Lecture 16: Positive Semidefinite Matrices and Cholesky Decomposition

1 Positive Semidefinite Matrices

We now study another important class of Hermitian matrices: positive semidefinite matrices.

These matrices arise naturally in least squares, optimization, statistics, and the singular value decomposition.

1.1 Definition

Definition (Positive Semidefinite Matrix)**.** *A Hermitian matrix*

$$A \in \mathbb{C}^{n \times n}$$

is called positive semidefinite *if*

$$x^* A x \geq 0 \qquad \text{for every } x \in \mathbb{C}^n.$$

We write

$$A \succeq 0.$$

Similarly, A is called *positive definite* if

$$x^* A x > 0 \qquad \text{for every } x \neq 0.$$

In this case, we write

$$A \succ 0.$$

Example 1.1. *Let*

$$A = \begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix}.$$

Then for

$$x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix},$$

we have

$$x^* A x = 2|x_1|^2 + |x_2|^2.$$

Thus

$$x^* A x > 0$$

for every $x \neq 0$, so A is positive definite.

1.2 Positive Semidefinite Matrices and Eigenvalues

Theorem 1.2. *Let $A \in \mathbb{C}^{n\times n}$ be Hermitian. Then*

$$A \succeq 0$$

if and only if every eigenvalue of A is nonnegative.

Proof. Suppose first that $A \succeq 0$.

Let $v \neq 0$ be an eigenvector of A with eigenvalue λ. Then

$$Av = \lambda v.$$

Therefore,

$$v^*Av = v^*(\lambda v) = \lambda \|v\|_2^2.$$

Since $A \succeq 0$,

$$v^*Av \geq 0.$$

Because $v \neq 0$,

$$\|v\|_2^2 > 0,$$

and hence

$$\lambda \geq 0.$$

Conversely, suppose all eigenvalues of A are nonnegative.

By the spectral theorem,

$$A = Q\Lambda Q^*,$$

where Q is unitary and

$$\Lambda = \operatorname{diag}(\lambda_1, \ldots, \lambda_n), \qquad \lambda_j \geq 0.$$

For any $x \in \mathbb{C}^n$, let

$$z = Q^*x.$$

Then

$$x^*Ax = x^*Q\Lambda Q^*x = z^*\Lambda z.$$

Thus

$$x^*Ax = \sum_{j=1}^{n} \lambda_j |z_j|^2 \geq 0.$$

Therefore,

$$A \succeq 0.$$

□

Similarly, we obtain the following characterization.

Theorem 1.3. *Let $A \in \mathbb{C}^{n\times n}$ be Hermitian. Then*

$$A \succ 0$$

if and only if every eigenvalue of A is strictly positive.

1.3 Why A^*A is Positive Semidefinite

Let

$$A \in \mathbb{C}^{m\times n}.$$

Then

$$A^*A \in \mathbb{C}^{n\times n}$$

is Hermitian.

Moreover, for any $x \in \mathbb{C}^n$,

$$x^*A^*Ax = (Ax)^*(Ax) = \|Ax\|_2^2 \geq 0.$$

Therefore,

Theorem 1.4. *For every matrix $A \in \mathbb{C}^{m\times n}$,*

$$A^*A \succeq 0.$$

Similarly,

$$AA^* \succeq 0.$$

This gives another way to understand why all eigenvalues of A^*A and AA^* are nonnegative.

1.4 When is A^*A Positive Definite?

The matrix A^*A is always positive semidefinite, but it is not always positive definite.

Indeed,

$$x^*A^*Ax = \|Ax\|_2^2.$$

Therefore,

$$x^*A^*Ax = 0$$

if and only if

$$Ax = 0.$$

Thus we obtain:

Theorem 1.5. *Let $A \in \mathbb{C}^{m\times n}$. Then*

$$A^*A \succ 0$$

if and only if

$$\mathcal{N}(A) = \{0\}.$$

Equivalently,

$$A^*A \succ 0$$

if and only if the columns of A are linearly independent.

Proof. We have

$$x^*A^*Ax = \|Ax\|_2^2.$$

Therefore,

$$x^*A^*Ax > 0 \qquad \text{for every } x \neq 0$$

if and only if

$$Ax \neq 0 \qquad \text{for every } x \neq 0.$$

This is equivalent to

$$\mathcal{N}(A) = \{0\},$$

which is equivalent to the columns of A being linearly independent. □

This result explains why, in least squares, the normal equations

$$A^*A\widehat{x} = A^*b$$

have a unique solution whenever A has linearly independent columns.

1.5 Square Root of a Positive Semidefinite Matrix

Let $A \succeq 0$ and write

$$A = Q\Lambda Q^*,$$

where

$$\Lambda = \operatorname{diag}(\lambda_1, \ldots, \lambda_n), \qquad \lambda_j \geq 0.$$

Define

$$\Lambda^{1/2} = \operatorname{diag}\left(\sqrt{\lambda_1}, \ldots, \sqrt{\lambda_n}\right).$$

Then define

$$A^{1/2} = Q\Lambda^{1/2}Q^*.$$

We have

$$A^{1/2}A^{1/2} = Q\Lambda^{1/2}Q^*Q\Lambda^{1/2}Q^* = Q\Lambda Q^* = A.$$

Thus every positive semidefinite matrix has a Hermitian positive semidefinite square root.

2 Cholesky Decomposition, Trace, and Determinant

2.1 From the PSD Square Root to Cholesky

Recall that if $A \in \mathbb{C}^{n\times n}$ is positive semidefinite, then

$$A^{1/2} = Q\Lambda^{1/2}Q^*$$

is Hermitian and satisfies

$$A^{1/2}A^{1/2} = A.$$

If A is positive definite, then $A^{1/2}$ has full rank.

Theorem 2.1 (Cholesky Decomposition)**.** *Let $A \in \mathbb{C}^{n\times n}$ be positive definite. Then there exists a lower triangular matrix $L \in \mathbb{C}^{n\times n}$ with positive real diagonal entries such that*

$$\boxed{A = LL^*.}$$

Proof. Let

$$B = A^{1/2}.$$

Since A is positive definite, B has full rank. Take a QR decomposition

$$B = QR,$$

where Q is unitary and R is upper triangular with positive real diagonal entries. Since $B = B^*$,

$$A = B^*B = (QR)^*(QR) = R^*Q^*QR = R^*R.$$

Let $L = R^*$. Then L is lower triangular with positive real diagonal entries and

$$A = LL^*.$$

□

Example 2.2. *Consider*

$$A = \begin{pmatrix} 4 & 2 \\ 2 & 5 \end{pmatrix}.$$

Seek

$$L = \begin{pmatrix} \ell_{11} & 0 \\ \ell_{21} & \ell_{22} \end{pmatrix}$$

such that $A = LL^T$. Since

$$LL^T = \begin{pmatrix} \ell_{11}^2 & \ell_{11}\ell_{21} \\ \ell_{11}\ell_{21} & \ell_{21}^2 + \ell_{22}^2 \end{pmatrix},$$

matching entries gives

$$\ell_{11} = 2, \qquad \ell_{21} = 1, \qquad \ell_{22} = 2.$$

Hence

$$\boxed{A = \begin{pmatrix} 2 & 0 \\ 1 & 2 \end{pmatrix}\begin{pmatrix} 2 & 1 \\ 0 & 2 \end{pmatrix}.}$$

If $A = LL^*$, then solving $Ax = b$ reduces to two triangular systems:

$$Ly = b, \qquad L^*x = y.$$