The Cholesky decomposition

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Consider the LU decomposition of a matrix M:

$$M = LU$$

Recall that U is upper triangular with the picots on the diagonal. In the case when M is symmetric, we can turn the LU decomposition into the LDL^T decomposition to get

$$M = LDL^T.$$

This is done by extracting the diagonal of pivots from U, forming a diagonal matrix D with those pivots on the diagonal,

$$D = \begin{pmatrix} U_{11} & 0 & \cdots & 0 \\ 0 & U_{22} & & \vdots \\ \vdots & & \ddots & 0 \\ 0 & \cdots & 0 & U_{nn} \end{pmatrix},$$

and noticing that U can be written as DL^T. (This is something we'd have to prove.)

If furthermore M is positive semi-definite, then the pivots are nonnegative, and we can consider the matrix

$$\sqrt{D} = \begin{pmatrix} \sqrt{U_{11}} & 0 & \cdots & 0 \\ 0 & \sqrt{U_{22}} & & \vdots \\ \vdots & & \ddots & 0 \\ 0 & \cdots & 0 & \sqrt{U_{nn}} \end{pmatrix}.$$

Then rewrite the LDL^T decomposition as $M = (L\sqrt{D})(\sqrt{D}L^T)$. Call $R = \sqrt{D}L^T$: it is an upper triangular matrix like L^T. Hence we have the so-called Cholesky decomposition

$$M = R^T R.$$

(During office hours I wrote RR^T but it really doesn't matter what choice you make for R, as long as it's clear that the first factor is lower triangular, and the second is its transpose.)

There is only one way to write a symmetric PSD matrix into $R^T R$ with R upper triangular, up to a sign: you may turn R into $-R$ and still have $M = (-R^T)(-R) = R^T R$. Hence the Cholesky decomposition is unique, up to a sign.