1.4.2 Cholesky Decomposition

We mention now the special form that LU decomposition takes for a matrix $A$ that is symmetric ($A^T=A$) and positive-definite, i.e.

$$y^T A y > 0 \text{ for all } y \in \mathbb{R}^N, y \neq 0 \quad (1.4.2-1)$$

The meaning of positive definiteness will be made clearer in our later discussion of matrix eigenvalues. For now, we merely state the definition above, and note that many matrices satisfy this property.

For example, the matrix below, common in the numerical solution of PDE’s

$$A = \begin{bmatrix}
2 & -1 & & \\
-1 & 2 & -1 & \\
& -1 & 2 & -1 & \\
& & -1 & 2
\end{bmatrix} \quad (1.4.2-2)$$

Is positive-definite since

$$A y = \begin{bmatrix}
2 & -1 & & \\
-1 & 2 & -1 & \\
& -1 & 2 & -1 & \\
& & -1 & 2
\end{bmatrix} \begin{bmatrix}
y_1 \\
y_2 \\
y_3 \\
y_4
\end{bmatrix} = \begin{bmatrix}
2y_1 - y_2 \\
y_1 + 2y_2 - y_3 \\
y_2 + 2y_3 - y_4 \\
y_3 + 2y_4
\end{bmatrix} \quad (1.4.2-3)$$

$$y^T A y = y \bullet (A y) = \begin{bmatrix}
y_1 & y_2 & y_3 & y_4
\end{bmatrix} \begin{bmatrix}
2y_1 - y_2 \\
y_1 + 2y_2 - y_3 \\
y_2 + 2y_3 - y_4 \\
y_3 + 2y_4
\end{bmatrix}$$

$$= y_1(2y_1 - y_2) + y_2(-y_1 + 2y_2 - y_3) + y_3(-y + 2y_3 - y_4) + y_4(-y_3 + 2y_4)$$

$$= 2y_1^2 - y_1 y_2 - y_1 y_2 + 2y_2^2 - y_2 y_3 + 2y_3^2 - y_3 y_4 + 2y_4^2 - y_3 y_4$$

$$= 2(y_1^2 + y_2^2 + y_3^2 + y_4^2) - 2(y_1 y_2 + y_2 y_3 + y_3 y_4) \quad (1.4.2-4)$$

As first term in positive and always larger in magnitude than the second, $y^T A y > 0.$
For such a matrix $A$ with $A^T = A$, $v^T A v > 0$, we can perform a Cholesky decomposition to write

$$A = LL^T \quad (1.4.2-5)$$

Note that

$$A^T = (LL^T)^T = (L^T)^T L^T = LL^T = A \quad (1.4.2-6)$$

And

$$v^T A v = v^T LL^T v = (L^T v)^T (L^T v) = (L^T v) \cdot (L^T v) > 0 \quad \text{for } v \neq 0, \text{ A non-singular} \quad (1.4.2-7)$$

Where we have used the property for determinants $(AB)^T = B^T A^T \quad (1.4.2-8)$

Therefore, the equation $A = LL^T$ immediately implies that $A$ is symmetric and positive-definitive.

Advantages of Cholesky decomposition, when it can be used:

- cut storage requirement since only need $L$
- stable even without pivoting
- faster than LU decomposition By a factor of 2

If we write out $(1.4.2-5)$ explicitly,

$$A = LL^T = \begin{bmatrix}
L_{11} & L_{21} & L_{31} & \ldots & L_{N1} \\
L_{21} & L_{22} & L_{32} & \ldots & L_{N2} \\
L_{31} & L_{32} & L_{33} & \ldots & L_{N3} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
L_{N1} & L_{N2} & L_{N3} & \ldots & L_{NN}
\end{bmatrix} \begin{bmatrix}
L_{11} & L_{12} & L_{13} & \ldots & L_{1N} \\
L_{21} & L_{22} & L_{23} & \ldots & L_{2N} \\
L_{31} & L_{32} & L_{33} & \ldots & L_{3N} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
L_{N1} & L_{N2} & L_{N3} & \ldots & L_{NN}
\end{bmatrix} \quad (1.4.2-9)$$

We can perform the multiplication to obtain,

$$L_{11} L_{11} = a_{11} \Rightarrow L_{11} = (a_{11})^{(1/2)} \quad (1.4.2-10)$$
Next, multiply row 1 of $L$ with column 2 of $L^T$,
\[ a_{12} = L_{11}L_{21} \quad \Rightarrow \quad L_{21} = a_{12}/L_{11} \quad (1.4.2-11) \]

Next, row #1 of $L$ with column #3 of $L^T$,
\[ a_{13} = L_{11}L_{31} \quad \Rightarrow \quad L_{31} = a_{13}/L_{11} \quad (1.4.2-12) \]

Similarly for $j = 4, \ldots, N$ we have $L_{j1} = a_{ij}/L_{11}$ \hspace{1cm} (1.4.2-13)

This gives us the values of the 1st column of $L$ (and 1st row of $L^T$).

Next, we move to the 2nd column of $L$.

Multiplying row #2 of $L$ with column #2 of $L^T$,
\[ L_{21}L_{21} + L_{22}L_{22} = a_{22} \quad \Rightarrow \quad L_{22} = (a_{22} - L_{21}^2)^{1/2} \quad (1.4.2-14) \]

Then, multiplying row #2 of $L$ with column #3 of $L^T$,
\[ L_{21}L_{31} + L_{22}L_{32} = a_{23} \quad \Rightarrow \quad L_{32} = (a_{23} - L_{21}L_{31})/L_{22} \quad (1.4.2-15) \]

And row #2 of $L$ with column #j (j=4,\ldots,N) of $L^T$,
\[ L_{21}L_{j1} + L_{22}L_{j2} = a_{2j} \quad \Rightarrow \quad L_{j2} = (a_{2j} - L_{21}L_{j1})/L_{22} \quad (1.4.2-16) \]

This gives us the elements of the 2nd column of $L$ (2nd row of $L^T$).

In general, to determine the elements of the ith column of $L$, we first multiply the ith row of $L$ with ith column of $L^T$ to obtain
\[ L_{i1}^2 + L_{i2}^2 + \ldots + L_{i,i-1}^2 + L_{ii}^2 = a_{ii} \quad (1.4.2-17) \]

\[ \Rightarrow \quad L_{ii} = [a_{ii} - \sum_{k=1}^{i-1} L_{ik}^2]^{1/2} \quad (1.4.2-18) \]
Then for \( j = i+1, i+2, \ldots, N \) we multiply the \( i \)th row of \( L \) by the \( j \)th column of \( L^T \) to obtain
\[
L_{i1}L_{j1} + L_{i2}L_{j2} + \ldots + L_{i,i-1}L_{j,i-1} + L_{ii}L_{ji} = a_{ij} \quad (1.4.2-19)
\]
So
\[
L_{ji} = \left[ a_{ij} - \sum_{k=1}^{i-1} L_{ik}L_{jk} \right] / L_{ii} \quad (1.4.2-20)
\]

This gives us the following algorithm for performing a Cholesky decomposition:

For \( i = 1, 2, \ldots, N \) \% each column of \( L \)
\[
\text{\( \sqrt{L_{ii}} \leftarrow [a_{ii} - \sum_{k=1}^{i-1} L_{ik}^2]^{(1/2)} \) }
\]
For \( j = i+1, i+2, \ldots, N \) \% each element below the diagonal in column \#\( i \) of \( L \)
\[
\text{\( L_{ji} = \left[ a_{ij} - \sum_{k=1}^{i-1} L_{ik}L_{jk} \right] / L_{ii} \) }
\]