

The Cholesky Factorization

What if, instead of factoring A into two matrices L and U , we could factor it into the product of one triangular matrix? That is, when does $A = R^T R$ for some upper-triangular matrix R ? Such a factorization is called a *Cholesky* factorization

Definition 1. An $n \times n$ matrix A is *symmetric* if $A^T = A$.

Example 1. Give an example of 2×2 matrix that is symmetric.

Question 2. Suppose $A = R^T R$. Is A symmetric?

So in order to have a Cholesky factorization, it is *necessary* that A be symmetric. This is not sufficient; here's an example that we will later see does not have one:

$$\begin{bmatrix} 1 & 3 \\ 3 & 1 \end{bmatrix}.$$

There's a second property of matrices that, combined with symmetry, will guarantee the existence of a Cholesky factorization.

Definition 3. An $n \times n$ matrix A is *positive definite* if $\mathbf{x}^T A \mathbf{x} > 0$ for all vectors $\mathbf{x} \neq 0$.

Example 2. Let $A = \begin{bmatrix} 1 & 3 \\ 3 & 1 \end{bmatrix}$, $\mathbf{x}_1 = \begin{bmatrix} 3 \\ 1 \end{bmatrix}$, and $\mathbf{x}_2 = \begin{bmatrix} -3 \\ 1 \end{bmatrix}$. Compute $\mathbf{x}^T A \mathbf{x}$ for each \mathbf{x} . Is this enough information to determine if A is or is not positive definite?

Example 3. Let $\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$ and $A = \begin{bmatrix} 1 & 3 \\ 3 & 1 \end{bmatrix}$. Find a formula for $\mathbf{x}^T A \mathbf{x}$.

Essentially, the process of showing a matrix is positive definite is exactly the same. If you can write the expression entirely as the (positive) sum of squares, the result is guaranteed to be positive. If you can't, then start experimenting with some numbers that make the expression negative. If you can find even one pair, then the claim that A is positive definite is false.

Example 4. Show that $A_1 = \begin{bmatrix} 2 & 2 \\ 2 & 5 \end{bmatrix}$, $A_2 = \begin{bmatrix} 1 & -1 & 0 \\ -1 & 5 & 4 \\ 0 & 4 & 8 \end{bmatrix}$, and $A_3 = \begin{bmatrix} 1 & -1 & 0 \\ -1 & 5 & 6 \\ 0 & 2 & 8 \end{bmatrix}$ are positive definite. Which ones are symmetric positive definite?

Some theory regarding positive definite matrices.

Theorem 4. *All symmetric positive definite matrices are invertible.*

Which also means that $A\mathbf{x} = \mathbf{b}$ has a unique solution for all \mathbf{b} , and that A has linearly independent columns, 0 is not an eigenvalue, etc. etc.

Theorem 5. *If the $n \times n$ matrix A is symmetric, then A is positive definite if and only if all of its eigenvalues are positive.*

We haven't touched on eigenvalues yet, other than mentioning that they also can only be found iteratively. That means that while this theorem is nice theoretically, it's not particularly helpful if a computer is trying to determine if A is symmetric positive definite.

Definition 6. A *principal submatrix* of a square matrix A is a square submatrix whose diagonal entries are diagonal entries of A .

Example 5. List the principal submatrices of $A = \begin{bmatrix} 1 & -1 & 0 \\ -1 & 5 & 4 \\ 0 & 4 & 8 \end{bmatrix}$.

Theorem 7. *If A is symmetric positive definite, then so are all its principle submatrices.*

Theorem 8. *If A is a square symmetric positive definite matrix, then there exists an upper triangular matrix such that $A = R^T R$.*

Cholesky Factorization

We compute the factorization by going along the diagonal. Let A be represented as

$$\left[\begin{array}{c|c} a & \mathbf{b}^T \\ \hline \mathbf{b} & C \end{array} \right]$$

1. First, update the diagonal element a . The square root of a goes into R . **

$$R = \left[\begin{array}{c|c} \sqrt{a} & \mathbf{b}^T \\ \hline \mathbf{0} & C \end{array} \right]$$

2. Next we update the vector \mathbf{b} by also scaling it with \sqrt{a} . Let $\mathbf{u} = \frac{1}{\sqrt{a}}\mathbf{b}$. Then we have

$$R = \left[\begin{array}{c|c} \sqrt{a} & \mathbf{u}^T \\ \hline \mathbf{0} & C \end{array} \right]$$

3. Finally we update the submatrix C . The new submatrix D is:

$$D = C - \mathbf{u}\mathbf{u}^T$$

so that R is now

$$R = \left[\begin{array}{c|c} \sqrt{a} & \mathbf{u}^T \\ \hline \mathbf{0} & D \end{array} \right]$$

4. Repeat steps 1-3 on the submatrix D until no submatrix remains.

** If at any point the diagonal element a is negative, then the matrix is not symmetric positive definite. This is actually the most efficient way for a computer to check if a matrix is symmetric positive definite - just start computing a Cholesky factorization. If it works, great! The matrix is positive definite. If at any point the first step of the factorization fails, then A is not symmetric positive definite.

Example 6. Find a Cholesky factor of $\begin{bmatrix} 1 & -1 & 0 \\ -1 & 5 & 4 \\ 0 & 4 & 8 \end{bmatrix}$.

Example 7. Find a Cholesky factor of $A = \begin{bmatrix} 2 & 2 \\ 2 & 5 \end{bmatrix}$.

Example 8. Find a Cholesky factor of $A = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 2 & 2 \\ 1 & 2 & 3 \end{bmatrix}$.

Question 9. Compare and contrast an $R^T R$ factorization verses an LU factorization.

Both could be used to solve $A\mathbf{x} = \mathbf{b}$ through back substitution. One advantage is saving storage space - we only have to store one matrix instead of two.

How about speed? With about half as many elements, it also works out to be about half as many operations as LU at $\frac{n^3}{3}$.