THE LDL^T AND CHOLESKY DECOMPOSITIONS

The LDL^T decomposition $\binom{1}{2}$ is a variant of the LU decomposition that is valid for positive-definite symmetric matrices; the Cholesky decomposition is a variant of the LDL^T decomposition.

Theorem. *Let S be a positive-definite symmetric matrix. Then S has unique decompositions*

$$S = LDL^T \quad \text{and} \quad S = L_1 L_1^T$$

where:

- *L is lower-unitriangular,*
- *D is diagonal with positive diagonal entries, and*
- *L_1 is lower-triangular with positive diagonal entries.*

See later in this note for an efficient way to compute an LDL^T decomposition (by hand or by computer) and an example.

Remark. Any matrix admitting either decomposition is symmetric positive-definite by Problem 13(a) on Homework 11.

Remark. Since L_1^T has full column rank, taking $A = L_1^T$ shows that any positive-definite symmetric matrix S has the form $A^T A$.

Remark. Suppose that S has an LDL^T decomposition with

$$D = \begin{pmatrix} d_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & d_n \end{pmatrix}.$$

Then we define

$$\sqrt{D} = \begin{pmatrix} \sqrt{d_1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \sqrt{d_n} \end{pmatrix},$$

so that $(\sqrt{D})^2 = D$, and we set $L_1 = L\sqrt{D}$. Then

$$L_1 L_1^T = L(\sqrt{D})(\sqrt{D})^T L^T = LDL^T = S,$$

so $L_1 L_1^T$ is the Cholesky decomposition of S.

Conversely, given a Cholesky decomposition $S = L_1 L_1^T$, we can write $L_1 = LD'$, where D' is the diagonal matrix with the same diagonal entries as L_1; then $L = L_1 D'^{-1}$ is the lower-unitriangular matrix obtained from L_1 by dividing each column by its diagonal entry. Setting $D = D'^2$, we have

$$S = (LD')(LD')^T = LD'^2 L^T = LDL^T,$$

which is the LDL^T decomposition of S.

Since the LDL^T decomposition and the Cholesky decompositions are interchangeable, we will focus on the former.

Remark. The matrix $U = DL^T$ is upper-triangular with positive diagonal entries. In particular, it is in row echelon form, so $S = LU$ is the LU decomposition of S. This gives another way to interpret the Theorem: it says that every positive-definite symmetric matrix S has an LU decomposition (no row swaps are needed); moreover, U has positive diagonal entries, and if D is the diagonal matrix with the same diagonal entries as U, then $L^T = D^{-1}U$ (dividing each row of U by its pivot gives L^T).

This shows that one can easily compute an LDL^T decomposition from an LU decomposition: use the same L, and let D be the diagonal matrix with the same diagonal entries as U. However, we will see that one can compute LDL^T twice as fast as LU, by hand or by computer: see the end of this note.

Proof that the LDL^T decomposition exists and is unique. The idea is to do row *and* column operations on S to preserve symmetry in elimination. Suppose that E is an elementary matrix for a row replacement, say

$$R_2 \mathrel{-}= 2R_1: \qquad E = \begin{pmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Then EA performs the row operation $R_2 \mathrel{-}= 2R_1$ on a 3×3 matrix A. On the other hand, AE^T performs the corresponding *column* operation $C_2 \mathrel{-}= 2C_1$: indeed, taking transposes, we have $(AE^T)^T = EA^T$, which performs $R_2 \mathrel{-}= 2R_1$ on A^T.

Starting with a positive-definite symmetric matrix S, first we note that the $(1,1)$-entry of S is positive: this is Problem 14(a) on Homework 11. Hence we can do row replacements (and no row swaps) to eliminate the last $n-1$ entries in the first column. Multiplying the corresponding elementary matrices together gives us a lower-unitriangular matrix L_1 such that the last $n-1$ entries of the first column of L_1S are zero. Multiplying L_1S by L_1^T on the right performs the same sequence of column operations; since S was symmetric, this has the effect of clearing the last $n-1$ entries of the first *row* of S. In diagrams:

$$S = \begin{pmatrix} a & b & c \\ b & * & * \\ c & * & * \end{pmatrix} \qquad L_1 = \begin{pmatrix} 1 & 0 & 0 \\ -b/a & 1 & 0 \\ -c/a & 0 & 1 \end{pmatrix}$$

$$L_1S = \begin{pmatrix} a & b & c \\ 0 & * & * \\ 0 & * & * \end{pmatrix} \qquad L_1SL_1^T = \begin{pmatrix} a & 0 & 0 \\ 0 & * & * \\ 0 & * & * \end{pmatrix}$$

Since S is symmetric, the matrix $S_1 = L_1SL_1^T$ is symmetric, and since S is positive-definite, the matrix S_1 is also positive-definite by Problem 13(a) on Homework 11. In particular, the $(2,2)$-entry of S_1 is nonzero, so we can eliminate the second column and the second row in the same way. We end up with another positive-definite symmetric matrix $S_2 = L_2S_1L_2^T = (L_2L_1)S(L_2L_1)^T$ where the only nonzero entries in the first two rows/columns are the diagonal ones. Continuing in this way, we eventually get a diagonal matrix $D = S_{n-1} = (L_{n-1} \cdots L_1)S(L_{n-1} \cdots L_1)^T$ with positive diagonal entries. Setting $L = (L_{n-1} \cdots L_1)^{-1}$ gives $S = LDL^T$.

As for uniqueness,[1] suppose that $S = LDL^T = L'D'L'^T$. Multiplying on the left by L'^{-1} gives $L'^{-1}LDL^T = D'L'^T$, and multiplying on the right by $(DL^T)^{-1}$ gives

$$L'^{-1}L = (D'L'^T)(DL^T)^{-1}.$$

The left side is lower-unitriangular and the right side is upper-triangular. The only matrix that is both lower-unitriangular and upper-triangular is the identity matrix. It follows that $L'^{-1}L = I_n$, so $L' = L$. Then we have $(D'L'^T)(DL^T)^{-1} = I_n$, so $D'L^T = DL^T$ (using $L' = L$), and hence $D' = D$ (because L is invertible). □

Remark (For experts). In abstract linear algebra, the expression $\langle x, y\rangle = x^T S y$ is called an *inner product*. This is a generalization of the usual dot product: $\langle x, y\rangle = x \cdot y$ when $S = I_n$. When S is positive-definite, one can run the Gram–Schmidt algorithm to turn the usual basis $\{e_1, \ldots, e_n\}$ of $\mathbf{R}^n$ into a basis $\{v_1, \ldots, v_n\}$ which is orthogonal with respect to $\langle \cdot, \cdot \rangle$. The corresponding change-of-basis matrix is a lower-unitriangular matrix L', and the matrix for $\langle \cdot, \cdot \rangle$ with respect to the orthogonal basis is a diagonal matrix D. This means $L'DL'^T = S$, so taking $L = L'^{-1}$, we have $S = LDL^T$.

Upshot: the LDL^T decomposition is exactly Gram–Schmidt as applied to the inner product $\langle x, y\rangle = x^T S y$.

Computational Complexity. The algorithm in the above proof appears to be the same as LU: the matrix $L = (L_{n-1} \cdots L_1)^{-1}$ is exactly what one would compute in an LU decomposition of an arbitrary matrix. However, one can save compute cycles by taking advantage of the symmetry of S.

In an ordinary LU decomposition, when clearing the first column, each row replacement involves $n-1$ multiplications (scale the first row) and $n-1$ additions (add to the ith row), for $2(n-1)$ floating point operations (flops). Hence it takes $2(n-1)^2$ flops to clear the first column. Clearing the second column requires $2(n-2)^2$ flops, and so on, for a total of

$$2\big((n-1)^2 + (n-2)^2 + \cdots + 1\big) = 2\frac{n(n-1)(2n-1)}{6} \approx \frac{2}{3}n^3$$

flops. However, when clearing the first row and column of a symmetric positive-definite matrix S, one only needs to compute the entries of $L_1 S L_1^T$ *on or above the diagonal*; the others are determined by symmetry. The first row replacement (the one that clears the $(2,1)$-entry) still needs $n-1$ multiplications and $n-1$ additions, but the second only needs $n-2$ multiplications and $n-2$ additions (because we don't need to compute the $(3,2)$-entry), and so on, for a total of

$$2\big((n-1) + (n-2) + \cdots + 1\big) = 2\frac{n(n-1)}{2} = n^2 - n$$

[1]What follows is essentially the same proof that the LU decomposition is unique for an invertible matrix.

flops to clear the first column. Clearing the second column requires $(n-1)^2-(n-1)$ flops, and so on, for a total of

$$\begin{aligned}\big(n^2-n\big)+&\big((n-1)^2-(n-1)\big)+\cdots+\big(1^2-1\big)\\ &=\big(n^2+(n-1)^2+\cdots+1\big)-\big(n+(n-1)+\cdots+1\big)\\ &=\frac{n(n+1)(2n+1)}{6}-\frac{n(n+1)}{2}\approx\frac{1}{3}n^3\end{aligned}$$

flops: half what was required for a full LU decomposition!

An Algorithm. The above discussion tells us how to modify the LU algorithm to compute the LDL^T decomposition. We use the two-column method as for an LU decomposition, but instead of keeping track of $L_1S, L_2L_1S, \ldots$ in the right column, we keep track of the *symmetric* matrices $S_1 = L_1SL_1^T$, $S_2 = L_2L_1S(L_2L_1)^T, \ldots$, for which we only have to compute the entries on or above the diagonal. Instead of ending up with the matrix U in the right column, we end up with D.

Very explicitly: to compute $S_1 = L_1SL_1^T$ from S, first do row operations to eliminate the entries below the first pivot, then do column operations to eliminate the entries to the right of the first pivot; since the entries below the first pivot are zero after doing the row operations, this only changes entries in the first row. We end up with a symmetric matrix, so we only need to compute the entries on and above the diagonal. Now clear the second row/column, and continue recursively. Computing L is done the same way as in the LU decomposition, by recording the column divided by the pivot at each step.

Example. Let us compute the LDL^T decomposition of the positive-definite symmetric matrix

$$S = \begin{pmatrix} 2 & 4 & -2 & 2 \\ 4 & 9 & -1 & 6 \\ -2 & -1 & 14 & 13 \\ 2 & 6 & 13 & 35 \end{pmatrix}.$$

The entries in blue came for free by symmetry and didn't need to be calculated; the entries in green come from dividing the column by the pivot, as in the usual LU decomposition.

	L	S_i
start	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ ? & 1 & 0 & 0 \\ ? & ? & 1 & 0 \\ ? & ? & ? & 1 \end{pmatrix}$	$\begin{pmatrix} 2 & 4 & -2 & 2 \\ 4 & 9 & -1 & 6 \\ -2 & -1 & 14 & 13 \\ 2 & 6 & 13 & 35 \end{pmatrix}$
clear first column (then row)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 2 & 1 & 0 & 0 \\ -1 & ? & 1 & 0 \\ 1 & ? & ? & 1 \end{pmatrix}$	$\begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 3 & 2 \\ 0 & 3 & 12 & 15 \\ 0 & 2 & 15 & 33 \end{pmatrix}$
clear second column (then row)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 2 & 1 & 0 & 0 \\ -1 & 3 & 1 & 0 \\ 1 & 2 & ? & 1 \end{pmatrix}$	$\begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 3 & 9 \\ 0 & 0 & 9 & 29 \end{pmatrix}$
clear third column (then row)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 2 & 1 & 0 & 0 \\ -1 & 3 & 1 & 0 \\ 1 & 2 & 3 & 1 \end{pmatrix}$	$\begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}$

Hence $S = LDL^T$ for

$$L = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 2 & 1 & 0 & 0 \\ -1 & 3 & 1 & 0 \\ 1 & 2 & 3 & 1 \end{pmatrix} \qquad D = \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}.$$

The Determinant Criterion We can also use the LDL^T decomposition to prove the determinant criterion that we discussed in class.

Theorem. *A symmetric matrix S is positive-definite if and only if all upper-left determinants are positive.*

Proof. First we show that if S is positive-definite then all upper-left determinants are positive. Let S_1 be an $r \times r$ upper-left submatrix:

$$S = \begin{pmatrix} & & & * \\ & S_1 & & * \\ & & & * \\ * & * & * & * \end{pmatrix}$$

Let $x = (x_1, \ldots, x_r, 0, \ldots, 0)$ be a nonzero vector in $\mathrm{Span}\{e_1, \ldots, e_r\}$. Then $x^T S x$ only depends on S_1:

$$(x_1\ x_2\ x_3\ 0) \begin{pmatrix} & & & * \\ & S_1 & & * \\ & & & * \\ * & * & * & * \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ 0 \end{pmatrix} = (x_1\ x_2\ x_3\ 0) \begin{pmatrix} S_1 \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \\ * \end{pmatrix} = (x_1\ x_2\ x_3) S_1 \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}.$$

Since $x^T S x > 0$, this shows that S_1 is also positive-definite. Hence the eigenvalues of S_1 are positive, so $\det(S_1) > 0$.

We will prove the converse by *induction:* that is, we'll prove it for 1×1 matrices, then for 2×2 matrices using that the 1×1 case is true, then for 3×3 matrices using that the 2×2 case is true, etc. The 1×1 case is easy: it says that the matrix (a) is positive-definite if and only if $\det(a) = a > 0$. Suppose then that we know that an $(n-1) \times (n-1)$ matrix with positive upper-left determinants is positive-definite. Let S be an $n \times n$ matrix with positive upper-left determinants, and let S_1 be the upper-left $(n-1) \times (n-1)$ submatrix of S:

$$S = \begin{pmatrix} & & & a_1 \\ & S_1 & & \vdots \\ & & & a_{n-1} \\ a_1 & \cdots & a_{n-1} & a_n \end{pmatrix}$$

Then we already know that S_1 is positive-definite, so it has an LDL decomposition: say $S_1 = L_1' D_1 L_1'^T$. Taking $L_1 = L_1'^{-1}$, we have $L_1 S_1 L_1^T = D_1$. Let L be the matrix obtained from L_1 by adding the vector e_n to the right and e_n^T to the bottom, and likewise for D and D_1:

$$L = \begin{pmatrix} & & & 0 \\ & L_1 & & \vdots \\ & & & 0 \\ 0 & \cdots & 0 & 1 \end{pmatrix} \qquad D = \begin{pmatrix} & & & 0 \\ & D_1 & & \vdots \\ & & & 0 \\ 0 & \cdots & 0 & 1 \end{pmatrix}.$$

Multiplying out LSL^T and keeping track of which entries are multiplied by which gives

$$LSL^T = \begin{pmatrix} & & & b_1 \\ & L_1 S_1 L_1^T & & \vdots \\ & & & b_{n-1} \\ b_1 & \cdots & b_{n-1} & b_n \end{pmatrix} = \begin{pmatrix} d_1 & & & b_1 \\ & \ddots & & \vdots \\ & & d_{n-1} & b_{n-1} \\ b_1 & \cdots & b_{n-1} & b_n \end{pmatrix},$$

where $d_1, \dots, d_{n-1} > 0$ are the diagonal entries of D_1, $(b_1, \dots, b_{n-1}) = L_1(a_1, \dots, a_{n-1})$, and $b_n = a_n$. Since the d_i are nonzero, we can do $n-1$ row operations $R_n \mathrel{-}= \frac{b_i}{d_i} R_i$ to clear the entries in the last row. Doing the same column operations $C_n \mathrel{-}= \frac{b_i}{d_i} C_i$ clears the entries in the last column as well. Letting E be the product of the (lower-unitriangular) elementary matrices for these row operations, we get

$$E(LSL^T)E^T = \begin{pmatrix} d_1 & & & 0 \\ & \ddots & & 0 \\ & & d_{n-1} & 0 \\ 0 & 0 & 0 & d_n \end{pmatrix}.$$

Note that $\det(E) = \det(L) = \det(L^T) = \det(E^T) = 1$, so $\det(S) = d_1 \cdots d_{n-1} d_n$. Since $\det(S) > 0$ and $d_1, \dots, d_{n-1} > 0$, we have $d_n > 0$ as well. Setting $L_2 = (EL)^{-1}$ and $D_2 = ELSL^T E^T$, this gives $S = L_2 D_2 L_2^T$. Since S has an LDL^T decomposition, it is positive-definite, as desired. □