Department of Mathematics, University of Utah

Analysis of Numerical Methods I

MTH6610 – Section 001 – Fall 2017

Lecture notes – Cholesky Decompositions

Friday, October 18, 2019

These notes are not a substitute for class attendance. Their main purpose is to provide a lecture overview summarizing the topics covered.

Reading: Trefethen & Bau III, Lectures 23

Let $A \in \mathbb{C}^{n\times n}$. Such a square matrix is Hermitian positive definite if it is both Hermitian, and if

$$x^* A x > 0, \qquad\qquad x \neq 0. \tag{1}$$

This is a very strong condition, and implies that the matrix is invertible, has real and positive eigenvalues, and is unitarily diagonalizable. By selecting $x = e_j$ for $j = 1, \ldots, n$, we also see that the diagonal elements of A must be real and positive.
The process of LU factorizations simplifies considerably when we have a Hermitian positive-definite matrix. Suppose we start with the Hermitian positive definite matrix

$$A = \begin{pmatrix} a & — & v^* & — \\ | & & & \\ v & & A_2 & \\ | & & & \end{pmatrix}, \qquad\qquad v \in \mathbb{C}^{n-1},$$

where the $(n-1)\times(n-1)$ matrix A_2 must also be Hermitian positive definite. (In condition (3), take $x \in \mathbb{C}^n$ as any vector whose first entry vanishes.) Since $a > 0$, then we can perform Gaussian elimination, seeking to eliminate the vector v:

$$A = \underbrace{\begin{pmatrix} 1 & — & 0 & — \\ | & & & \\ \frac{v}{a} & & I & \\ | & & & \end{pmatrix}}_{L_1} \underbrace{\begin{pmatrix} a & — & v^* & — \\ | & & & \\ 0 & & A_2 - \frac{vv^*}{a} & \\ | & & & \end{pmatrix}}_{B^*} \tag{2a}$$

We have defined the matrix B^*, so that

$$B = \begin{pmatrix} a & — & 0 & — \\ | & & & \\ v & & A_2 - \frac{vv^*}{a} & \\ | & & & \end{pmatrix}$$

One could again consider performing one LU decomposition step to eliminate the vector v in the first column of B:

$$B = \begin{pmatrix} 1 & — & 0 & — \\ | & & & \\ \frac{v}{a} & & I & \\ | & & & \end{pmatrix} \begin{pmatrix} a & — & 0 & — \\ | & & & \\ 0 & & A_2 - \frac{vv^*}{a} & \\ | & & & \end{pmatrix} \tag{2b}$$

By combining the relations (2), we have shown that

$$A = \begin{pmatrix} 1 & — & 0 & — \\ | & & & \\ \frac{v}{a} & & I & \\ | & & & \end{pmatrix} \begin{pmatrix} a & — & 0 & — \\ | & & & \\ 0 & & A_2 - \frac{vv^*}{a} & \\ | & & & \end{pmatrix} \begin{pmatrix} 1 & — & \frac{v^*}{a} & — \\ | & & & \\ 0 & & I & \\ | & & & \end{pmatrix}.$$

Finally, we factor out a $\sqrt{a}$ from the (1,1) entry in the middle matrix, and notice that the first and third matrices are Hermitian conjugates:

$$A = \begin{pmatrix} \sqrt{a} & — & 0 & — \\ | & & & \\ \frac{v}{\sqrt{a}} & & I & \\ | & & & \end{pmatrix} \begin{pmatrix} 1 & — & 0 & — \\ | & & & \\ 0 & & A_2 - \frac{vv^*}{a} & \\ | & & & \end{pmatrix} \begin{pmatrix} \sqrt{a} & — & 0 & — \\ | & & & \\ \frac{v}{\sqrt{a}} & & I & \\ | & & & \end{pmatrix}$$

We can define the first matrix on the right-hand side as L_1. Now note that the middle matrix is again a Hermitian positive-definite matrix. (Positive-definite since A was positive-definite and L_1 is invertible.) Therefore, the (1,1) entry of the submatrix $A_2 - \frac{vv^*}{a}$ is also positive, and we may repeat our symmetric LU procedure iteratively. The result is that we can perform the decompsition

$$A = (L_1 L_2 \cdots L_{n-1})(L_1 L_2 \cdots L_{n-1})^* =: LL^*$$

I.e., we have shown that Hermitian positive-definite matrices have a symmetric LU factorization. This is called the Cholesky factorization. In fact, we have existence and uniqueness:

Theorem 1. *If A is a Hermitian positive-definite matrix, then it has a unique Cholesky factorization $A = LL^*$.*

If A is only positive *semi*-definite, i.e., if

$$x^* A x \geq 0, \qquad x \neq 0, \tag{3}$$

then the Cholesky procedure may fail since the (1,1) entry may be zero. However, if one is willing to allow zeros on the diagonal of L and allows pivoting, then such a factorization is still possible:

Theorem 2. *If A is a Hermite positive semi-definite matrix, then it has a pivoted Cholesky factorization $A = PLL^*P^*$, where P is a permutation matrix, and L may have zeros on its diagonal. Such a factorization is in general not unique.*