Section 5.9. Factorizations of Nonnegative Definite Matrices

Note. We address the square root of a symmetric nonnegative definite matrix again and define the Cholesky factorization.

Note. Recall from Theorem 3.8.15 that for symmetric positive definite matrix A there is orthogonal V and nonnegative definite S such that $(VSV^T)^2 = A$. Matrix VSV^T is the square root of A, denoted $A^{1/2}$. We have not yet established the uniqueness of $A^{1/2}$ and we do so now.

Theorem 5.9.1. Let A be a symmetric nonnegative definite matrix and let B be a symmetric nonnegative definite matrix such that $B^2 = A$. Then $B = VC^{1/2}V^T = VSV^T$ where $S = C^{1/2} = \text{diag}(c_1^{1/2}, c_2^{1/2}, \ldots, c_n^{1/2})$ where $c_1, c_2, \ldots, c_n$ are the eigenvalues of A and V is orthogonal.

Definition. Let A be a symmetric positive definite matrix. If $A = T^TT$ where T is an upper triangular matrix with positive diagonal entries, then $A = T^TT$ is a *Cholesky factorization* of A.

Note. The following two theorems, Theorem 5.9.2 and Theorem 5.9.A, on Cholesky factorizations are based on Markus Garsmair's online document On the Existence of a Cholesky Factorization (accessed 4/25/2020).

Theorem 5.9.2. If A is a symmetric positive definite matrix, then A has a Cholesky factorization.

Note. Gentle gives an algorithm to calculate matrix T in the Cholesky factorization of symmetric positive definite $n \times n$ matrix A as follows. We let $T = [t_{ij}]$ be the $n \times n$ upper triangular matrix with entries defined recursively as follows:

Define $t_{11} = \sqrt{a_{11}}$.

Define $t_{1j} = a_{1j}/t_{11}$ for $j = 2, 3, \ldots, n$ (notice that A is positive definite so $a_{11} \neq 0$ and $t_{11} \neq 0$).

Define $t_{ii} = \left(a_{ii} - \sum_{k=1}^{i-1} t_{ki}^2\right)^{1/2}$ for $i = 1, 2, 3, \ldots, n$.

Define $t_{ij} = \left(a_{ij} - \sum_{k=1}^{i-1} t_{ki}t_{kj}\right)\Big/\, t_{ii}$ for $i = 2, 3, \ldots, n$ and $j = i+1, i+2, \ldots, n$.

Define all other t_{ij} as 0 (so T is upper triangular).

Note. For an invertible matrix A, the converse of Theorem 5.9.2 holds, as follows.

Theorem 5.9.A. An invertible matrix A has a Cholesky factorization if and only if A is symmetric and positive definite.

Note. In Exercise 5.9.B, it is to be shown that the Cholesky factorization of a symmetric positive definite matrix is unique.

Note. We now make a few observations about the Grammian matrix X^TX.

Note. X^TX is symmetric, so by Theorem 3.8.A is orthogonally diagonalizable: $X^TX = VCV^T$ where V is orthogonal (notice Theorem 3.7.1, $V^{-1} = V^T$).

Note. If X has a QR factorization (where Q is orthogonal and R is upper triangular with positive diagonal entries), which is the case if X is full column rank by Theorem 5.7.C, then $X^TX = (QR)^TQR = R^TQ^TQR = R^TR$, since $Q^TQ = \mathcal{I}$ because Q is orthogonal (by Theorem 3.7.1). So X^TX has the Cholesky factorization R^TR.

Note. Every matrix has a singular value decomposition by Theorem 3.8.16, so $X = UDV^T$ where U and V are orthogonal and D is diagonal. So

$$\begin{aligned} X^TX &= (UDV^T)^T(UDV^T) = VD^TU^TUDV^T \\ &= VD^TDV^T \text{ since } U \text{ is orthogonal (Theorem 3.7.1)} \end{aligned}$$

and $X^TX = (DV^T)^T(DV^T)$. Now D^TD is diagonal, so $X^TX = V(D^TD)V^T$ is an orthogonal diagonalization of the Grammian matrix X^TX. By Theorem 3.8.7(4), the real eigenvalues of X^TX are the squares of the eigenvalues of X.