Numerical Analysis

Grinshpan

Positive definite and positive semidefinite matrices

Let A be a matrix with real entries. We say that A is positive semidefinite if, for any vector x with real components, the dot product of Ax and x is nonnegative,

$$\langle Ax, x \rangle \geq 0.$$

In geometric terms, the condition of positive semidefiniteness says that, for every x, the angle between x and Ax does not exceed $\frac{\pi}{2}$. Indeed, $\langle Ax, x \rangle = \|Ax\| \; \|x\| \; \cos\theta$ and so $\cos\theta \geq 0$.

EXAMPLE 1. Let $A = \left(\begin{smallmatrix} 1 & 0 \\ 0 & 2 \end{smallmatrix}\right)$. Then $Ax = \left(\begin{smallmatrix} x_1 \\ 2x_2 \end{smallmatrix}\right)$, $\langle Ax, x \rangle = x_1^2 + 2x_2^2 \geq 0$ implying that A is positive semidefinite.

EXAMPLE 2. Let $A = \left(\begin{smallmatrix} 1 & 1 \\ 1 & 1 \end{smallmatrix}\right)$. Then $Ax = \left(\begin{smallmatrix} x_1+x_2 \\ x_1+x_2 \end{smallmatrix}\right)$ and $\langle Ax, x \rangle = (x_1 + x_2)^2 \geq 0$ implying that A is positive semidefinite.

EXAMPLE 3. Let $A = \left(\begin{smallmatrix} 1 & 2 \\ -2 & 1 \end{smallmatrix}\right)$. Then $Ax = \left(\begin{smallmatrix} x_1+2x_2 \\ -2x_1+x_2 \end{smallmatrix}\right)$ and $\langle Ax, x \rangle = x_1^2 + x_2^2 \geq 0$ implying that A is positive semidefinite.

EXAMPLE 4. Let $A = \left(\begin{smallmatrix} 1 & 2 \\ -2 & -1 \end{smallmatrix}\right)$. Then $\langle Ax, x \rangle = x_1^2 - x_2^2$ is not nonnegative for $|x_1| < |x_2|$. Hence A is not positive semidefinite.

A symmetric matrix is positive semidefinite if and only if its eigenvalues are nonnegative.

EXERCISE. Show that if A is positive semidefinite then every diagonal entry of A must be nonnegative.

A real matrix A is said to be positive definite if

$$\langle Ax, x \rangle > 0,$$

unless x is the zero vector. Examples 1 and 3 are examples of positive definite matrices. The matrix in Example 2 is not positive definite because $\langle Ax, x \rangle$ can be 0 for nonzero x (e.g., for $x = \left(\begin{smallmatrix} -3 \\ 3 \end{smallmatrix}\right)$). A symmetric matrix is positive definite if and only if its eigenvalues are positive.

The Cholesky Decomposition

Theorem. Every symmetric positive definite matrix A has a unique factorization of the form

$$A = LL^t,$$

where L is a lower triangular matrix with positive diagonal entries.

L is called the (lower) Cholesky factor of A.

We will use induction on n, the size of A, to prove the theorem.

Case $n = 1$ is trivial: $A = (a)$, $a > 0$, and $L = (\sqrt{a})$. There is only one way to write a as a product of two equal positive numbers.

Case $n = 2$ is the heart of the matter. Let $A = \left(\begin{smallmatrix} a & b \\ b & d \end{smallmatrix}\right)$ be positive definite and form a 2×2 matrix $L = \left(\begin{smallmatrix} \lambda & 0 \\ x & \delta \end{smallmatrix}\right)$. Then the equation $LL^t = \left(\begin{smallmatrix} \lambda & 0 \\ x & \delta \end{smallmatrix}\right)\left(\begin{smallmatrix} \lambda & x \\ 0 & \delta \end{smallmatrix}\right) = \left(\begin{smallmatrix} \lambda^2 & \lambda x \\ \lambda x & x^2+\delta^2 \end{smallmatrix}\right) = A$ is equivalent to

$$\begin{aligned} \lambda^2 &= a \\ \lambda x &= b \\ x^2 + \delta^2 &= d. \end{aligned}$$

Solving for λ, x, and δ,

$$\begin{aligned} \lambda &= \sqrt{a} \\ x &= \lambda^{-1} b \\ \delta &= \sqrt{d - x^2}, \end{aligned}$$

we obtain the desired lower triangular L. But why are a and $d - x^2$ positive? This is a consequence of positive definiteness:

$$\begin{aligned} &\langle \left(\begin{smallmatrix} a & b \\ b & d \end{smallmatrix}\right)\left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right), \left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right) \rangle = \langle \left(\begin{smallmatrix} a \\ b \end{smallmatrix}\right), \left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right) \rangle = a > 0 \\ &\langle \left(\begin{smallmatrix} a & b \\ b & d \end{smallmatrix}\right)\left(\begin{smallmatrix} b \\ -a \end{smallmatrix}\right), \left(\begin{smallmatrix} b \\ -a \end{smallmatrix}\right) \rangle = \langle \left(\begin{smallmatrix} 0 \\ b^2 - ad \end{smallmatrix}\right), \left(\begin{smallmatrix} b \\ -a \end{smallmatrix}\right) \rangle = a^2(d - x^2) > 0. \end{aligned}$$

This justifies the construction.

We need a lemma generalizing the preceding calculation.

Lemma. Let Q be nonsingular, x be a column vector, d be a number, and let $A = \left(\begin{smallmatrix} QQ^t & Qx \\ (Qx)^t & d \end{smallmatrix}\right)$ be positive definite. Then $\|x\|^2 < d$.

Proof. Let $u = \left(\begin{smallmatrix} Q^{-t}x \\ -1 \end{smallmatrix}\right)$. [1] Then $Au = \left(\begin{smallmatrix} 0 \\ \|x\|^2 - d \end{smallmatrix}\right)$ because

$$\begin{aligned} QQ^tQ^{-t}x - Qx &= Qx - Qx = 0 \\ (Qx)^tQ^{-t}x &= x^tQ^tQ^{-t}x = x^tx = \|x\|^2. \end{aligned}$$

---

[1] Q^{-t} is the inverse transpose of Q, $Q^{-t} = (Q^t)^{-1} = (Q^{-1})^t$.

Consequently $\langle Au, u\rangle = -\|x\|^2 + d > 0$. □

Back to the theorem.

Induction.

Assume that the theorem holds for all matrices of size $m \times m$. The induction step from $n = m$ to $n = m+1$ is analogous to the case of $n = 2$. Let $A = \left(\begin{smallmatrix} \tilde{A} & b \\ b^t & d \end{smallmatrix}\right)$, where $\tilde{A}$ is the $m \times m$ principal submatrix of A, b is the m-vector $(a_{i,m+1})$, and $d = a_{m+1,m+1}$. By the inductive hypothesis, there exists a unique $m \times m$ lower triangular matrix Q with positive diagonal entries (hence nonsingular) such that $QQ^t = \tilde{A}$.

Form an $(m+1) \times (m+1)$ lower triangular matrix $L = \left(\begin{smallmatrix} Q & 0 \\ x^t & \delta \end{smallmatrix}\right)$. Then the equation $LL^t = \left(\begin{smallmatrix} Q & 0 \\ x^t & \delta \end{smallmatrix}\right)\left(\begin{smallmatrix} Q^t & x \\ 0 & \delta \end{smallmatrix}\right) = \left(\begin{smallmatrix} QQ^t & Qx \\ (Qx)^t & \|x\|^2+\delta^2 \end{smallmatrix}\right) = A$ is equivalent to

$$\begin{aligned} QQ^t &= \tilde{A} \\ Qx &= b \\ \|x\|^2 + \delta^2 &= d. \end{aligned}$$

Letting

$$\begin{aligned} x &= Q^{-1}b \\ \delta &= \sqrt{d - \|x\|^2} \qquad\qquad (\delta \text{ exists by Lemma}) \end{aligned}$$

we obtain the desired lower triangular L. □

The inductive construction of the proof can be turned into an algorithm.

Example. $A = \left(\begin{smallmatrix} 4 & 1 & -1 \\ 1 & 2 & 1 \\ -1 & 1 & 2 \end{smallmatrix}\right)$ is a symmetric positive definite matrix. Retracing the computation of the proof, we can find its lower Cholesky factor:

$$L = \left(\begin{smallmatrix} 2 & 0 & 0 \\ * & * & 0 \\ * & * & * \end{smallmatrix}\right) = \begin{pmatrix} 2 & 0 & 0 \\ \frac{1}{2} & \frac{\sqrt{7}}{2} & 0 \\ * & * & * \end{pmatrix} = \begin{pmatrix} 2 & 0 & 0 \\ \frac{1}{2} & \frac{\sqrt{7}}{2} & 0 \\ -\frac{1}{2} & \frac{5}{2\sqrt{7}} & \sqrt{\frac{6}{7}} \end{pmatrix}.$$

Certainly, A is positive semidefinite whenever $A = LL^t$. Cholesky factors for a positive semidefinite matrix always exist with a nonnegative diagonal. However they may not be unique.

Zero matrix has a unique Cholesky decomposition. $\left(\begin{smallmatrix} 0 & 0 \\ 0 & 1 \end{smallmatrix}\right)$ has infinitely many Cholesky decompositions:

$$\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ \sin\theta & \cos\theta \end{pmatrix}\begin{pmatrix} 0 & \sin\theta \\ 0 & \cos\theta \end{pmatrix}.$$

In general, a triangular factorization does not always exist. For instance, $\left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$ cannot be written as a product of two triangular matrices.