1.7 DOOLITTLE'S METHOD WITH ROW INTERCHANGES

We have seen that Doolittle factorization of a matrix A may fail the moment at stage i we encounter a u_{ii} which is zero. This occurrence corresponds to the occurrence of zero pivot at the i^{th} stage of simple Gaussian elimination method. Just as we avoided this problem in the Gaussian elimination method by introducing partial pivoting we can adopt this procedure in the modified Doolittle's procedure. The Doolittle's method which is used to factorize A as LU is used from the point of view of reducing the system

$Ax = y$

to two triangular systems

$Lz = y$

$Ux = z$

as already mentioned on page 19.

Thus instead of actually looking for a factorization A = LU we shall be looking for a system,

$A^*x = y^*$

and for which A^* has LU decomposition.

We illustrate this by the following example: The basic idea is at each stage calculate all the u_{ii} that one can get by the permutation of rows of the matrix and choose that matrix which gives the maximum absolute value for u_{ii}.

As an example consider the system

$Ax = y$

where

$$A = \begin{pmatrix} 3 & 1 & -2 & -1 \\ 2 & -2 & 2 & 3 \\ 1 & 5 & -4 & -1 \\ 3 & 1 & 2 & 3 \end{pmatrix} \qquad y = \begin{pmatrix} 3 \\ -8 \\ 3 \\ -1 \end{pmatrix}$$

We want LU decomposition for some matrix that is obtained from A by row interchanges.

We keep $l_{ii} = 1$ for all i.

<u>Stage 1:</u>

1^{st} diagonal of U. By Doolittle decomposition,

$u_{11} = a_{11} = 3$

If we interchange 2^{nd} or 3^{rd} or 4^{th} rows with 1^{st} row and then find the u_{11} for the new matrix we get respectively u_{11} = 2 or 1 or 3. Thus interchange of rows does not give any advantage at this stage as we have already got 3, without row interchange, for u_{11}.

So we keep the matrix as it is and calculate 1st row of U, by Doolittle's method.

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

The first column of L:

$$l_{11} = 1; l_{21} = \frac{a_{21}}{u_{11}} = 2/3; l_{31} = \frac{a_{31}}{u_{11}} = \frac{1}{3}; l_{41} = \frac{a_{41}}{u_{11}} = \frac{3}{3} = 1.$$

Thus

L is of the form $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 2/3 & 1 & 0 & 0 \\ 1/3 & l_{32} & 1 & 0 \\ 1 & l_{42} & l_{43} & l_{44} \end{pmatrix}$; and

U is of the form $\begin{pmatrix} 3 & 1 & -2 & -1 \\ 0 & u_{22} & u_{23} & u_{24} \\ 0 & 0 & u_{33} & u_{34} \\ 0 & 0 & 0 & u_{44} \end{pmatrix}$; A and Y remaining unchanged.

<u>Stage 2</u>

We now calculate the second diagonal of U: By Doolittle's method we have

$$u_{22} = a_{22} - l_{21}u_{12}$$
$$= -2 - \left(\frac{2}{3}\right)(1) = -\frac{8}{3}$$

Suppose we interchange 2nd row with 3rd row of A and calculate u_{22} : our new a_{22} is 5.

But note that l_{21} and l_{31} get interchanged. Therefore new l_{21} is 1/3.

Suppose instead of above we interchange 2nd row with 4th row of A:

New a_{22} = 1 and new l_{21} = 1 and therefore new u_{22} = 1 – (1) (1) = 0

Of these 14/3 has largest absolute value. So we prefer this. Therefore we interchange 2nd and 3rd row.

$$NewA = \begin{pmatrix} 3 & 1 & -2 & -1 \\ 1 & 5 & -4 & -1 \\ 2 & -2 & 2 & 3 \\ 3 & 1 & 2 & 3 \end{pmatrix}; Newy = \begin{pmatrix} 3 \\ 3 \\ -8 \\ -1 \end{pmatrix}$$

$$NewL = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1/3 & 1 & 0 & 0 \\ 2/3 & * & 1 & 0 \\ 1 & * & * & 1 \end{pmatrix}; NewU = \begin{pmatrix} 3 & 1 & -2 & -1 \\ 0 & 14/3 & * & * \\ 0 & 0 & * & * \\ 0 & 0 & 0 & * \end{pmatrix}$$

Now we do the Doolittle calculation for this new matrix to get 2nd row of U and 2nd column of L.

$$u_{23} = a_{23} - l_{21}u_{13}$$

$$= (-4) - \left(\frac{1}{3}\right)(-2) = -\frac{10}{3}$$

$$u_{24} = a_{24} - l_{21}u_{14}$$

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

<u>2nd column of L</u>:

$$l_{32} = [a_{32} - l_{31}u_{12}] \div u_{22}$$

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

$$= -\frac{4}{7}$$

$$l_{42} = [a_{42} - l_{41}u_{12}] \div u_{11}$$

$$= [3 - (1)(1)] \div \frac{14}{3}$$

= 0

Therefore new L has form $\begin{pmatrix} 1 & 0 & 0 & 0 \\ 1/3 & 1 & 0 & 0 \\ 2/3 & -4/7 & 1 & 0 \\ 1 & 0 & * & 1 \end{pmatrix}$

New U has form $\begin{pmatrix} 3 & 1 & -2 & -1 \\ 0 & 14/3 & -10/3 & -2/3 \\ 0 & 0 & * & * \\ 0 & 0 & 0 & * \end{pmatrix}$

This completes the 2nd stage of our computation.

Note: We had three choices of u_{22} to be calculated, namely –8/3, 14/3, 0 before we chose 14/3. It appears that we are doing more work than Doolittle. But this is not really so. For, observe, that the rejected u_{22} namely – 8/3 and 0 when divided by the chosen u_{22} namely 14/3 give the entries of L below the second diagonal.

3rd Stage:

3rd diagonal of U:

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

$$= 2 - \left(\frac{2}{3}\right)(-2) - \left(-\frac{4}{7}\right)\left(-\frac{10}{3}\right)$$

$$= \frac{10}{7}$$

Suppose we interchange 3rd row and 4th row of new A obtained in 2nd stage. We get new $a_{33} = 2$.

But in L also the second column gets 3rd and 4th row interchanges

Therefore new $l_{31} = 1$ and new $l_{32} = 0$

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

$$= 2 - (1)(-2) + (0)\left(-\frac{10}{3}\right)$$

$= 4.$

Of these two choices of u_{33} we have 4 has the largest magnitude. So we interchange 3rd and 4th rows of the matrix of 2nd stage to get

$$NewA = \begin{pmatrix} 3 & 1 & -2 & -1 \\ 1 & 5 & -4 & -1 \\ 3 & 1 & 2 & 3 \\ 2 & -2 & 2 & 3 \end{pmatrix} NewY = \begin{pmatrix} 3 \\ 3 \\ -1 \\ -8 \end{pmatrix}$$

$$NewL = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1/3 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 2/3 & -4/7 & * & 1 \end{pmatrix}; NewU = \begin{pmatrix} 3 & 1 & -2 & -1 \\ 0 & 14/3 & -10/3 & -2/3 \\ 0 & 0 & 4 & * \\ 0 & 0 & 0 & * \end{pmatrix}$$

Now for this set up we calculate the 3rd stage entries as in Doolittle's method:

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

$$= 3 - (1)(-1) - (0)\left(-\frac{2}{3}\right) = 4$$

$$l_{43} = \left(a_{43} - l_{41}u_{13} - l_{42}u_{23}\right) \div u_{33}$$

$$= \left[2 - \left(\frac{2}{3}\right)(-2) - \left(-\frac{4}{7}\right)\left(-\frac{10}{3}\right)\right] \div 4$$

= 5/14.

$$\therefore NewL = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1/3 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 2/3 & -4/7 & 5/14 & 1 \end{pmatrix}; NewU = \begin{pmatrix} 3 & 1 & -2 & -1 \\ 0 & 14/3 & -10/3 & -2/3 \\ 0 & 0 & 4 & 4 \\ 0 & 0 & 0 & * \end{pmatrix}$$

Note: The rejected u_{33} divided by chosen u_{33} gives l_{43}.

4th Stage

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

$$= 3 - \left(\frac{2}{3}\right)(-1) - \left(-\frac{4}{7}\right)\left(-\frac{2}{3}\right) - \left(\frac{5}{14}\right)(4)$$

= 13/7.

$$\therefore NewA = A^* = \begin{pmatrix} 3 & 1 & -2 & -1 \\ 1 & 5 & -4 & -1 \\ 3 & 1 & 2 & 3 \\ 2 & -2 & 2 & 3 \end{pmatrix} NewY = Y^* = \begin{pmatrix} 3 \\ 3 \\ -1 \\ -8 \end{pmatrix}$$

New L = L* , New U = U*

$$L^* = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1/3 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 2/3 & -4/7 & 5/14 & 1 \end{pmatrix}; U^* = \begin{pmatrix} 3 & 1 & -2 & -1 \\ 0 & 14/3 & -10/3 & -2/3 \\ 0 & 0 & 4 & 4 \\ 0 & 0 & 0 & 13/7 \end{pmatrix},$$

and $A^* = L^*U^*$

The given system Ax=y is equivalent to the system

$A^*x=y^*$

and hence can be split into the triangular systems,

$L^*z = y^*$

$U^*x = z$

Now $L^*z = y^*$ gives by forward substitution:

$Z_1 = 3$

$$\frac{1}{3}z_1 + z_2 = 3 \Rightarrow z_2 = 3 - 1 = 2$$

$$z_1 + z_3 = -1 \Rightarrow z_3 = -1 - z_1 = -4$$

$$\frac{2}{3}z_1 - \frac{4}{7}z_2 + \frac{5}{14}z_3 + z_4 = -8$$

$$\left(\frac{2}{3}\right)(3) - \left(\frac{4}{7}\right)(2) + \left(\frac{5}{14}\right)(-4) + z_4 = -8$$

$$\Rightarrow z_4 = -\frac{5^2}{7}$$

$$\therefore z = \begin{pmatrix} 3 \\ 2 \\ -4 \\ -\frac{52}{7} \end{pmatrix}$$

Therefore U*x = z gives by back-substitution;

$\frac{13}{7}x_4 = -\frac{52}{7}$ therefore $x_4 = -4$.

$$4x_3 + 4x_4 = -4 \Rightarrow x_3 + x_4 = -1 \Rightarrow x_3 = -1 - x_4 = 3$$

therefore $x_3 = 3$

$$\frac{14}{3}x_2 - \frac{10}{3}x_3 - \frac{2}{3}x_4 = 2$$

$$\frac{14}{3}x_2 - \left(\frac{10}{3}\right)(3)\left(-\frac{2}{3}\right)(-4) = 2$$

$$\Rightarrow \; x_2 = 2$$

$$3x_1 + x_2 - 2x_3 - x_4 = 3$$

$$\Rightarrow 3x_1 + 2 - 6 + 4 - 3 \Rightarrow x_1 = 1$$

Therefore the solution of the given system is

$$x = \begin{pmatrix} 1 \\ 2 \\ 3 \\ -4 \end{pmatrix}$$

<u>Some Remarks:</u>

The factorization of a matrix A as the product of lower and upper triangular matrices is by no means unique. In fact, the diagonal elements of one or the other factor can be chosen arbitrarily; all the remaining elements of the upper and lower triangular matrices may then be uniquely determined as in Doolittle's method; which is the case when we choose all the diagonal entries of L as 1. The name of Crout is often associated with triangular decomposition methods, and in Crout's method the diagonal elements of U are all chosen as unity. Apart from this, there is little distinction, as regards procedure or accuracy, between the two methods.

As already mentioned, Wilkinson's (see Page 25), suggestion is to get a LU decomposition in which $|l_{ii}| = |u_{ii}|; 1 \le i \le n$.

We finally look at the Cholesky decomposition for a symmetric matrix:

Let A be a symmetric matrix.

Let A = LU be its LU decomposition

Then $A^T = U^T L^T$ where the superscript T denotes the Transpose.

We have

U^T is lower triangular and L^T is upper triangular

Therefore $U^T L^T$ is a decomposition of A^T as product of lower and upper triangular matrices. But $A^T = A$ since A is symmetric.

Therefore $LU = U^T L^T$

We ask the question whether we can choose L as U^T; so that

$A = U^T U$ (or same as LL^T)

In that case, determining U automatically gets $L = U^T$

We now do the Doolittle method for this. Note that it is enough to determine the rows of U.

<u>Stage 1:</u> <u>1st row of U:</u>

$$a_{11} = \sum_{k=1}^{n} l_{1k} u_{k1} = \sum_{k=1}^{n} u_{kl}^2 \quad \text{since } l_{1k} = u_{k1} \qquad \because \mathrm{L} = \mathrm{U}^{\mathrm{T}}$$

$= u_{11}^2$ since $u_{k1} = 0$ for k>1 as U is upper triangular.

$$\therefore u_{11} = \sqrt{a_{11}}$$

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

$= u_{11} u_{1i}$ since $u_{k1} = 0 \text{ for } k > 1$

$$u_{11} = \sqrt{a_{11}}$$

$\therefore u_{1i} = a_{1i} / u_{11}$ determines the first row of U.

and hence the first column of L.

Having determined the 1st i-1 rows of U; we determine the ith row of U as follows:

$$a_{ii} = \sum_{k=1}^{n} l_{ik} u_{ki} = \sum_{k=1}^{n} u_{kl}^2 \text{ since } l_{ik} = u_{ki}$$

$$= \sum_{k=1}^{i} u_{ki}^{2} \text{ since } u_{ki} = 0 \text{ for } k > i$$

$$= \sum_{k=1}^{i-1} u_{ki}^{2} + u_{ii}^{2}$$

$$\therefore\ u_{ii}^{2} = a_{ii} - \sum_{k=1}^{i-1} u_{ki}^{2}$$

$$\therefore\ u_{ii} = \sqrt{a_{ii} - \sum_{k=1}^{i-1} u_{ki}^{2}} \quad ;$$

(Note that u_{ki} are known for $k \le i - 1$,because 1st i-1 rows have already been obtained).

$$a_{ij} = \sum_{k=1}^{n} l_{ik} u_{kj} = \sum_{k=1}^{n} u_{ki} u_{kj}$$ Now we need u_{ij} for $j > i$

$$= \sum_{k=1}^{i} u_{ki} u_{kj}$$ Because $u_{ki} = 0$ for $k > i$

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

Therefore

$$u_{ij} = \left[a_{ij} - \sum_{k=1}^{i-1} u_{ki} u_{kj} \right] \div u_{ii}$$

$$\therefore \begin{cases} u_{ii} = \sqrt{a_{ii} - \sum_{k=1}^{i-1} u_{ki}{}^{2}} \\ u_{ij} = \left[a_{ij} - \sum_{k=1}^{i-1} u_{ki} u_{kj} \right] \div u_{ij} \end{cases}$$

determines the ith row of U in terms of the previous rows. Thus we get U and L is U^1. This is called CHOLESKY decomposition.

Example:

Let $A = \begin{pmatrix} 1 & -1 & 1 & 1 \\ -1 & 5 & -3 & 3 \\ 1 & -3 & 3 & 1 \\ 1 & 3 & 1 & 10 \end{pmatrix}$

This is a symmetric matrix. Let us find the Cholesky decomposition.

1st row of U

$$\begin{cases} u_{11} = \sqrt{a_{11}} = 1 \\ u_{12} = a_{12} \div u_{11} = -1 \\ u_{13} = a_{13} \div u_{11} = 1 \\ u_{14} = a_{14} \div u_{11} = 1 \end{cases}$$

2nd row of U

$$\begin{cases} u_{22} = \sqrt{a_{22} - u^{2}{}_{12}} = \sqrt{5-1} = 2 \\ u_{23} = (a_{23} - u_{12}u_{13}) \div u_{22} = (-3-(-1)(1)) \div 2 = -1 \\ u_{24} = (a_{24} - u_{12}u_{14}) \div u_{22} = (3-(-1)(1)) \div 2 = 2 \end{cases}$$

3rd row of U

$$\begin{cases} u_{33} = \sqrt{a_{33} - u^2{}_{13} - u^2{}_{23}} = \sqrt{3-1-1} = 1 \\ u_{34} = (a_{34} - u_{13}u_{14} - u_{23}u_{24}) \div u_{33} = (1-(1)(1)-(-1)(2)) \div 1 = 2 \end{cases}$$

<u>4th row of U</u>

$$u_{44} = \sqrt{a_{44} - u^2{}_{14} - u^2{}_{24} - u^2{}_{34}} = \sqrt{10-1-4-4} = 1$$

$$\therefore U = \begin{pmatrix} 1 & -1 & 1 & 1 \\ 0 & 2 & -1 & 2 \\ 0 & 0 & 1 & 2 \\ 0 & 0 & 0 & 1 \end{pmatrix} \qquad \therefore U^1 = L = \begin{pmatrix} 1 & 0 & 0 & 0 \\ -1 & 2 & 0 & 0 \\ 1 & -1 & 1 & 0 \\ 1 & 2 & 2 & 1 \end{pmatrix} \text{ and}$$

A = LU
= LL^T
= U^TU