Symmetric Decomposition of a Positive Definite Matrix*

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1. Theoretical Background

The methods are based on the following theorem due to Cholesky [I].

If \( A \) is a symmetric positive definite matrix then there exists a real non-singular lower-triangular matrix \( L \) such that

\[
LL^T = A.
\] (1)

Further if the diagonal elements of \( L \) are taken to be positive the decomposition is unique.

The elements of \( L \) may be determined row by row or column by column by equating corresponding elements in (1). In the row by row determination we have for the \( i \)-th row

\[
\sum_{k=1}^{i} l_{ik} l_{kj} = a_{ij} \quad \text{giving} \quad l_{ij} = \left( a_{ij} - \sum_{k=1}^{j-1} l_{ik} l_{kj} \right) / l_{jj} \quad (j = 1, \ldots, i - 1),
\] (2)

\[
\sum_{k=1}^{i} l_{ik} l_{ki} = a_{ii} \quad \text{giving} \quad l_{ii} = \left( a_{ii} - \sum_{k=1}^{i-1} l_{ik} l_{ki} \right)^{1/2}.
\] (3)

There are thus \( n \) square roots and approximately \( \frac{1}{6} n^3 \) multiplications.

An alternative decomposition may be used in which the square roots are avoided as follows. If we define \( \tilde{L} \) by the relation

\[
L = \tilde{L} \text{ diag}(l_{ii}),
\] (4)

where \( L \) is the matrix given by the Cholesky factorization, then \( \tilde{L} \) exists (since the \( l_{ii} \) are positive) and is a unit lower-triangular matrix. We have then

\[
A = L L^T = \tilde{L} \text{ diag}(l_{ii}) \text{ diag}(l_{ii}) \tilde{L}^T = \tilde{L} D \tilde{L}^T,
\] (5)

where \( D \) is a positive diagonal matrix.

This factorization can be performed in \( n \) major steps in the \( i \)-th of which the \( i \)-th row of \( \tilde{L} \) and \( \tilde{d}_i \) are determined. The corresponding equations are

\[
\sum_{k=1}^{i} \tilde{l}_{ik} \tilde{d}_k \tilde{l}_{jk} = a_{ij} \quad \text{giving} \quad \tilde{l}_{ij} \tilde{d}_j = a_{ij} - \sum_{k=1}^{i-1} \tilde{l}_{ik} \tilde{d}_k \tilde{l}_{jk} \quad (j = 1, \ldots, i - 1),
\] (6)

\[
\sum_{k=1}^{i} \tilde{l}_{ik} \tilde{d}_k \tilde{l}_{ki} = a_{ii} \quad \text{giving} \quad \tilde{d}_i = a_{ii} - \sum_{k=1}^{i-1} \tilde{l}_{ik} \tilde{d}_k \tilde{l}_{ki}
\] (7)

since $\tilde{I}_{ij} = 1$. Expressed in this form the decomposition appears to take twice as many multiplications as that of CHOLESKY, but if we introduce the auxiliary quantities $\tilde{a}_{ij}$ defined by

$$\tilde{a}_{ij} = \tilde{I}_{ij} d_j$$

(8)
equations (6) and (7) become

$$\tilde{a}_{ij} = a_{ij} - \sum_{k=1}^{i-1} \tilde{a}_{ik} \tilde{I}_{jk} \quad (j = 1, \ldots, i - 1),$$

(9)

$$d_i = a_{ii} - \sum_{k=1}^{i-1} \tilde{a}_{ik} \tilde{I}_{ik}.$$  

(10)

We can therefore determine the $\tilde{a}_{ij}$ successively and then use them to determine the $\tilde{I}_{ij}$ and $d_i$. Notice that the $\tilde{a}_{ij}$ corresponding to the $i$-th row are not required when dealing with subsequent rows. The number of multiplications is still approximately $\frac{1}{6} n^3$ and there are no square roots.

Either factorization of $A$ enables us to calculate its determinant since we have

$$\text{det} (A) = \text{det} (L) \text{det} (L^T) = \prod_{i=1}^{n} l_{ii}^2$$

(11)

and

$$\text{det} (A) = \text{det} (\tilde{L}) \text{det} (\tilde{D}) \text{det} (\tilde{L}^T) = \prod_{i=1}^{n} d_i.$$  

(12)

We can also compute the solution of the set of equations

$$Ax = b$$

corresponding to any given right-hand side. In fact if

$$Ly = b \quad \text{and} \quad L^T x = y$$

(14)

we have

$$Ax = LL^T x = Ly = b.$$  

(15)

Equations (15) may be solved in the steps

$$y_i = \left( b_i - \sum_{k=1}^{i-1} l_{ik} y_k \right) / l_{ii} \quad (i = 1, \ldots, n),$$

(16)

$$x_i = \left( y_i - \sum_{k=i+1}^{n} l_{ki} x_k \right) / l_{ii} \quad (i = n, \ldots, 1)$$

(17)

involving $n^2$ multiplications in all and $2n$ divisions. Similarly if

$$\tilde{L} y = b, \quad \tilde{L}^T x = D^{-1} y,$$

(18)

we have

$$Ax = \tilde{L} \tilde{D} \tilde{L}^T x = \tilde{L} DD^{-1} y = b.$$  

(19)

Equations (18) may be solved in the steps

$$y_i = b_i - \sum_{k=1}^{i-1} \tilde{I}_{ik} y_k \quad (i = 1, \ldots, n),$$

(20)