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| **Matrix Computations** | **Fall 2020** |

# Lecture 10: LU decomposition Revisited

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**The intention of this notes is to further explain the definition of LU decomposition and to modify some ambiguity in Homework 2.**

**Definition 1** (General definition of LU decomposition[1]). *A matrix* $\mathbf{A} \in \mathbb{R}^{n\times n}$ *is said to have an LU decomposition/factorization if it can be factored as*

$$\mathbf{A} = \mathbf{LU}\,,$$

*where* $\mathbf{L} \in \mathbb{R}^{n\times n}$ *is unit lower triangular (lower triangular with unit diagonal elements, i.e.,* $\ell_{ii} = 1$ *for all* $i$*), and* $\mathbf{U} \in \mathbb{R}^{n\times n}$ *is upper triangular.*

In this case, a natural question is, does every matrix have an LU decomposition? The answer is no.

**Theorem 1.** *If* $\mathbf{A} \in \mathbb{R}^{n\times n}$ *and* $\det(\mathbf{A}_{\{1,\dots,k\}}) \neq 0$ *for* $k = 1, \dots, n-1$*, then* $\mathbf{A}$ *has an LU decomposition. If this is the case and* $\mathbf{A}$ *is nonsingular, then the factorization is unique* [2].

So far, we have shown the sufficient condition for the LU decomposition. However, what if $\mathbf{A}$ is singular, does $\mathbf{A}$ still admit an LU decomposition?

From the general definition of LU decomposition, as long as we can find matrices $\mathbf{L}$ and $\mathbf{U}$ which are unit lower triangular and upper triangular such that $\mathbf{A} = \mathbf{LU}$, we can claim that $\mathbf{A}$ has LU decomposition. For example, recall Problem 2 of Homework 2, consider the $4 \times 4$ matrix

$$\begin{bmatrix} a & a & a & a \\ a & b & b & b \\ a & b & c & c \\ a & b & c & d \end{bmatrix}$$

we can find its LU decomposition via

$$\begin{bmatrix} a & a & a & a \\ a & b & b & b \\ a & b & c & c \\ a & b & c & d \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} a & a & a & a \\ 0 & b-a & b-a & b-a \\ 0 & 0 & c-b & c-b \\ 0 & 0 & 0 & d-c \end{bmatrix}. \tag{1}$$

When $a = 0$, or $b = a$, or $c = b$, $\mathbf{U}$ is singular and consequently $\mathbf{A}$ is singular. Therefore, even singular matrix can have an LU decomposition in the general sense. And in this case, is the LU

[1] This definition is consistent with the definition given in Slides.

[2] *The proof of this theorem is omitted here, you can find the proof in Section 3.2.5 of [2].*

decomposition unique? The answer is no. For example, when $a = 0$ and $b, c, d$ are randomly given, then $\mathbf{A}$ can be factored as

$$\begin{bmatrix} a & a & a & a \\ a & b & b & b \\ a & b & c & c \\ a & b & c & d \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ \ell_{21} & 1 & 0 & 0 \\ \ell_{31} & 1 & 1 & 0 \\ \ell_{41} & 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} a & a & a & a \\ 0 & b-a & b-a & b-a \\ 0 & 0 & c-b & c-b \\ 0 & 0 & 0 & d-c \end{bmatrix},$$

where $\ell_{21}, \ell_{31}, \ell 41$ can take any values. Therefore, such LU decomposition is not unique.

**Definition 2** (General definition of LDM/LDU decomposition)**.** *A matrix $\mathbf{A} \in \mathbb{R}^{n\times n}$ is said to have an LDM/LDU decomposition/factorization if it can be factored as*

$$\mathbf{A} = \mathbf{L}\mathbf{D}\mathbf{M}^T,$$

*where $\mathbf{L} \in \mathbb{R}^{n\times n}$ and $\mathbf{M}$ are unit lower triangular (lower triangular with unit diagonal elements), and $\mathbf{D} = \mathrm{diag}(d_1, \ldots, d_n)$ is a diagonal matrix.*

If $\mathbf{A}$ is nonsingular and has LU decomposition $\mathbf{A} = \mathbf{L}\mathbf{U}$ (in this case, the diagonal elements of $\mathbf{U}$ are all nonzero), then the LDM decomposition can be given as

$$\mathbf{A} = \mathbf{L}\mathbf{D}\mathbf{M}^T,$$

where

$$\mathbf{D} = \mathrm{diag}(u_{11}, \ldots, u_{nn}), \quad \mathbf{M} = \mathbf{U}^T\mathbf{D}^{-1},$$

therefore, in the case of nonsingular $\mathbf{A}$, the existence of LDM decomposition follows the existence of LU decomposition.

In the case of singular $\mathbf{A}$, take (2) for example, the LDM decomposition can be given by

$$\begin{bmatrix} a & a & a & a \\ a & b & b & b \\ a & b & c & c \\ a & b & c & d \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} a & 0 & 0 & 0 \\ 0 & b-a & 0 & 0 \\ 0 & 0 & c-b & 0 \\ 0 & 0 & 0 & d-c \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 \end{bmatrix}. \tag{2}$$

But if the existence of LDM decomposition follows the existence of LU decomposition in the singular case? Let the LU decomposition for singular $\mathbf{A}$ be given by (denote $\mathbf{L} = (\ell_{i,j})_{n\times n}, \mathbf{U} = (u_{i,j})_{n\times n}$ ).

$$\mathbf{A} = (a_{i,j})_{n\times n} = \begin{bmatrix} 1 & & & & \\ \ell_{21} & 1 & & & \\ \ell_{31} & \ell_{32} & 1 & & \\ \vdots & \vdots & & \ddots & \\ \ell_{n1} & \ell_{n2} & & \cdots & 1 \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & \cdots & u_{1n} \\ & u_{22} & \cdots & u_{2n} \\ & & \ddots & \vdots \\ & & & u_{nn} \end{bmatrix},$$

suppose that $u_{ii} = 0$ for some $i$, but $u_{i,j} \neq 0$ for some $j \in \{i+1, \ldots, n\}$, then consider the LDM decomposition (denote $\mathbf{M} = (m_{i,j})_{n\times n}$)

$$\mathbf{A} = (a_{i,j})_{n\times n} = \begin{bmatrix} 1 & & & & \\ \ell_{21} & 1 & & & \\ \ell_{31} & \ell_{32} & 1 & & \\ \vdots & \vdots & & \ddots & \\ \ell_{n1} & \ell_{n2} & & \cdots & 1 \end{bmatrix} \begin{bmatrix} u_{11} & & & & & \\ & u_{22} & & & & \\ & & \ddots & & & \\ & & & u_{ii} = 0 & & \\ & & & & \ddots & \\ & & & & & u_{nn} \end{bmatrix} \begin{bmatrix} 1 & m_{21} & \cdots & m_{n1} \\ & 1 & \cdots & m_{n2} \\ & & \ddots & \vdots \\ & & & 1 \end{bmatrix},$$

which indicates that $u_{ij} = \mathbf{D}(i,:)\mathbf{M}(:,j) = 0$ and it contradicts the assumption. Therefore, in this case, $\mathbf{A}$ which has an LU decomposition does not have an LDM decomposition. Whereas, if the LU decomposition for $\mathbf{A}$ satisfies $u_{ii} = 0$ for some $i$, and $u_{i,j} = 0$ for $j = i+1, \dots, n$, then the LDM decomposition for $\mathbf{A}$ exists,

$$\mathbf{A} = (a_{i,j})_{n\times n} = \begin{bmatrix} 1 & & & & \\ \ell_{21} & 1 & & & \\ \ell_{31} & \ell_{32} & 1 & & \\ \vdots & \vdots & & \ddots & \\ \ell_{n1} & \ell_{n2} & & \cdots & 1 \end{bmatrix} \begin{bmatrix} u_{11} & & & & & \\ & u_{22} & & & & \\ & & \ddots & & & \\ & & & u_{ii} = 0 & & \\ & & & & \ddots & \\ & & & & & u_{nn} \end{bmatrix} \begin{bmatrix} 1 & m_{21} = \frac{u_{12}}{u_{11}} & & \cdots & & & m_{n1} = \frac{u_{1n}}{u_{11}} \\ & 1 & & \cdots & & & m_{n2} = \frac{u_{2n}}{u_{22}} \\ & & \ddots & & & & \vdots \\ & & & 1 & m_{i+1,i} & \cdots & m_{n,i} \\ & & & & \ddots & & \vdots \\ & & & & & & 1 \end{bmatrix}$$

where $m_{j,i}$ $(j = i+1, \dots, n)$ can take any take, and therefore is not unique in general. To sum up, the problem description in problem 4 of Homework 2 is ambiguous. The modified version can be found in 1 (The modified part is marked with red).

However, when discussing LU decomposition, we almost always consider the problem of solving linear equations,

$$\mathbf{A}\mathbf{x} = \mathbf{b}\,,$$

and $\mathbf{A}$ is nonsingular by default. And the singular $\mathbf{A}$ case may be trivial. In other contexts, the definitions of LU decomposition may vary. For example, in section 3.10 of [1], the LU factorization this textbook discussed is restricted to nonsingular $\mathbf{A}$ case. In section 3.2.10 of [2], LU decomposition of a rectangular matrix is defined. You can read section 3.2 of [2] for more details.

# 1 Problem 4 of Homework 2 modified

Given a matrix $\mathbf{A} \in \mathbb{R}^{n\times n}$, suppose that the LDM (LDU) decomposition of $\mathbf{A}$ exists, prove that

1. suppose $\mathbf{A}$ is nonsingular, then the LDM (LDU) decomposition of $\mathbf{A}$ is *uniquely* determined;
2. if $\mathbf{A}$ is a nonsingular symmetric matrix, then its LDM (LDU) decomposition must be $\mathbf{A} = \mathbf{L}\mathbf{D}\mathbf{L}^T$, which is called LDL decomposition in this case;
3. $\mathbf{A}$ is a symmetric and positive definite matrix if and only if its Cholesky decomposition exists (i.e., there exists a matrix $\mathbf{G} \in \mathbb{R}^{n\times n}$ such that $\mathbf{A} = \mathbf{G}\mathbf{G}^T$, where $\mathbf{G}$ is lower triangular with *positive* diagonal entries);
4. if $\mathbf{A}$ is a symmetric and positive definite matrix, then its Cholesky decomposition is *uniquely* determined.

**Hint:** You can directly utilize the following lemmas,

- the inverse (if it exists) of a lower (resp. upper) triangular matrix is also lower (resp. upper) triangular;
- the product of two lower (resp. upper) triangular matrices is lower (resp. upper) triangular;
- also, if such two lower (resp. upper) triangular matrices have unit diagonal entries, then their product also has unit diagonal entries.

**Solution:**

1. Assume that $\mathbf{A}$ has two **LDM** decompositions as $\mathbf{A} = \mathbf{L}_1\mathbf{D}_1\mathbf{M}_1^T = \mathbf{L}_2\mathbf{D}_2\mathbf{M}_2^T$, we expect to prove that $\mathbf{L}_1 = \mathbf{L}_2$, $\mathbf{D}_1 = \mathbf{D}_2$, and $\mathbf{M}_1 = \mathbf{M}_2$. For nonsingular matrix $\mathbf{A}$, ~~*First*, note that the existence of the LDM decomposition implies that $\mathbf{A}$ is nonsingular. Hence,~~ the determinant of $\mathbf{A}$ satisfies $|\mathbf{A}| \neq 0$. Besides, since $|\mathbf{A}| = |\mathbf{L}_1| \times |\mathbf{D}_1| \times |\mathbf{M}_1| = |\mathbf{L}_2| \times |\mathbf{D}_2| \times |\mathbf{M}_2|$, we have that $\mathbf{L}_1$, $\mathbf{D}_1$, $\mathbf{M}_1$, $\mathbf{L}_2$, $\mathbf{D}_2$, and $\mathbf{M}_2$ are all nonsingular (*i.e.*, invertible).
   *Second*, since $\mathbf{L}_1\mathbf{D}_1\mathbf{M}_1^T = \mathbf{L}_2\mathbf{D}_2\mathbf{M}_2^T$, we have
   $$\mathbf{L}_2^{-1}\mathbf{L}_1 = \mathbf{D}_2\mathbf{M}_2^T(\mathbf{M}_1^T)^{-1}\mathbf{D_1}^{-1}.$$
   We can check that the left hand side $\mathbf{L}_2^{-1}\mathbf{L}_1$ is lower triangular, while the right hand side $\mathbf{D}_2\mathbf{M}_2^T(\mathbf{M}_1^T)^{-1}\mathbf{D_1}^{-1}$ is upper triangular. Hence, the left hand side and the right hand side are both diagonal matrices.
   *Third*, the diagonal entries of the left hand side $\mathbf{L}_2^{-1}\mathbf{L_1}$ must be one, which implies $\mathbf{L}_2^{-1}\mathbf{L}_1 = \mathbf{I}$ and accordingly $\mathbf{L}_1 = \mathbf{L}_2$. Similarly, we can derive that $\mathbf{M}_2^T(\mathbf{M}_1^T)^{-1} = \mathbf{D}_2^{-1}\mathbf{L}_2^{-1}\mathbf{L}_1\mathbf{D}_1$, which can further deduce that $\mathbf{M}_1 = \mathbf{M}_2$. Finally, we have $\mathbf{D}_1 = \mathbf{L}_1^{-1}\mathbf{A}(\mathbf{M}_1^T)^{-1} = \mathbf{L}_2^{-1}\mathbf{A}(\mathbf{M}_2^T)^{-1} = \mathbf{D}_2$, which concludes this proof.
2. For nonsingular $\mathbf{A}$, $\mathbf{A}$ must have LDM decomposition and it is unique. Let $\mathbf{A} = \mathbf{L}\mathbf{D}\mathbf{M}^T$, and since $\mathbf{A}$ is symmetric, we have $\mathbf{L}\mathbf{D}\mathbf{M}^T = \mathbf{A} = \mathbf{A}^T = \mathbf{M}\mathbf{D}\mathbf{L}^T$. From the proof in 1), we learn that $\mathbf{L}$ and $\mathbf{M}^T$ are both invertible. Then we can derive that
   $$\mathbf{D}\mathbf{M}^T(\mathbf{L}^T)^{-1} = \mathbf{L}^{-1}\mathbf{M}\mathbf{D}.$$
   Note that $(\mathbf{L}^T)^{-1}$ and $\mathbf{M}^T$ are both upper triangular, while $\mathbf{L}^{-1}$ and $\mathbf{M}$ are both lower triangular. We can check that the left hand side $\mathbf{D}\mathbf{M}^T(\mathbf{L}^T)^{-1}$ is upper triangular and the right hand side $\mathbf{L}^{-1}\mathbf{M}\mathbf{D}$ is lower triangular. Hence, the left hand side and the right hand side are both diagonal matrices. Since $\mathbf{D}$ is a diagonal matrix, $\mathbf{L}^{-1}\mathbf{M}$ is also a diagonal matrix. Moreover, the diagonal entries of $\mathbf{L}^{-1}\mathbf{M}$ must be one, which implies $\mathbf{L}^{-1}\mathbf{M} = \mathbf{I}$ and accordingly $\mathbf{L} = \mathbf{M}$.

3. $\mathbf{A}$ is a symmetric and positive definite matrix $\Rightarrow$ its Cholesky decomposition exists)
Note that a positive definite matrix must be nonsingular. According to the conclusion in 2), we have $\mathbf{A} = \mathbf{LDL}^T$. For any vector $\mathbf{x} \in \mathbb{R}^n$, there exists a vector $\mathbf{y} \in \mathbb{R}^n$ such that $\mathbf{y} = \mathbf{L}^T\mathbf{x}$. Since $A$ is a positive definite matrix, we can derive that
$$\mathbf{y}^T\mathbf{D}\mathbf{y} = \mathbf{x}^T\mathbf{LDL}^T\mathbf{x} = \mathbf{x}^T\mathbf{A}\mathbf{x} > 0.$$
Hence, the diagonal entries of $\mathbf{D}$ are all positive. Let $\mathbf{D}^{'}$ denote a diagonal matrix, where $\mathbf{D}^{'}_{ii} = \sqrt{\mathbf{D}_{ii}}$ for $i = 1, 2, 3, ..., n$. Then we have
$$\mathbf{A} = \mathbf{LDL}^T = \mathbf{LD}^{'}(\mathbf{D}^{'})^T\mathbf{L}^T = \mathbf{LD}^{'}(\mathbf{LD}^{'})^T.$$
Let $\mathbf{G} = \mathbf{LD}^{'}$, then $\mathbf{A} = \mathbf{GG}^T$, where $\mathbf{G}$ is lower triangular with positive diagonal elements.
($\mathbf{A}$ is a symmetric and positive definite matrix $\Leftarrow$ its Cholesky decomposition exists)
*First*, since $\mathbf{A}^T = (\mathbf{GG}^T)^T = \mathbf{GG}^T = \mathbf{A}$, we can learn that $\mathbf{A}$ is a symmetric matrix.
*Second*, for any non-zero vector $\mathbf{x} \in \mathbb{R}^n$, we have
$$\mathbf{x}^T\mathbf{A}\mathbf{x} = \mathbf{x}^T\mathbf{GG}^T\mathbf{x} = (\mathbf{G}^T\mathbf{x})^T(\mathbf{G}^T\mathbf{x}) > 0,$$
which implies that $A$ is a positive definite matrix.

4. First we have that $\mathbf{A}$ is nonsingular since $\mathbf{A}$ is PD. Assume that $\mathbf{A}$ has two Cholesky decompositions as $\mathbf{A} = \mathbf{G}_1\mathbf{G}_1^T = \mathbf{G}_2\mathbf{G}_2^T$, we expect to prove that $\mathbf{G}_1 = \mathbf{G}_2$.
*First*, since $\mathbf{G}_1$ and $\mathbf{G}_2$ are both lower triangular with positive diagonal entries, $\mathbf{G}_1$ and $\mathbf{G}_2$ must be invertible. *Second*, since $\mathbf{A} = \mathbf{G}_1\mathbf{G}_1^T = \mathbf{G}_2\mathbf{G}_2^T$, we have
$$\mathbf{G}_1^{-1}\mathbf{G}_2 = (\mathbf{G}_1^{-1}\mathbf{G}_2)^T.$$
We can check that the left hand side $\mathbf{G}_1^{-1}\mathbf{G}_2$ is lower triangular, while the right hand side $(\mathbf{G}_1^{-1}\mathbf{G}_2)^T$ is upper triangular. Hence, the left hand side and the right hand side are both diagonal matrices. Let $\mathbf{G}_0 = \mathbf{G}_1^{-1}\mathbf{G}_2$, then $\mathbf{G}_0$ is a diagonal matrix.
*Third*, by $\mathbf{G}_1\mathbf{G}_1^T = \mathbf{G}_2\mathbf{G}_2^T$, we can also derive that
$$\mathbf{I} = \mathbf{G}_1^{-1}\mathbf{G}_2\mathbf{G}_2^T(\mathbf{G}_1^T)^{-1} = \mathbf{G}_0\mathbf{G}_0^T.$$
Hence, the diagonal entries of $\mathbf{G}_0$ must be 1 or $-1$. Note that $\mathbf{G}_2 = \mathbf{G}_1\mathbf{G}_0$. Considering the diagonal entries of $\mathbf{G}_2$ and $\mathbf{G}_1$, we have $(\mathbf{G}_2)_{ii} = (\mathbf{G}_1)_{ii} \times (\mathbf{G}_0)_{ii}$ for $i = 1, 2, ..., n$. Since the diagonal entries of $\mathbf{G}_2$ and $\mathbf{G}_1$ are required to be positive, $(\mathbf{G}_0)_{ii}$ can only be 1 for $i = 1, 2, ..., n$, *i.e.*, $\mathbf{G}_0 = \mathbf{I}$. Accordingly, $\mathbf{G}_1 = \mathbf{G}_2$, which concludes this proof.

## References

[1] Meyer, Carl D. Matrix analysis and applied linear algebra. Vol. 71. Siam, 2000.

[2] Gene H. Golub, Chales F. Van Loan. Matrix Computations. The John Hopkins University Press.