Cholesky Factorisation*

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The Cholesky Factorisation of a matrix A is given by a matrix L such that $LL^T = A$, where L is lower triangular.

This factorisation is a special case of LU factorisation which is possible if and only if the original matrix was symmetric positive definite: that is, $A = A^T$ (the symmetric part) and for any vector $\mathbf{x}$ other than the zero vector, $\mathbf{x}^T A\mathbf{x}$ is strictly greater than zero (the positive definite part).

Once such a factorisation has been found, the original system $A\mathbf{x} = \mathbf{b}$ can be solved as for LU factorisation, with L^T taking the place of U. Thus the only difference is making use of the symmetry to simplify the derivation.

Deriving a Cholesky Factorisation

As with LU factorisation, the matrix L is built up by a series of column vectors which are obtained by an iterative process using the matrix A and previously determined columns. There is no longer any need to track U, since this will simply be L^T; however, additional computation is introduced by the use of square roots. So to start the process, define L_1 as the first column of A divided through by $\sqrt{a_{1,1}}$. Construct a new matrix A^2 by $A^2 = A - L_1 L_1^T$ (again, this is not a scalar product, else the difference makes no sense). Obtain L_2 from the second column of A^2 divided by $\sqrt{a_{2,2}^2}$. Proceed iteratively, finding L_i by $A_i^i / \sqrt{a_{i,i}^i}$, until all N columns have been found. Then check LL^T gives A.

Possible problems

If any of the diagonal entries of A is zero or negative, then dividing by the square root won't be possible (working in the reals). However, by the iff relation between being symmetric positive definite and having a Cholesky factorisation, this should not occur. In fact, this can be used as a test for A being SPD, rather than the potentially awkward $\mathbf{x}^T A\mathbf{x} > 0$: attempt to find the Cholesky factors and if the process ever fails, you didn't have an SPD matrix.

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A sample Cholesky factorisation

Let A be the matrix

$$\begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix}$$

Then L_1 is $A_1/\sqrt{a_{1,1}} = \begin{bmatrix} 2 \\ -1 \\ 0 \end{bmatrix} / \sqrt{2}$. It's easiest to carry the square root outside the vector, as it'll be squared back up again when we construct A^2:

$$A - L_1 L_1^T = \begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix} - \begin{pmatrix} 2 & -1 & 0 \\ -1 & \frac{1}{2} & 0 \\ 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \frac{3}{2} & -1 \\ 0 & -1 & 2 \end{pmatrix}$$

The second column of A^2 divided by $\sqrt{a_{2,2}^2} = \sqrt{\frac{3}{2}}$ gives us $L_2 = \begin{bmatrix} 0 \\ \frac{3}{2} \\ -1 \end{bmatrix} / \sqrt{\frac{3}{2}}$. Repeat again to get A^3 which is just

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{4}{3} \end{pmatrix}$$

Which makes $L_3 = \begin{bmatrix} 0 \\ 0 \\ \frac{4}{3} \end{bmatrix} / \sqrt{\frac{4}{3}} = \begin{bmatrix} 0 \\ 0 \\ \frac{2}{\sqrt{3}} \end{bmatrix}$. Combining these columns we get for L:

$$\begin{pmatrix} \frac{2}{\sqrt{2}} & 0 & 0 \\ \frac{-1}{\sqrt{2}} & \sqrt{\frac{3}{2}} & 0 \\ 0 & -\sqrt{\frac{2}{3}} & \frac{2}{\sqrt{3}} \end{pmatrix}$$