1.6 DOOLITTLE'S LU DECOMPOSITION

We shall now consider the LU decomposition of a general matrix. The method we describe is due to Doolittle.

Let $A = (a_{ij})$. We seek as in the case of a tridiagonal matrix, an LU decomposition in which the diagonal entries l_{ii} of L are all 1. Let $L = (l_{ii})$; $U = (u_{ij})$. Since L is a lower triangular matrix, we have

$l_{ij} = 0$ if $j > i$; and by our choice, $l_{ii} = 1$.

Similarly, since U is an upper triangular matrix, we have

$u_{ij} = 0$ if $i > j$.

We determine L and U as follows : The 1st row of U and 1st column of L are determined as follows :

$$a_{11} = \sum_{k=1}^{n} l_{1k} u_{k1}$$

$$= l_{11} u_{11} \qquad \text{since } l_{1k} = 0 \text{ for } k>1$$

$$= u_{11} \qquad \text{since } l_{11} = 1.$$

Therefore

$u_{11} = a_{11}$

In general,

$$a_{1j} = \sum_{k=1}^{n} l_{1k} u_{kj}$$

$$= l_{11} u_{1j}. \qquad \text{since } l_{1k} = 0 \text{ for } k>1$$

$$= u_{1j} \qquad \text{since } l_{11} = 1.$$

$$\Rightarrow \quad u_{1j} = a_{1j} \; \ldots\ldots\ldots \text{(I)}$$

Thus the first row of U is the same as the first row of A. The first column of L is determined as follows:

$$a_{j1} = \sum_{k=1}^{n} l_{jk} u_{k1}$$

$$= l_{j1} u_{11} \qquad \text{since } u_{k1} = 0 \text{ if } k>1$$

$$\Rightarrow \quad l_{j1} = a_{j1}/u_{11} \; \ldots\ldots\ldots \text{(II)}$$

Note : u_{11} is already obtained from (I).

Thus (I) and (II) determine respectively the first row of U and first column of L. The other rows of U and columns of L are determined recursively as given below: Suppose we have determined the first i-1 rows of U and the first i-1 columns of L. Now we proceed to describe how one then determines the i^{th} row of U and i^{th} column of L. Since first i-1 rows of U have been determined, this means, u_{kj} ; are all known for $1 \le k \le i-1$; $1 \le j \le n$. Similarly, since first i-1 columns are known for L, this means, l_{ik} are all known for $1 \le i \le n$; $1 \le k \le i-1$.

Now

$$a_{ij} = \sum_{k=1}^{n} l_{ik} u_{kj}$$

$$= \sum_{k=1}^{i} l_{ik} u_{kj} \qquad \text{since } l_{ik} = 0 \text{ for } k>i$$

$$= \sum_{k=1}^{i-1} l_{ik} u_{kj} + l_{ii} u_{ij}$$

$$= \sum_{k=1}^{i-1} l_{ik} u_{kj} + u_{ij} \qquad \text{since } l_{ii} = 1.$$

$$\Rightarrow \quad u_{ij} = a_{ij} - \sum_{k=1}^{i-1} l_{ik} u_{kj} \qquad \text{. . . . .(III)}$$

Note that on the RHS we have a_{ij} which is known from the given matrix. Also the sum on the RHS involves l_{ik} for $1 \le k \le i-1$ which are all known because they involve entries in the first i-1 columns of L ; and they also involve u_{kj} ; $1 \le k \le i-1$ which are also known since they involve only the entries in the first i-1 rows of U. Thus (III) determines the i^{th} row of U in terms of the known given matrix and quantities determined upto the previous stage. Now we describe how to get the i^{th} column of L :

$$a_{ji} = \sum_{k=1}^{n} l_{jk} u_{ki}$$

$$= \sum_{k=1}^{i} l_{jk} u_{ki} \qquad \text{Since } u_{ki} = 0 \text{ if } k>i$$

$$= \sum_{k=1}^{i-1} l_{jk} u_{ki} + l_{ji} u_{ii}$$

$$\Rightarrow \quad l_{ji} = \frac{1}{u_{ii}} \left[a_{ji} - \sum_{k=1}^{i-1} l_{jk} u_{ki} \right] \qquad \text{.....(IV)}$$

Once again we note the RHS involves u_{ii}, which has been determined using (III); a_{ji} which is from the given matrix; l_{jk}; $1 \le k \le i-1$ and hence only entries in the first i-1 columns of L; and u_{ki}, $1 \le k \le i-1$ and hence only entries in the first i-1 rows of U. Thus RHS in (IV) is completely known and hence l_{ji}, the entries in the i^{th} column of L are completely determined by (IV).

Summarizing, Doolittle's procedure is as follows:

$l_{ii} = 1$; 1st row U = 1st row of A ; Step 1 determining 1st row of U and
$l_{j1} = a_{j1}/u_{11}$ 1st column of L.

For $i \ge 2$; we determine, (by (III) and (IV)),

$$u_{ij} = a_{ij} - \sum_{k=1}^{i-1} l_{ik} u_{kj}$$; j = i, i+1, i+2, …….,n

(Note for j<i we have $u_{ij} = 0$)

$$l_{ji} = \frac{1}{u_{ii}} \left[a_{ji} - \sum_{k=1}^{i-1} l_{jk} u_{ki} \right]$$; j = i, i+1, i+2,…..,n

(Note for j<i we have $l_{ji} = 0$)

We observe that the method fails if $u_{ii} = 0$ for some i.

<u>Example:</u>

Let

$$A = \begin{pmatrix} 2 & 1 & -1 & 3 \\ -2 & 2 & 6 & -4 \\ 4 & 14 & 19 & 4 \\ 6 & 0 & -6 & 12 \end{pmatrix}$$

Let us determine the Doolittle decomposition for this matrix.

<u>First step:</u>

1st row of U : same as 1st row of A.

Therefore $u_{11} = 2$; $u_{12} = 1$; $u_{13} = -1$; $u_{14} = 3$

<u>1st column of L:</u>

$l_{11} = 1$;

$l_{21} = a_{21}/u_{11} = -2/2 = -1$.

$l_{31} = a_{31}/u_{11} = 4/2 = 2$.

$l_{41} = a_{41}/u_{11} = 6/2 = 3.$

Second step:

2^{nd} row of U : $u_{12} = 0$ (Because upper triangular)

$u_{22} = a_{22} - l_{21}\, u_{12} = 2 - (-1)\,(1) = 3.$

$u_{23} = a_{23} - l_{21}\, u_{13} = 6 - (-1)\,(-1) = 5.$

$u_{24} = a_{24} - l_{21}\, u_{14} = -\,4 - (-1)\,(3) = -1.$

2^{nd} column of L : $l_{12} = 0$ (Because lower triangular)

$l_{22} = 1.$

$l_{32} = (a_{32} - l_{31}\, u_{12})\, /u_{22}$

$= [14 - (2)(1)]/3 = 4.$

$l_{42} = (a_{42} - l_{41}\, u_{12})\, /u_{22}$

$= [0 - (3)(1)]/3 = -1.$

Third Step:

3^{rd} row of U: $\left.\begin{array}{l} u_{31} = 0 \\ u_{32} = 0 \end{array}\right\}$ (because U is upper triangular)

$u_{33} = a_{33} - l_{31}\, u_{13} - l_{32}\, u_{23}$

$= 19 - (2)\,(-1) - (4)(5) = 1.$

$u_{34} = a_{34} - l_{31}\, u_{14} - l_{32}\, u_{24}$

$= 4 - (2)\,(3) - (4)(-1) = 2.$

3^{rd} column of L : $\left.\begin{array}{l} l_{13} = 0 \\ l_{23} = 0 \end{array}\right\}$ (because L is lower triangular)

$l_{33} = 1$

$l_{43} = (a_{43} - l_{41}\, u_{13} - l_{42}\, u_{23})/\, u_{33}$

$= [-6 - (3)\,(-1) - (-1)\,(5)]/1$

$= 2.$

Fourth Step:

4^{th} row of U: $u_{41} = 0$

$u_{42} = 0$ (because upper triangular)

$u_{43} = 0$

$u_{44} = a_{44} - l_{41}u_{14} - l_{42}u_{24} - l_{43}u_{34}$

$= 12 - (3)(3) - (-1)(-1) - (2)(2)$

$= -2.$

4^{th} column of L : $l_{14} = 0 = l_{24} = l_{34}$ Because lower triangular

$l_{44} = 1.$

Thus

$$L = \begin{pmatrix} 1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 2 & 4 & 1 & 0 \\ 3 & -1 & 2 & 1 \end{pmatrix}; \qquad U = \begin{pmatrix} 2 & 1 & -1 & 3 \\ 0 & 3 & 5 & -1 \\ 0 & 0 & 1 & 2 \\ 0 & 0 & 0 & -2 \end{pmatrix} \text{ . . . .(V)}$$

and

A = LU.

This gives us the LU decomposition by Doolittle's method for the given A.

As we observed in the case of the LU decomposition of a tridiagonal matrix; it is not advisable to choose the l_{ii} as 1; but to choose in such a way that the diagonal entries of L and the corresponding diagonal entries of U are of the same magnitude. We describe this procedure as follows:

Once again 1^{st} row and 1^{st} column of U & L respectively is our first concern:

Step 1: $a_{11} = l_{11}u_{11}$

Choose $l_{11} = \sqrt{|a_{11}|}; u_{11} = (\text{sgn}.a_{11})\sqrt{|a_{11}|}$

Next $a_{ij} = \sum_{k=1}^{n} l_{1k}u_{kj} = l_{11}u_{1j}$ as $l_{1k} = 0$ for $k > 1$

$$\Rightarrow u_{ij} = a_{1j} / l_{11}$$

Thus note that u_{1j} have been scaled now as compared to what we did earlier.

Similarly,

$$l_{j1} = {}^{a_{j1}}\!\big/_{u_{11}}$$

These determine the first row of U and first column of L. Suppose we have determined the first i-1 rows of U and first i-1 columns of L. We determine now the i^{th} row of U and i^{th} column of L as follows:

$$a_{ii} = \sum_{k=1}^{n} l_{ik} u_{ki}$$

$$= \sum_{k=1}^{i} l_{ik} u_{ki} \qquad \text{for } l_{ik} = 0 \quad \text{if } k>i$$

$$= \sum_{k=1}^{i-1} l_{ik} u_{ki} + l_{ii} u_{ii}$$

Therefore

$$l_{ii}u_{ii} = a_{ii} - \sum_{k=1}^{i-1} l_{ik}u_{ki} = p_i, \text{ say}$$

Choose $\quad l_{ii} = \sqrt{|p_i|} = \sqrt{\left|a_{ii} - \sum_{k=1}^{i-1} l_{ik}u_{ki}\right|}$

$$u_{ii} = -\operatorname{sgn} p_i \sqrt{|p_i|}$$

$$a_{ij} = \sum_{k-1}^{n} l_{ik}u_{kj} = \sum_{k=1}^{i} l_{ik}u_{kj} \because l_{ik} = 0 \text{ for } k > i$$

$$= \sum_{k=1}^{i-1} l_{ik} u_{kj} + l_{ii} u_{ij}$$

$$\Rightarrow u_{ij} = \left(a_{ij} - \sum_{k=1}^{i-1} l_{ik}u_{kj}\right) \Big/ \; l_{ii}$$

determining the i^{th} row of U.

$$a_{ji} = \sum_{k=1}^{n} l_{jk} u_{ki}$$

$$= \sum_{k=1}^{i} l_{jk} u_{ki} \because u_{ki} = 0 \text{ if } k > i$$

$$= \sum_{k=1}^{i-1} l_{jk} u_{ki} + l_{ji} u_{ii}$$

$$\Rightarrow l_{ji} = \left(a_{ji} - \sum_{k=1}^{i-1} l_{jk} u_{ki} \right) / u_{ii} ,$$

thus determining the i^{th} column of L.

Let us now apply this to matrix A in the example in page 32.

First Step:

$$l_{11} u_{11} = a_{11} = 2 \therefore l_{11} = \sqrt{2}; u_{11} = \sqrt{2}$$

$$u_{12} = \frac{a_{12}}{l_{11}} = \frac{1}{\sqrt{2}} u_{13} = \frac{a_{13}}{l_{11}} = -\frac{1}{\sqrt{2}}; u_{14} = \frac{a_{14}}{l_{11}} = \frac{3}{\sqrt{2}}$$

$$u_{11} = \sqrt{2}; u_{12} = \frac{1}{\sqrt{2}}; u_{13} = -\frac{1}{\sqrt{2}}; u_{14} = \frac{3}{\sqrt{2}}$$

$$l_{21} = \frac{a_{21}}{u_{11}} = -\frac{2}{\sqrt{2}} = -\sqrt{2}$$

$$l_{31} = \frac{a_{31}}{u_{11}} = \frac{4}{\sqrt{2}} = 2\sqrt{2}$$

$$l_{41} = \frac{a_{41}}{u_{11}} = \frac{6}{\sqrt{2}} = 3\sqrt{2}$$

Therefore

$$l_{11} = \sqrt{2}$$
$$l_{21} = -\sqrt{2}$$
$$l_{31} = 2\sqrt{2}$$
$$l_{41} = 3\sqrt{2}$$

Second Step:

$$l_{22} u_{22} = a_{22} - l_{21} u_{12}$$

$$= 2 - \left(-\sqrt{2}\right)\left(\frac{1}{\sqrt{2}}\right) = 3$$

$$\therefore l_{22} = \sqrt{3}; u_{22} = \sqrt{3}$$

$$u_{23} = \left(a_{23} - l_{21}u_{13}\right) / l_{22}$$

$$= \left[6 - \left(-\sqrt{2}\right)\left(-\frac{1}{\sqrt{2}}\right)\right] / \sqrt{3} \quad = 5/\sqrt{3}$$

$$u_{24} = \left(a_{24} - l_{21}u_{14}\right) / l_{22}$$

$$= \left[(-4) - \left(-\sqrt{2}\right)\left(\frac{3}{\sqrt{2}}\right)\right] / \sqrt{3} \quad = -1/\sqrt{3}$$

Therefore

$$u_{21} = 0; u_{22} = \sqrt{3}; u_{23} = \frac{5}{\sqrt{3}}; u_{24} = -\frac{1}{\sqrt{3}}$$

$$l_{32} = \left(a_{32} - l_{31}u_{12}\right) / u_{22}$$

$$= \left[14 - \left(2\sqrt{2}\right)\left(\frac{1}{\sqrt{2}}\right)\right] / \sqrt{3}$$

$$= 4\sqrt{3}$$

$$l_{42} = \left(a_{42} - l_{41}u_{12}\right) / u_{22}$$

$$= \left(0 - \left(3\sqrt{2}\right)\left(\frac{1}{\sqrt{2}}\right)\right) / \sqrt{3}$$

$$= -\sqrt{3}$$

Therefore

$$l_{12} = 0$$
$$l_{22} = \sqrt{3}$$
$$l_{32} = 4\sqrt{3}$$
$$l_{42} = \sqrt{3}$$

Third Step:

$$l_{33}u_{33} = a_{33} - l_{31}u_{13} - l_{32}u_{23}$$

$$= 19 - \left(2\sqrt{2}\right)\left(-\frac{1}{\sqrt{2}}\right) - \left(4\sqrt{3}\right)\left(\frac{5}{\sqrt{3}}\right)$$

= 1

$$\therefore l_{33} = 1; u_{33} = 1$$

$$u_{34} = \left(a_{34} - l_{31}u_{14} - l_{32}u_{24}\right) \Big/ l_{33}$$

$$= \left[\left(4 - \left(2\sqrt{2}\right)\left(\frac{3}{\sqrt{2}}\right) - \left(4\sqrt{3}\right)\left(-\frac{1}{\sqrt{3}}\right)\right)\right] \Big/ 1$$

= 2

$$\therefore u_{31} = 0; u_{32} = 0; u_{33} = 1, u_{34} = 2$$

$$l_{43} = \left[a_{43} - l_{41}u_{13} - l_{42}u_{23}\right] \Big/ u_{33}$$

$$= \left(-6 - \left(3\sqrt{2}\right)\left(-\frac{1}{\sqrt{2}}\right) - \left(-\sqrt{3}\right)\left(\frac{5}{\sqrt{3}}\right)\right) \Big/ 1$$

= 2

Therefore

$$\begin{bmatrix} l_{13} & = & 0 \\ l_{23} & = & 0 \\ l_{33} & = & 1 \\ l_{43} & = & 2 \end{bmatrix}$$

Fourth Step:

$$l_{44}u_{44} = a_{44} - l_{41}u_{14} - l_{42}u_{24} - l_{43}u_{34}$$

$$= 12 - \left(3\sqrt{2}\right)\left(\frac{3}{\sqrt{2}}\right) - \left(-\sqrt{3}\right)\left(-\frac{1}{\sqrt{3}}\right) - (2)(2)$$

= -2

$$\therefore l_{44} = \sqrt{2}; u_{44} = -\sqrt{2}$$

$$\therefore u_{41} = 0; u_{42} = 0; u_{43} = 0; u_{44} = -\sqrt{2}$$

$$\begin{bmatrix} l_{14} & = & 0 \\ l_{24} & = & 0 \\ l_{34} & = & 0 \\ l_{44} & = & \sqrt{2} \end{bmatrix}$$

Thus we get the LU decompositions,

$$L = \begin{pmatrix} \sqrt{2} & 0 & 0 & 0 \\ -\sqrt{2} & \sqrt{3} & 0 & 0 \\ 2\sqrt{2} & 4\sqrt{3} & 1 & 0 \\ 3\sqrt{2} & -\sqrt{3} & 2 & \sqrt{2} \end{pmatrix} \quad ; \quad U = \begin{pmatrix} \sqrt{2} & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & \frac{3}{\sqrt{2}} \\ 0 & \sqrt{3} & \frac{5}{\sqrt{3}} & -\frac{1}{\sqrt{3}} \\ 0 & 0 & 1 & 2 \\ 0 & 0 & 0 & -\sqrt{2} \end{pmatrix}$$

in which $|l_{ii}| = |u_{ii}|$, i.e. the corresponding diagonal entries of L and U have the same magnitude.

Note: Compare this with the L and U of page 35. What is the difference.

The U we have obtained above can be obtained from the U of page 34 by

(1) replacing the 'numbers' in the diagonal of the U of Page 34 by their square roots of their magnitude and keeping the same sign. Thus the first diagonal 2 is replaced by $\sqrt{2}$; 2nd diagonal 3 is replaced by $\sqrt{3}$, third diagonal 1 by 1 and 4th diagonal –2 by -$\sqrt{2}$. These then give the diagonals of the U we have obtained above.

(2) Divide each entry to the right of a diagonal in the U of page 35 by these replaced diagonals.

Thus 1st row of the U of Page 34 changes to 1st row of U in page 40

2nd row of the U of Page 34 changes to 2nd row of U in page 40

3rd row of the U of Page 34 changes to 3rd row of U in page 40

4th row of the U of Page 34 changes to 4th row of U in page 40

This gives the U of page 40 from that of page 35.

The L in page 40 can be obtained from the L of page 35 as follows:

(1) Replace the diagonals in L by magnitude of the diagonals in U of page 40.

(2) Multiply each entry below the diagonal of L by this new diagonal entry.

We get the L of page 35 changing to the L of page 40.