The Cholesky Factorization
(Numerical Linear Algebra, Spring 2016)

Consider a square matrix $A \in \mathbb{R}^{n\times n}$. The Cholesky factorization (decomposition) is applied to symmetric ($A = A^T$) and positive definite ($\mathrm{eig}(A) > 0$) matrices. Let us denote such matrices as SPD matrices.

For SPD matrices, Gaussian elimination ($A = LU$) can be performed without pivoting. In addition to this, an SPD matrix A can be decomposed in the form $A = LL^T$, where L is a lower-triangular matrix, and $U = L^T$, and, therefore, L and U have the same diagonal entries. $A = LL^T$ is called the Cholesky decomposition (or factorization), and L is called the Cholesky factor.

Remember that we pursue the same goal here: we want to solve $A\mathbf{x} = \mathbf{b}$. If $A = LL^T$, we write $LL^T\mathbf{x} = \mathbf{b}$, and first solve $L\mathbf{y} = \mathbf{b}$ for $\mathbf{y}$, and then $L^T\mathbf{x} = \mathbf{y}$ for $\mathbf{x}$.

Given a SPD matrix A and its LU factorization, you can notice the following: $A = LDD^{-1}U = LDM^T$. Here we have $D = \mathrm{diag}(u_{11}, u_{22}, \dots, u_{nn})$ and $M = D^{-1}U$. Since $A = A^T$, then $LDM^T = MDL^T$ and $A = LDL^T$ (so-called LDL decomposition). Since A is SPD, it can be shown that D has positive entries. Let us rewrite A as follows: $A = LD^{1/2}D^{1/2}L^T = \hat{L}\hat{L}^T$, with $\hat{L} = L \cdot \mathrm{diag}(\sqrt{u_{11}}, \sqrt{u_{22}}, \dots, \sqrt{u_{nn}})$.

Algorithm and Example:

In general, to find the Cholesky factorization, we partition matrices in $A = LL^T$ as

$$A = \begin{pmatrix} a_{11} & A_{21}^T \\ A_{21} & A_{22} \end{pmatrix} = \begin{pmatrix} l_{11} & 0 \\ L_{21} & L_{22} \end{pmatrix} \begin{pmatrix} l_{11} & L_{21}^T \\ 0 & L_{22} \end{pmatrix} = \begin{pmatrix} l_{11}^2 & l_{11}L_{21}^T \\ l_{11}L_{21} & L_{21}L_{21}^T + L_{22}L_{22}^T \end{pmatrix}$$

Step 1. Determine $l_{11} = \sqrt{a_{11}}$ ($a_{11} > 0$ as A is PD) and $L_{21} = \dfrac{1}{l_{11}}A_{21}$.
Step 2. Compute L_{22} from $A_{22} - L_{21}L_{21}^T = L_{22}L_{22}^T$.
This is a Cholesky factorization of order $n-1$. It can be shown that if the algorithm works for $n = k$, it will work for $n = k-1$. If $n = 1$, it obviously works. therefore, it works for all n.

Consider the following matrix A, we want to find $A = LL^T$:

$$A = \begin{pmatrix} 25 & 15 & -5 \\ 15 & 18 & 0 \\ -5 & 0 & 11 \end{pmatrix} = \begin{pmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{pmatrix} \begin{pmatrix} l_{11} & l_{21} & l_{31} \\ 0 & l_{22} & l_{32} \\ 0 & 0 & l_{33} \end{pmatrix}$$

Find the first column of L:

$$A = \begin{pmatrix} 25 & 15 & -5 \\ 15 & 18 & 0 \\ -5 & 0 & 11 \end{pmatrix} = \begin{pmatrix} 5 & 0 & 0 \\ 3 & l_{22} & 0 \\ -1 & l_{32} & l_{33} \end{pmatrix} \begin{pmatrix} 5 & 3 & -1 \\ 0 & l_{22} & l_{32} \\ 0 & 0 & l_{33} \end{pmatrix}$$

Find the second column of L:

$$\begin{pmatrix} 18 & 0 \\ 0 & 11 \end{pmatrix} - \begin{pmatrix} 3 \\ -1 \end{pmatrix} \begin{pmatrix} 3 & -1 \end{pmatrix} = \begin{pmatrix} l_{22} & 0 \\ l_{32} & l_{33} \end{pmatrix} \begin{pmatrix} l_{22} & l_{32} \\ 0 & l_{33} \end{pmatrix}$$

$$\begin{pmatrix} 9 & 3 \\ 3 & 10 \end{pmatrix} = \begin{pmatrix} 3 & 0 \\ 1 & l_{33} \end{pmatrix} \begin{pmatrix} 3 & 1 \\ 0 & l_{33} \end{pmatrix}$$

Find the third column of L, i.e., l_{33}.

We have $l_{33}l_{33} = 10 - 1 \cdot 1 = 9$ or $l_{33} = 3$.

The result is

$$\begin{pmatrix} 25 & 15 & -5 \\ 15 & 18 & 0 \\ -5 & 0 & 11 \end{pmatrix} = \begin{pmatrix} 5 & 0 & 0 \\ 3 & 3 & 0 \\ -1 & 1 & 3 \end{pmatrix} \begin{pmatrix} 5 & 3 & -1 \\ 0 & 3 & 1 \\ 0 & 0 & 3 \end{pmatrix}$$

Cost of the algorithms grows with n at the order of $(1/3)n^3$. The rest, i.e., the backward and forward substitution to find y and then x, has order $O(n^2)$ each.