,1) | finds 1st column elements
enddo
do for j = 1, n
  U(1,j) = A(1,j)/L(1,1) | finds 1st row elements
enddo
do for j = 2, n
  do for i = j, n
    do for k = 1, j-1
      accumulate sum of L(i,k)*U(k,j)
    enddo
    L(i,j) = A(i,j) - sum
  enddo
  U(j,j) = 1
  do for i = j+1, n
    do for k = 1, j-1
      accumulate sum of L(j,k)*U(k,i)
    enddo
    U(j,i) = (A(j,i)-sum)/L(j,j)
  enddo
enddo
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Now, we try to have a sample code listing for that operation that we just explain to get element values in coefficient matrix L and U. So, do for i is equal to 1 to n $L_{i,1} = A_{i,1}$, so this step finds first column elements in L matrix. Similarly for U $U_{1,j}$ run from 1 to n $A_{1,j}$ divided by $L_{1,1}$ and this gives first row elements for U matrix. Then we find out other elements in L matrix and U matrix with the help of recursive relationship we displayed just now. The same relationship is written in the form a programming listing here. so for j is equal to 2 to n and for i j to n k 1 to j minus 1 you accumulate the sum of $L_{i,k}$ and $U_{k,j}$ end do we find elements of coefficient matrix L. Similarly for U matrix that is also listed here. What is shown here is not actual program is the only skeleton of what can go in the code meant for writing to find out LU decomposition any language can be used what is show here is based on Fortran coding language.

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LU Decomposition

Once L and U are determined, the solution to the Equations is obtained as follows:

$$Ax = b$$


where, $x = (x_1, x_2 \dots x_n)^T$; $b = (b_1, b_2 \dots b_n)^T$

$$LUx = b$$

The solution is obtained in two steps:

1. $Ux = y$, where $y = (y_1, y_2 \dots y_n)^T$
2. $Ly = b$

So the solution is $y_1 = b_1, y_i = b_i - \sum_{k=1}^{i-1} l_{ik} \cdot y_k$ where $i = 2, 3 \dots n$

$$x_n = \frac{y_n}{u_{nn}}$$
$$x_i = \frac{y_i - \sum_{k=i+1}^n u_{ik} \cdot x_k}{u_{ii}} \text{ where } i = n-1 \dots 2, 1$$


So once L and U are determined, solution to the equation the original equation is obtained has explain here $Ax = b$ is the original set of linear equation, where x is unknown column vector and form of transpose it is here; b is again known value matrix on the right hand side that also in the given form of transpose here. We have decomposed the original A matrix into L U. So, we rewrite A as LU to $x = b$. So, solutions is obtained in two steps; first we write $Ux = y$ where y is equal to y_1 to y_n transpose then $Ly = b$. So, solution is obtained as $y_1 = b_1$ and y_i is equal to this recursive relationship and where i is equal to 2 to n. And x_n , this is now backward substitution is again by recursive relationship as shown here.

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LU Decomposition

- Find the solution of $X = \begin{bmatrix} x \\ y \\ z \end{bmatrix}$ of $\begin{bmatrix} 1 & 2 & 4 \\ 3 & 8 & 14 \\ 2 & 6 & 13 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 3 \\ 13 \\ 4 \end{bmatrix}$
- The first step is to calculate the LU Decomposition of the coefficient matrix on the left hand side

$$L = \begin{bmatrix} 1 & 0 & 0 \\ L_{21} & 1 & 0 \\ L_{31} & L_{32} & 1 \end{bmatrix} \text{ and } U = \begin{bmatrix} U_{11} & U_{12} & U_{13} \\ 0 & U_{22} & U_{23} \\ 0 & 0 & U_{33} \end{bmatrix}$$

- Multiplying L and U and set the answer equal to the coefficient matrix

$$\begin{bmatrix} U_{11} & U_{12} & U_{13} \\ L_{21}U_{11} & L_{21}U_{12} + U_{22} & L_{21}U_{13} + U_{23} \\ L_{31}U_{11} & L_{31}U_{12} + L_{32}U_{22} & L_{31}U_{13} + L_{32}U_{23} + U_{33} \end{bmatrix} = \begin{bmatrix} 1 & 2 & 4 \\ 3 & 8 & 14 \\ 2 & 6 & 13 \end{bmatrix}$$

Let us explain the LU decomposition procedure and finding the solution with the help of an example. So, it is given find X of the unknown vector x y z with the coefficient matrix as shown here 1 2 4 3 8 14 2 6 13 and D matrix as shown here as 3 13 4. The first step is to get LU decomposition of the given coefficient matrix, and we rewrite L as given here. So, L matrix as diagonal element as 1 and L 2 1 L 3 1 L 3 2 are elements in a L matrix, and upper part of the L matrix are 0. Similarly for U matrix and lower part of the matrix are 0, and you have along diagonal values U 1 1 U 2 2 U 3 3 and then upper part. So, if you multiply L and U and equated to given coefficient then you are able to find values of L and U and that is what we are going to show here.

So if you multiply, for example, this is 3 by 3 matrix, this is again 3 by 3 matrix, so it is possible to multiply. So 1 into U 1 1 that becomes a first element for the product matrix L and U; similarly for other coefficient elements. You can observe, for example, last row L3 1 multiplying U 1 1 and then L 3 2 multiplying U 1 2 plus L 3 2 multiplying U 2 2 and you get similarly expression for all the elements in that product matrix L and U. This is equated to the original coefficient matrix A that is what is shown here 1 2 4 3 8 14 2 6 13 and that is what displayed here. Now all that we do we set up an equation three equations.


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LU Decomposition

- Now we have to use this to find the entries in L and U. It is easier in this example.

$$U_{11} = 1, U_{12} = 2, U_{13} = 4$$

- Now consider the second row

$$\begin{aligned} L_{21}U_{11} &= 3 \rightarrow L_{21} * 1 = 3 \rightarrow L_{21} = 3 \\ L_{21}U_{12} + U_{22} &= 8 \rightarrow 3 * 2 + U_{22} = 8 \rightarrow U_{22} = 2 \\ L_{21}U_{13} + U_{23} &= 14 \rightarrow 3 * 4 + U_{23} = 14 \rightarrow U_{23} = 2 \end{aligned}$$


So, we have to use this to find entries in the L and U. It is easier in this example; however, it is good to understand. So, U 1 1 directly get the values of 1, U 1 2 gets the value of 2, and U 13 gets the value of 4. Now, we write equation for other entries. So, L 2 1 U 1 1 is equal to 3, if you substitute U 1 1 you get the value of L 2 1 as 3. Similarly, L 2 1, U 1 2, U 2 2 is equal to 8; if you substitute values for U 2 2 we get if the substitute value U 1 2 you get values for U 2 2 as 2. You can extend for this third row and following algebraic you finally get values for U 2 3 as 2.


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LU Decomposition

- Now consider the last/third row

$$\begin{aligned} L_{31}U_{11} &= 2 \rightarrow L_{31} * 1 = 2 \rightarrow L_{31} = 2 \\ L_{31}U_{12} + L_{32}U_{22} &= 6 \rightarrow 2 * 2 + L_{32} * 2 = 6 \rightarrow L_{32} = 1 \\ L_{31}U_{13} + L_{32}U_{23} + U_{33} &= 13 \rightarrow (2 * 4) + (1 * 2) + U_{33} = 13 \rightarrow U_{33} = 3 \end{aligned}$$

- Thus the LU Decomposition of the given matrix

$$A = \begin{bmatrix} 1 & 2 & 4 \\ 3 & 8 & 14 \\ 2 & 6 & 13 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 3 & 1 & 0 \\ 2 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 & 4 \\ 0 & 2 & 2 \\ 0 & 0 & 3 \end{bmatrix}$$


Again continue that exercise to find coefficient values in the L matrix, and all the steps are shown here, and you get values of L_{31} L_{32} and then remaining U_{33} . So, if you substitute finally, we get LU decomposition of a given matrix as shown here. So, given matrix A is shown here is equal to product of L matrix and U matrix. As defined before in L matrix diagonal elements are having value of 1 and the lower part of the diagonal elements that is they are having value as 3 2 1 and upper part having zero value. Similarly U matrix, you have values along the diagonal and an upper part again there are some values, but the lower part has zero value.


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LU Decomposition

- To solve a system of equation by LU Decomposition the following procedure should be followed
 1. Given A, find L and U so that $A=LU$. Hence $LUx=B$
 2. Let $Y=UX$ so that $LY=B$. Solve this triangular system for Y
 3. Finally solve the triangular system $UX=Y$ for X

- We have the decomposed coefficient matrix

$$L = \begin{bmatrix} 1 & 0 & 0 \\ 3 & 1 & 0 \\ 2 & 1 & 1 \end{bmatrix} \text{ and } U = \begin{bmatrix} 1 & 2 & 4 \\ 0 & 2 & 2 \\ 0 & 0 & 3 \end{bmatrix}$$



Now, once you find L and U decomposition of the given matrix, now we have to find a column vector x y z. So to solve a system application by LU D decomposition you need follow procedure given below give a find L and U which you have already done. Now set y is equal to U x so that becomes L Y equal to B. Now if you solve this because L is now triangular system and Y is now becoming unknown B is again known from the original set. So, when you solve this equation L Y is equal to B then we get Y. Then once you get Y, we already defined Y is equal to U X, now if you solve by backward substitution you get X, and that is what is the initial interest. Let us apply this steps for the example problem that we have just now explained, so L is already obtained as shown here, and U also obtain as shown here.


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LU Decomposition

- Solve $LY=B$ for the vector $Y = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}$

$$LY = \begin{bmatrix} 1 & 0 & 0 \\ 3 & 1 & 0 \\ 2 & 1 & 1 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} 3 \\ 13 \\ 4 \end{bmatrix}$$

Which can be solved by **forward substitution**. From the top equation we see that $y_1 = 3$. The middle equation states that $3y_1 + y_2 = 13$ and $y_2 = 4$. Finally the bottom equation states that $2y_1 + y_2 + y_3 = 4$, from which we see that $y_3 = -6$.



So, LY is equal to B for the vector Y as defined as y_1, y_2, y_3 . Now LY is equal to B ; so B values also given in the problem; L is shown here and Y is y_1 to y_3 . Now you can solve this by what is known as forward substitution; if you perform operation from the top, for example, that is directly known y_1 is equal to 3. Now perform the operation for the second row we get $3y_1 + y_2 = 13$, y_1 is already determined substituting you get the value y_2 to be 4. Now from the last row, we get $2y_1 + y_2 + y_3 = 4$ this y_2 is known y_1 is known, solve for y_3 you get value of minus 3. So, in the set up LY is equal to B , we have now got Y .


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LU Decomposition

- Now that we have found Y we finish the procedure by solving $UX=Y$ for X . That is we solve

$$UX = \begin{bmatrix} 1 & 2 & 4 \\ 0 & 2 & 2 \\ 0 & 0 & 3 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 3 \\ 4 \\ -6 \end{bmatrix} = Y$$

By using **back substitution**. Starting with the bottom equation from $3z = -6$, we get $z = -2$. The middle equation implies that $2y + 2z = 4$ and it follows that $y = 4$. The top equation states that $x + 2y + 4z = 3$ and consequently $x = 3$. So the solution is,

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 3 \\ 4 \\ -2 \end{bmatrix}$$



So, once we set up this equation, we solve by backward substitution. You can immediately observe the last row, so $3z$ is equal to minus 6. If you solve you get value of z to be minus 2. Now take the second row, so $2y + 2z$ is equal to 4, again value of z is known substitute you get value of y to be 4. Now take the first row top equation, so $x + 2y + 4z$ is equal to 3, and if you solve for the substituting value of y and z get x value to be 3. So, final solution is x, y, z equal to 3, 4, minus 2. So we have explained given a coefficient matrix how to decompose into L and U . And how to follow from there to get solution; first steps is forward substitution using L matrix; second step is backward substitution using U matrix.

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LU Decomposition

- It is very popular
- It is easily programmable.
- There is no need to store the '0's in either L or U .
- Similarly '1's on the diagonal of L can also be omitted.
- In can store valuable elements of U . As well as, where '0's appear in the L array.
- Though it appears two (additional) separate matrices, the original matrix A can be transformed (used) as

$$\begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \dots & \dots & \dots & \dots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix} \longrightarrow \begin{bmatrix} u_{11} & u_{12} & \dots & u_{1n} \\ l_{21} & u_{22} & \dots & u_{2n} \\ \dots & \dots & \dots & \dots \\ l_{n1} & l_{n2} & \dots & u_{nn} \end{bmatrix}$$



So, if you look at advantages with respect to gauss elimination. It is very popular, it is easy to program, there is no need to store zeros either for L matrix or U matrix. So, if you observe carefully given coefficient matrix A split into L and U and upper triangular part for L has zero value, lower triangular for U as zero value. And though they are actually represent that in actual program for while doing the program to get L and U matrix you do not handling zeros at all. Similarly, L matrix has value of 1 along the diagonal, because it is fixed for any coefficient matrix and do not be stored; instead 1 is possible to store coefficient values of U matrix in L matrix itself wherever zeros are appearing in L matrix.

Hence finally, though it appears as if given matrix A is split into two different matrices; natural coding it is not so. The given matrix A itself is used to store both L and U as shown here. So, given matrix a_{11} a_{12} a_{1n} all the way up to a_{nn} is now replaced with L and U as shown here. We already know for L matrix diagonal element values are 1. And we also just now mentioned, there is no need to store 1 because it is default for any coefficient matrix that place is used to store values of U matrix U_{11} along the diagonal all the way up to U_{nn} ; and upper part of the L matrix has zero value and that is used to store U matrix as shown here U_{12} all the way other elements. Hence the given coefficient matrix A itself is used to write L and U . so, this becomes easier to program and it also become very popular because it is easy to solve any matrix.

So, in this today's class, particularly we talked in detail about LU decomposition way of solving a given coefficient matrix, we explain procedure with the help of a simple example problem. We also listed a sample coding for structure, it is possible to write the code in any language appropriately for getting L U decomposition and then proceed to get answer for a given coefficient matrix. Next class, we will talk about another procedure what is known as iterative procedure.

Thank you.