MATHEMATICS OF COMPUTATION, VOLUME 29, NUMBER 132
OCTOBER 1975, PAGES 1051–1077

Methods for Computing and Modifying the LDV Factors of a Matrix

By Philip E. Gill, Walter Murray and Michael A. Saunders

Abstract. Methods are given for computing the LDV factorization of a matrix B and modifying the factorization when columns of B are added or deleted. The methods may be viewed as a means for updating the orthogonal (LQ) factorization of B without the use of square roots. It is also shown how these techniques lead to two numerically stable methods for updating the Cholesky factorization of a matrix following the addition or subtraction, respectively, of a matrix of rank one. The first method turns out to be one given recently by Fletcher and Powell; the second method has not appeared before.

1. Introduction. Any $m \times n$ matrix B of rank m $(m \leqslant n)$ has an LQ factorization of the form $B = [L \ 0]Q$, where L is a nonsingular lower-triangular matrix and Q is orthogonal ($Q^TQ = QQ^T = I$). The columns of L and the first m rows of Q are uniquely defined, apart from sign. Let l_{ii} be the diagonal elements of L and let a diagonal matrix $D = \mathrm{diag}(d_1, d_2, \ldots, d_n)$ be defined by

$$d_i = \begin{cases} l_{ii}^2, & i = 1, 2, \ldots, m, \\ 1, & i = m + 1, \ldots, n. \end{cases}$$

An LDV factorization of B may then be written in the form $B = [\hat{L} \ 0]DV$, where $\hat{L}$ and V are defined in terms of L, Q and D by the equations

$$[\hat{L} \ 0]D^{1/2} = [L \ 0], \qquad D^{1/2}V = Q.$$

The diagonals of $\hat{L}$ are unity and the rows of V are orthogonal. The following relations are easily proved:

$$VV^T = D^{-1}, \tag{1a}$$

$$V^TDV = I. \tag{1b}$$

Henceforth we shall use the notation L for both L and $\hat{L}$ above, since it will always be clear from the context whether or not L has a unit diagonal.

In this paper we derive methods for computing the LDV factorization of a matrix and methods for modifying the factorization when columns are added and deleted. The resulting methods are described in Sections 3 and 4 and may be applied immediately to the Simplex method for linear programming. The motive for working with LDV factors

Received December 3, 1974.

AMS (MOS) subject classifications (1970). Primary 65F30; Secondary 15A06, 15A39, 90C05, 90C20, 90C30.

rather than LQ factors is that square roots are eliminated and the amount of computation and storage is reduced.

In Section 5 we show how these results lead naturally to two methods for computing the Cholesky factors $\bar{L}$ and $\bar{D}$ of the matrix $\bar{L}\bar{D}\bar{L}^T = LDL^T + \sigma zz^T$ for some vector z and scalar σ. The method for the case $\sigma > 0$ turns out to be one given by Fletcher and Powell (1973), while the method for the case $\sigma < 0$ has not appeared before.

The keynote to this work is the construction of LQ factors for two elementary matrices of the form

$$\begin{bmatrix} I & p \\ & 1 \end{bmatrix} \quad \text{and} \quad I - qq^T$$

for given vectors p and q, where $\|q\|_2 = 1$. The special structure of these factors is given in the Appendix. Although the derivation of the recurrence relations involved is relatively complicated, we emphasize that the recurrence relations themselves are very simple.

1.1. *Notation.* We shall use the notation $\widetilde{M} = \widetilde{M}(p, \beta, \gamma)$ to denote a *special lower-triangular matrix* constructed from the vectors p, β and γ according to

$$\widetilde{M}_{ij} = \begin{cases} 0, & i < j, \\ \gamma_i, & i = j, \\ p_i\beta_j, & i > j. \end{cases}$$

If the diagonal elements of $\widetilde{M}$ form the vector $e = (1, 1, \ldots, 1)^T$ we shall write either $\widetilde{M} = \widetilde{M}(p, \beta, e)$ or just $\widetilde{M} = \widetilde{M}(p, \beta)$.

The notation $\|v\|$ will always mean the 2-norm $\|v\|_2 = (v^Tv)^{1/2}$ of a vector v, and a diagonal matrix D with diagonals d_i $(i = 1, 2, \ldots, n)$ will be written $D = \text{diag}(d_1, d_2, \ldots, d_n)$.

2. ***LDV* Factors.** We have defined in Section 1 what will be called a *proper LDV* factorization of a general rectangular matrix B. For later use the notion needs to be generalized in the following way. Suppose that L is unit lower triangular, D is a diagonal matrix with positive diagonal elements, and V is a matrix such that

$$B = [L \;\; 0]DV. \tag{2}$$

If there exist nonsingular diagonal matrices D_1 and D_2 such that the matrix $Q = D_1VD_2$ is orthogonal (unitary), then we shall call (2) an LDV factorization of B. (In other words we require that V can be transformed into an orthogonal matrix by simple row and column scaling.)

We now define (2) to be a *proper LDV* factorization in the event that

$$D_1 = D^{1/2} \quad \text{and} \quad D_2 = I,$$

in which case $Q = D^{1/2}V$ and the relations

$$VV^T = D^{-1} \quad \text{and} \quad V^TDV = I$$

hold as stated in Section 1.

We shall be particularly interested in the case where some of the columns of B are null. Matrices B of this kind will always arise in such a context that they are expressible in a form LDV such that, corresponding to each Be_j which is null, $Le_j = e_j$, $Ve_j = e_j$, $e_j^T V_j = e_j^T$ and $De_j = 0$, where e_j is the jth column of the identity matrix. If $D^+ = \text{diag}(d_1^+, d_2^+, \ldots, d_n^+)$ is defined by

$$d_i^+ = \begin{cases} d_i, & d_i > 0, \\ 1, & d_i = 0, \end{cases}$$

then the relations $VV^T = (D^+)^{-1}$ and $V^TD^+V = I$ hold in place of (1). It should be emphasized that when several columns of B are null, the LDV factorization is far from unique; the particular form of the factorization LDV described above will arise in a natural way in the algorithms we describe.

3. Computing the LDV Factorization of an $m \times m$ Matrix B. Let A be a matrix made up of j columns of B and $m - j$ columns of the zero matrix (initially we shall not specify any particular ordering of the columns of A), and assume that the LDV factorization of A, denoted by $A = LDV$, is known. We shall describe a method for computing the LDV factors of the matrix $\bar{A}$ obtained by replacing a zero column of A by a new column b. This technique leads naturally to a method for computing the LDV factorization of B since, if B_0 denotes the zero matrix with factorization $B_0 = L_0D_0V_0$, where $L_0 = I$, $D_0 = 0$ and $V_0 = I$, the columns of B can be added one by one to B_0.

From our remarks in Section 2, the diagonal matrix associated with the factorization $A = LDV$ has $m - j$ zero elements and V has $m - j$ columns of the identity matrix Let p be the vector such that $Lp = b$, and p_s the first element of p such that $p_s \neq 0$ and $d_s = 0$. Define

$$\bar{A} = A + be_s^T$$

(that is, the column b is added into the sth position). The recurrence relations we shall derive are invalid if $p_s = 0$. However, if B is nonsingular it can be shown that there exists at least one $|p_j| > 0$ (otherwise the new column is a linear combination of those that have already been processed). Using the LDV factorization of A, we have

$$\bar{A} = LDV + be_s^T = L(DV + pe_s^T).$$

By definition, the sth row of V is e_s, giving

$$\bar{A} = L(D + pe_s^T)V. \tag{3}$$

From Theorem A2 we have that the LDV factorization of $D + pe_s^T$ is of the form

$$D + pe_s^T = \tilde{L}\tilde{D}\tilde{V}, \tag{4}$$

where

$$(5)\qquad \tilde{L} = \begin{bmatrix}
1 \\
p_2\beta_1 & 1 \\
p_3\beta_1 & p_3\beta_2 & 1 \\
\cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot \\
p_s\beta_1 & p_s\beta_2 & p_s\beta_3 & \cdot & 1 \\
p_{s+1}\beta_1 & p_{s+1}\beta_2 & p_{s+1}\beta_3 & \cdot & p_{s+1}\beta_s & 1 \\
p_{s+2}\beta_1 & p_{s+2}\beta_2 & p_{s+2}\beta_3 & \cdot & p_{s+2}\beta_s & 0 & 1 \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
p_m\beta_1 & p_m\beta_2 & p_m\beta_3 & \cdot & p_m\beta_s & 0 & 0 & \cdot & \cdot & \cdot & 1
\end{bmatrix},$$

$$(6)\qquad \tilde{V} = \begin{bmatrix}
1-\beta_1p_1 & & & & & \beta_1 \\
-\beta_2p_1 & 1-\beta_2p_2 & & & & \beta_2 \\
-\beta_3p_1 & -\beta_3p_2 & 1-\beta_3p_3 & & & \beta_3 \\
\cdot & \cdot & \cdot & \cdot & & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \beta_{s-1} \\
-\beta_sp_1 & -\beta_sp_2 & -\beta_sp_3 & \cdot & \cdot & \beta_s \\
0 & 0 & 0 & \cdot & \cdot & \cdot & \cdot & \cdot & 1 \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\
0 & 0 & 0 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 0 & 0 & 1
\end{bmatrix},$$

$$\begin{aligned}\tilde{D} &= \operatorname{diag}(\tilde{d}_1, \tilde{d}_2, \ldots, \tilde{d}_m)\\ &= \operatorname{diag}(\hat{d}_1, \hat{d}_2, \ldots, \hat{d}_{s-1}, \hat{d}_s, d_{s+1}, \ldots, d_m),\end{aligned}$$

and the matrix $(\tilde{D}^+)^{1/2}\tilde{V}(D^+)^{-1/2}$ is orthogonal. The vectors $\hat{d}$ and β are generated by the following recurrence relations:

(i) define $t_0 = 1$;

(ii) for $k = 1, 2, \ldots, s-1$ compute the following: if $d_k = 0$, then set $\nu_k = 0$, otherwise set $\nu_k = p_k/d_k$, $t_k = t_{k-1} + \nu_k p_k$, $\hat{d}_k = d_k t_k/t_{k-1}$, $\beta_k = \nu_k/t_k$;

(iii) define $\hat{d}_s = p_s^2/t_{s-1}$ and $\beta_s = 1/p_s$.

Substituting (4) in (3) gives $\bar{A} = L\tilde{L}\tilde{D}\tilde{V}V$. From the orthogonality of $(\tilde{D}^+)^{1/2}\tilde{V}(D^+)^{-1/2}$ we have

(7) $$\tilde{V}(D^+)^{-1}\tilde{V}^T = (\tilde{D}^+)^{-1}.$$

Now

$$(\tilde{V}V)(\tilde{V}V)^T = \tilde{V}VV^T\tilde{V}^T = \tilde{V}(D^+)^{-1}\tilde{V}^T = (\tilde{D}^+)^{-1}, \quad \text{from (7).}$$

Consequently, if we write $\tilde{V}V = \bar{V}$, $\tilde{D} = \bar{D}$ and $L\tilde{L} = \bar{L}$, then we have a factorization of $\bar{A}$ of the form required.

By adding each column of B in turn and using the results just obtained we can generate a product form of the factorization (2). As the factorization proceeds, a new element of the diagonal matrix D becomes nonzero and a new column of L and column of V are defined. Let D_j, V_j and L_j denote the matrices $\tilde{D}$, $\tilde{V}$ and $\tilde{L}$ defined at (4) which are associated with the matrix made up of j columns of B. Then we have

$$B = L_1L_2 \cdots L_mD_mV_m \cdots V_2V_1,$$

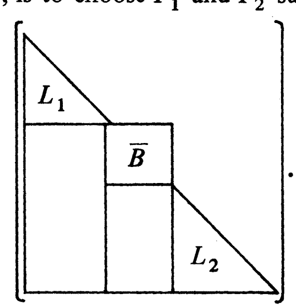
or $B = LDV$, if we write $L = L_1L_2 \cdots L_m$, $V = V_m \cdots V_2V_1$ and $D = D_m$.

The important feature of the matrices L_j and V_j is that they both can be constructed from the pair of vectors p and β. We shall show in Section 4.1 how their special form can be exploited to obtain the solution of equations of the form $L_jy = z$ and products of the form $y = V_jz$.

3.1. *Stability and Sparseness Considerations.* The general algorithm just given could be numerically unstable if the columns of B were added in random order. Just as with LU factorization, some "pivoting" strategy is required to ensure that the new column at each stage has a sufficiently large pivot element (p_s above). A preliminary ordering of the rows and columns of B would reduce the amount of column interchanging required. In the context of linear programming, the preassigned pivot procedures of Hellerman and Rarick (1971, 1972) would be useful.

In general, the purpose of preassigned pivot procedures is to rearrange the rows and columns of an arbitrarily sparse matrix before the factorization commences in order to reduce the subsequent storage requirements. In mathematical terms we seek permutation matrices P_1 and P_2 such that the fill-in during the solution of the equations $P_1BP_2y = P_1b$, is less than that during the solution of $Bx = b$. The solution x can be obtained from y using $x = P_2y$. One useful rearrangement of B, in view of the factorization being considered, is to choose P_1 and P_2 such that P_1BP_2 is of the form

(8)



This matrix is lower triangular except for the matrix $\bar{B}$, defined as a *bump*. The lower-triangular matrices L_1 and L_2 are known as the forward triangle and backward triangle, respectively. Hellerman and Rarick (1971 and 1972) have given two algorithms for determining a further reordering of the matrix $\bar{B}$. These algorithms give a matrix P_1BP_2 as in (8) together with a matrix $\bar{B}$ which is itself lower triangular save for further bumps $B_1, B_2, \ldots, B_j$ (there may be any number), each of which is lower triangular save for columns of nonzero elements called *spikes*. For example, a bump B_j could be of the form

$$B_j = \begin{bmatrix} x & \cdot & \cdot & \cdot & \cdot & x \\ \cdot & x & \cdot & \cdot & \cdot & x \\ x & \cdot & x & x & \cdot & x \\ \cdot & \cdot & x & x & \cdot & \cdot \\ \cdot & x & x & \cdot & x & x \\ x & x & \cdot & x & x & \cdot \end{bmatrix} \tag{9}$$

with x denoting the nonzero elements. Our example has spikes in the fourth and last columns.

If we apply the LDV factorization to a matrix which has been obtained by applying the Hellerman and Rarick scheme to B, then significant savings in fill-in are achieved. In this case, corresponding to a nonspike column, the L_j is an elementary matrix and the V_j is an identity matrix with its jth diagonal element replaced by $1/\beta_j$. The number of nontrivial V_j's is equal to the number of spike columns.

Rather than computing the LDV factors of B directly, there is an alternative strategy which maintains numerical stability and at the same time improves the sparsity of the factors. It is:

(1) compute a triangular factorization $B = LU$, using Gaussian elimination with column interchanges to preserve stability;

(2) use the above algorithm to compute an LDV factorization of U. In this case it is natural to add the columns of U in order from left to right.

The final result is a factorization of B in the form

$$B = LU = LL_1L_2 \cdots L_mD_mV_mV_{m-1} \cdots V_1.$$

Note that since U is upper triangular the elements $p_{s+1}, \ldots, p_m$ are zero for each factor L_s.

This strategy has been implemented and tested on some medium-scale linear programs. The procedure P^3 (Hellerman and Rarick (1971)) was used to specify an initial row and column ordering for B. (In practice only a few additional column interchanges are then required to ensure stability in the LU factorization.) The recurrence relations defining the LU factorization of P_1BP_2 imply that fill-in occurs only in the spike columns. For example, the LU factorization of (9) is of the form

$$
\begin{bmatrix}
x & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & x & \cdot & \cdot & \cdot & \cdot \\
x & \cdot & x & \cdot & \cdot & \cdot \\
\cdot & \cdot & x & x & \cdot & \cdot \\
\cdot & x & x & x & x & \cdot \\
x & x & \cdot & x & x & x
\end{bmatrix}
\begin{bmatrix}
x & \cdot & \cdot & \cdot & \cdot & x \\
\cdot & x & \cdot & \cdot & \cdot & x \\
\cdot & \cdot & x & x & \cdot & x \\
\cdot & \cdot & \cdot & x & \cdot & x \\
\cdot & \cdot & \cdot & \cdot & x & x \\
\cdot & \cdot & \cdot & \cdot & \cdot & x
\end{bmatrix}.
$$

The important facts are that

(a) the bulk of the LU factorization is in L, and

(b) U is almost strictly *diagonal* (except for the spikes).

In practice we find that there is virtually *no further fill-in* in the spike columns during the LDV factorization of U. To summarize, this means that for a general sparse matrix B (of the type encountered in *LP*) it is possible to compute an orthogonal factorization $B = LDV$ in product form, whose density is only slightly greater than that of the triangular factorization $B = LU$. This is a surprising result.

4. Adding and Deleting Columns of B. When combined, the two theorems in this section show how the LDV factors of a nonsingular square matrix B can be modified when one column of B is replaced by a new column.

THEOREM 1 (ADDING A COLUMN). *Let B be an $m \times m$ nonsingular matrix and let the $m \times (m + 1)$ matrix $[B\ 0]$ have a proper LDV factorization $[B\ 0] = [L\ 0]DV$, where L is unit lower triangular, $D = \mathrm{diag}(d_1, d_2, \ldots, d_m, 1)$ and $D^{1/2}V$ is orthogonal. If a column a_s is added to B to give the matrix $\overline{B}$, then $\overline{B}$ has a proper LDV factorization $\overline{B} = [B\ a_s] = [\overline{L}\ 0]\overline{D}\overline{V}$, with*

$$\overline{L} = L\widetilde{M}, \quad \overline{D} = \mathrm{diag}(d_1, d_2, \ldots, d_m, \alpha_1^2), \quad \overline{V} = \hat{V}V,$$

where

$$Lp = a_s, \quad \widetilde{M} = \widetilde{M}(p, \beta), \quad \widetilde{N} = \widetilde{M}(p, \beta)^T - \beta p^T, \quad \hat{V} = \begin{bmatrix} \widetilde{N} & \beta \\ -p^T & 1 \end{bmatrix},$$

and $\overline{D}^{1/2}\overline{V}$ is orthogonal. The quantities $\overline{d}_j$, β_j and α_1^2 are defined by the following recurrence relations:

$$
(10) \qquad \left.
\begin{array}{ll}
10(\mathrm{i}) & \textit{define } t_0 = 1; \\
10(\mathrm{ii}) & \textit{for } j = 1, 2, \ldots, m \textit{ set} \\
 & t_j = t_{j-1} + p_j^2/d_j, \\
 & \overline{d}_j = d_j t_j / t_{j-1}, \\
 & \beta_j = p_j/(d_j t_j); \\
10(\mathrm{iii}) & \textit{define } \alpha_1^2 = 1/t_m.
\end{array}
\right\}
$$

Proof. Adding the column to B gives

$$(11) \qquad \overline{B} = [B\ 0] + a_s e_{m+1}^T = [L\ 0]DV + Lpe_{m+1}^T = [L\ 0]\left(DV + \begin{bmatrix} p \\ 0 \end{bmatrix} e_{m+1}^T\right),$$

where p is the solution of $Lp = a_s$. Now $D^{1/2}V$ is orthogonal and the last column of $[B\ 0]$ is zero; hence $D^{1/2}V$ is really of the form

$$D^{1/2}V = \begin{bmatrix} Q & 0 \\ 0 & 1 \end{bmatrix},$$

where Q is the orthogonal matrix in the LQ factorization of B itself. Since $d_{m+1}^{1/2} = 1$ this means that $e_{m+1}^T V = e_{m+1}^T$. Substituting into (11) gives

$$\overline{B} = [L\ 0]\left(D + \begin{bmatrix} p \\ 0 \end{bmatrix} e_{m+1}^T\right) V = [L\ 0]\hat{L}\hat{D}\hat{V}V \equiv [\overline{L}\ 0]\overline{D}\overline{V},$$

where we are now using the corollary of Theorem A2 to write down an LDV factorization of $D + [{p \atop 0}] e_{m+1}^T$. Using the notation of the corollary of Theorem A2, we have

$$\text{(a)} \qquad [\overline{L}\ 0] = [L\ 0]\hat{L} = [L\ 0]\begin{bmatrix} \widetilde{M} & 0 \\ \beta^T & 1 \end{bmatrix} = [L\widetilde{M}\ 0],$$

so that

$$\text{(b)} \qquad \overline{L} = L\widetilde{M}; \quad \overline{D} = \hat{D};$$

$$\text{(c)} \qquad \overline{V} = \hat{V}V.$$

The structure of $\hat{V}$, $\widetilde{M}$ and $\widetilde{N}$ and the recurrence relations (10) also follow from the corollary of Theorem A2. Finally we have

$$\overline{D}^{1/2}\overline{V} = \hat{D}^{1/2}\hat{V}V = (\hat{D}^{1/2}\hat{V}D^{-1/2})(D^{1/2}V),$$

where both parenthesized quantities are orthogonal matrices. It follows that $\overline{D}^{1/2}\overline{V}$ is orthogonal and the theorem is proved. □

THEOREM 2 (DELETING A COLUMN). *Let B be an $m \times (m + 1)$ matrix with a proper LDV factorization $B = [L\ 0]DV$, where L is unit lower triangular, $D = \operatorname{diag}(d_1, d_2, \ldots, d_m, \alpha_1^2)$ is positive definite and $D^{1/2}V$ is orthogonal. If $\overline{B}$ is the matrix remaining after the rth column a_r is deleted from B, then $\overline{B}$ is nonsingular, and $[\overline{B}\ 0]$ has a proper LDV factorization $[\overline{B}\ 0] = [\overline{L}\ 0]\overline{D}\overline{V}$, with*

$$\overline{L} = L\widetilde{M}, \quad \overline{D} = \operatorname{diag}(\overline{d}_1, \overline{d}_2, \ldots, \overline{d}_m, 1), \quad \overline{V} = \hat{V}V\Pi,$$

where

$$\begin{bmatrix} p \\ \alpha_2 \end{bmatrix} = DVe_r, \quad \widetilde{M} = \widetilde{M}(p, \beta), \quad \hat{V} = \begin{bmatrix} \widetilde{M}^T & \alpha_2\beta \\ p^T & \alpha_2 \end{bmatrix}, \qquad \Pi = \text{a permutation matrix}$$

and $\overline{D}^{1/2}\overline{V}$ is orthogonal. The quantities $\overline{d}_j$ and β_j are defined by the following recurrence relations:

$$(12) \qquad \left.\begin{array}{l} \text{12(i) } \textit{define } t_{m+1} = \alpha_2^2/\alpha_1^2; \\ \text{12(ii) } \textit{for } j = m, m-1, \ldots, 1 \textit{ set} \\ \quad t_j = t_{j+1} + p_j^2/d_j, \\ \quad \overline{d}_j = d_j t_{j+1}/t_j, \\ \quad \beta_j = -p_j/(d_j t_{j+1}). \end{array}\right\}$$

Proof. If Π is the permutation matrix which interchanges columns r and $m + 1$ of B, we have the identity

$$[\bar{B}\ 0] = (B - a_r e_r^T)\Pi. \tag{13}$$

Also, if we compute the rth column of DV as $\begin{bmatrix} p \\ \alpha_2 \end{bmatrix} = DVe_r$ we have

$$a_r = Be_r = [L\ 0]DVe_r = [L\ 0]\begin{bmatrix} p \\ \alpha_2 \end{bmatrix}$$

and

$$e_r = V^T\begin{bmatrix} p \\ \alpha_2 \end{bmatrix},$$

since $V^T DV = I$ from (1b). Substituting for a_r and e_r in (13) gives

$$[\bar{B}\ 0] = [L\ 0]\left(D - \begin{bmatrix} p \\ \alpha_2 \end{bmatrix}[p^T\ \alpha_2]\right)V\Pi.$$

Now from the definition of p and α_2 we have $\|D^{-1/2}\begin{bmatrix} p \\ \alpha_2 \end{bmatrix}\| = \|D^{1/2}Ve_r\| = 1$ since $D^{1/2}V$ is orthogonal. Hence the conditions of Theorem A4 are satisfied and we can write down an LDV factorization of $D - \begin{bmatrix} p \\ \alpha_2 \end{bmatrix}[p^T\ \alpha_2]$ to give

$$[\bar{B}\ 0] = [L\ 0]\hat{L}\hat{D}\hat{V}V\Pi \equiv [\bar{L}\ 0]\bar{D}\bar{V}.$$

Using the notation of Theorem A4, we have

$$[\bar{L}\ 0] = [L\ 0]\hat{L} = [L\ 0]\begin{bmatrix} \tilde{M} & \\ \alpha_2 p^T & 0 \end{bmatrix} = [L\tilde{M}\ 0], \tag{a}$$

so that

$$\bar{L} = L\tilde{M}; \quad \bar{D} = \hat{D}; \tag{b}$$

$$\bar{V} = \hat{V}V\Pi. \tag{c}$$

The structure of $\hat{V}$ and $\tilde{M}$ and the recurrence relations (12) also follow from Theorem A4. Finally we have

$$\bar{D}^{1/2}\bar{V} = \hat{D}^{1/2}\hat{V}V\Pi = (\hat{D}^{1/2}\hat{V}D^{-1/2})(D^{1/2}V)(\Pi),$$

where all parenthesized quantities are orthogonal matrices. It follows that $\bar{D}^{1/2}\bar{V}$ is orthogonal and the theorem is proved.

Note also that the last row of $\bar{D}^{1/2}\bar{V}$ is

$$e_{m+1}^T\bar{D}^{1/2}\bar{V} = e_{m+1}^T\hat{D}^{1/2}\hat{V}V\Pi = e_{m+1}^T\hat{V}V\Pi = [p^T\ \alpha_2]V\Pi$$
$$= e_r^T V^T DV\Pi = e_r^T\Pi = e_{m+1}^T,$$

and hence $\bar{D}^{1/2}\bar{V}$ is of the form

$$\bar{D}^{1/2}\bar{V} = \begin{bmatrix} \bar{Q} & \\ & 1 \end{bmatrix},$$

where $\bar{Q}$ is the orthogonal matrix in the LQ factorization of $\bar{B}$. □

Theorems 1 and 2 imply that when a column of B is replaced by a new column we can extend the product form of Section 3 by adding new factors L_{m+1}, V_{m+1}, L_{m+2}, V_{m+2} and updating D_m to become D_{m+2}.

4.1. *Use of the Special Matrices $\widetilde{M}$ and $\hat{V}$.* The matrices $\widetilde{M} = \widetilde{M}(p, \beta)$ in Theorems 1 and 2 will be used to solve systems of the form

$$\widetilde{M}y = z \quad \text{or} \quad \widetilde{M}^T y = z.$$

Algorithms are given in Saunders (1972) which show that y can be computed using two multiplication operations for each nonzero element in p. Similarly the matrices $\hat{V}$ in Theorems 1 and 2 will be used to compute products of the form

$$y = \hat{V}z \quad \text{or} \quad y = \hat{V}^T z,$$

and it is easy to show that y can again be computed using only two multiplies per nonzero element in p.

5. Modification of the Cholesky Factors. This section is concerned with the modification of the Cholesky factors of a symmetric positive-definite matrix A after a rank-one correction. In mathematical terms, the problem is to compute the Cholesky factors $\bar{L}\bar{D}\bar{L}^T$ such that

$$\bar{L}\bar{D}\bar{L}^T = \bar{A} = A + \sigma zz^T = LDL^T + \sigma zz^T. \tag{14}$$

It will be assumed throughout that the elements d_j and $\bar{d}_j$ are positive, which implies that the matrices $\bar{A}$ and A are positive definite. We shall scale the vector z such that the modification (14) is either of the form

$$\bar{L}\bar{D}\bar{L}^T = LDL^T + vv^T, \tag{15}$$

or

$$\bar{L}\bar{D}\bar{L}^T = LDL^T - vv^T. \tag{16}$$

Although this scaling requires an additional n divisions and a square root, it minimizes the probability of overflow/underflow on the occasions when σ is large and $\|z\|$ is small.

Since A is positive definite, it can be written in the form $A = BB^T$, where B is a nonsingular $m \times m$ matrix. If B has the proper LDV factorization $B = LDV$, then L and D are the Cholesky factors of A. The two methods given in 5.1 and 5.2 for performing the modifications (15) and (16), respectively, are based upon the theorems given in the appendix for modifying the LDV factorization of B without storing V.

5.1. $\bar{L}\bar{D}\bar{L}^T = LDL^T + vv^T$. We have the identity

$$\bar{A} = L(D + pp^T)L^T, \tag{17}$$

where p is the solution of the equations

$$Lp = v. \tag{18}$$

We can now apply Lemma A3 to write down the LDL^T factors of $D + pp^T$ as

$$D + pp^T = \widetilde{M}\widetilde{D}\widetilde{M}^T,$$

where $\widetilde{M} = \widetilde{M}(p, \beta)$ and $\widetilde{D} = \operatorname{diag}(\bar{d}_1, \dots, \bar{d}_m)$ can be computed using the recurrence relations

$$\left.\begin{array}{l} \text{19(i) define } t_0 = 1; \\ \text{19(ii) for } j = 1, 2, \dots, m \text{ set} \\ \qquad t_j = t_{j-1} + p_j^2/d_j, \\ \qquad \bar{d}_j = d_j t_j / t_{j-1}, \\ \qquad \beta_j = p_j/(d_j t_j). \end{array}\right\} \tag{19}$$

Clearly the required Cholesky factors are given by $\bar{L} = L\widetilde{M}$ and $\bar{D} = \widetilde{D}$. These recurrence relations for computing β_j and $\bar{d}_j$ are identical to those given by Fletcher and Powell (1973) although they have been derived in a different way.

The special structure of the matrix $\widetilde{M}$ enables the product $L\widetilde{M}$ to be efficiently computed in terms of the β_j using the following forward recurrence relations suggested by Gill, Golub, Murray and Saunders (1974):

(i) define $v^{(1)} = Lp$;

(ii) for $j = 1, 2, \dots, m$ set

$$\left.\begin{array}{l} v_r^{(j+1)} = v_r^{(j)} - p_j l_{rj} \\ \bar{l}_{rj} = l_{rj} + \beta_j v_r^{(j+1)} \end{array}\right\}, \qquad r = j + 1, \dots, m. \tag{20}$$

The vector $v^{(1)}$ needed to initialize the recurrence relations is known, since $v^{(1)} = Lp = v$. Also, each of the vectors $v^{(j)}$ $(j = 1, 2, \dots, m)$ can be obtained during the jth stage of the initial forward substitution (20) since

$$v_r^{(j)} = \sum_{i=j}^{m} l_{ri} p_i = v_r - \sum_{i=1}^{j-1} l_{ri} p_i, \qquad r = j, j + 1, \dots, m.$$

We note also that, using the expression for $v_r^{(j+1)}$, we can rearrange the equation for $\bar{l}_{rj}$ in the form

$$\begin{aligned} \bar{l}_{rj} &= l_{rj} + \beta_j(v_r^{(j)} - p_j l_{rj}) = (1 - p_j\beta_j) l_{rj} + \beta_j v_r^{(j)} \\ &= (d_j/\bar{d}_j) l_{rj} + \beta_j v_r^{(j)}. \end{aligned} \tag{21}$$

This method requires $3m^2/2 + O(m)$ multiplications to completely update the factors, whereas only $m^2 + O(m)$ are required using (19) with (20).

Rounding-error analysis of the recurrence relations (19) and (20) and of (19) and (21) have been carried out by Fletcher and Powell (1973). This analysis shows that the corresponding rounding errors involve a term with coefficient $\bar{d}_j/d_j$ and $d_j/\bar{d}_j$, respectively. The recurrence relations (19ii) indicate that $\bar{d}_j > d_j$ for all j; and, consequently, the formula (21) should be used to obtain the new factor, since the term $d_j/\bar{d}_j$ has a damping effect on the error. The resulting algorithm has the unsatisfactory feature that an additional $m^2/2$ multiplications are required. However, Gentleman (1973) has suggested using formula (20) until the ratio $\bar{d}_j/d_j$ exceeds a certain fixed quantity. It has been observed in practice that the amount of work for this modified process is still approximately $m^2 + O(m)$ since large values of $\bar{d}_j/d_j$ are only likely to occur on one or two occasions during a single updating. For example, if $\bar{d}_k/d_k$ exceeds the bound, only $m - k$ additional multiplications are required.

In summary, the algorithm for performing the modification (15) is given by

(i) define $t_0 = 1$, $v^{(1)} = v$;

(ii) for $j = 1, 2, \ldots, m$ compute

$p_j = v_j^{(j)}$,

$t_j = t_{j-1} + p_j^2/d_j$,

$\bar{d}_j = d_j t_j/t_{j-1}$,

$\beta_j = p_j/(d_j t_j)$,

if $\bar{d}_j/d_j > 4$, then set

$$\left.\begin{aligned} \bar{l}_{rj} &= (t_{j-1}/t_j) l_{rj} + \beta_j v_r^{(j)} \\ v_r^{(j+1)} &= v_r^{(j)} - p_j l_{rj} \end{aligned}\right\}, \qquad r = j+1, \ldots, m,$$

otherwise set

$$\left.\begin{aligned} v_r^{(j+1)} &= v_r^{(j)} - p_j l_{rj} \\ \bar{l}_{rj} &= l_{rj} + \beta_j v_r^{(j+1)} \end{aligned}\right\}, \qquad r = j+1, \ldots, m.$$

5.2. $\bar{L}\bar{D}\bar{L}^T = LDL^T - vv^T$. In this case, instead of (17) we have

$$\bar{A} = L(D - pp^T)L^T, \tag{22}$$

where p satisfies (18). Consider the quantity $\alpha^2 = 1 - p^T D^{-1} p$. From (22) we have

$$\det(\bar{A}) = [\det(L)]^2 \det(D - pp^T).$$

Since L is unit lower triangular $\det(L) = 1$, and consequently

$$\det(\bar{A}) = \det(D - pp^T) = \alpha^2 \det(D).$$

Since by assumption $\bar{A}$ is positive definite, $\det(\bar{A}) > 0$ and α^2 is positive. This implies that we can apply Lemma A4 to give the factorization $D - pp^T = \tilde{M}\tilde{D}\tilde{M}^T$, using the recurrence relations:

(i) define $t_{m+1} = \alpha^2$;

(ii) for $j = m, m-1, \ldots, 1$ set

$$t_j = t_{j+1} + p_j^2/d_j, \quad \bar{d}_j = d_j t_{j+1}/t_j, \quad \beta_j = -p_j/(d_j t_{j+1}).$$

Since the elements of the vector β are computed in the order $\beta_m, \beta_{m-1}, \ldots, \beta_1$, it is convenient to compute the product $L\tilde{M}$ using the backward recurrence relations:

for $j = m, m-1, \ldots, 1$ set

$$v_j^{(j)} = p_j,$$

$$\left.\begin{aligned} \bar{l}_{rj} &= l_{rj} + \beta_j v_r^{(j+1)} \\ v_r^{(j)} &= v_r^{(j+1)} + p_j l_{rj} \end{aligned}\right\}; \qquad r = j+1, \ldots, m. \tag{23}$$

In this case there is no need to consider an alternative recurrence relation for $\bar{l}_{rj}$

since, as mentioned earlier in 5.1, the error involved using a recurrence relation of the form (23) is multiplied by the factor $\bar{d}_j/d_j$ and $\bar{d}_j \leqslant d_j$ for all j.

Unlike the recurrence relations for adding a rank-one matrix, the formation of $\bar{L}$ cannot take place during the computation of the vectors p and β since *all* of p must be known before the recurrence relations for β can commence. For this reason the computation of the modified factors requires $3m^2/2 + O(m)$ multiplications. It is a feature of this method that, provided $\alpha^2 > 0$, the modified matrix is positive definite regardless of any rounding errors made.

The final algorithm to perform the modification (16) is thus as follows:

(i) Solve the equations $Lp = v$ and define $t_{m+1} = 1 - p^TD^{-1}p$; if $t_{m+1} \leqslant 0$ set $t_{m+1} = \epsilon$, where ϵ ($\epsilon > 0$) is the machine precision;

(ii) for $j = m, m-1, \ldots, 1$ set

$$t_j = t_{j+1} + p_j^2/d_j,$$
$$\bar{d}_j = d_j t_{j+1}/t_j,$$
$$\beta_j = -p_j/(d_j t_{j+1}),$$
$$v_j^{(j)} = p_j,$$
$$\left.\begin{aligned} \bar{l}_{rj} &= l_{rj} + \beta_j v_r^{(j+1)} \\ v_r^{(j)} &= v_r^{(j+1)} + p_j l_{rj} \end{aligned}\right\}, \qquad r = j+1, \ldots, m.$$

Acknowledgments. The authors would like to thank Dr. J. H. Wilkinson for his careful reading of the manuscript and a number of helpful suggestions.

Appendix. Here we give the lemmas and theorems referred to earlier which develop the special structure of the following matrices:

(a) the product P of certain sequences of elementary orthogonal matrices which reduce an n-vector z to a multiple of the unit vector e_n, thus:

$$Pz = \|z\| e_n$$

with $P = P_{n-1}P_{n-2} \cdots P_2P_1$ and $P = P_1P_2 \cdots P_{n-2}P_{n-1}$, where each P_j is a plane rotation;

(b) the LQ factors of matrices of the form

$$\begin{bmatrix} I & p \\ & 1 \end{bmatrix} \quad \text{and} \quad I - qq^T \qquad (\|q\| = 1);$$

(c) the LDV factors of matrices of the form

$$\begin{bmatrix} D & p \\ & 1 \end{bmatrix} \quad \text{and} \quad D - qq^T \qquad (\|D^{-1/2}q\| = 1)$$

where D is a positive-definite diagonal matrix;

(d) the Cholesky factors of matrices of the form

$$D + pp^T \quad \text{and} \quad D - pp^T.$$

LEMMA A1. *Let z be an n-vector and P an orthogonal matrix such that*

(1) $$Pz = \|z\| e_n.$$

In particular, let P be the product of plane rotations

$$P = P_{n-1} \cdots P_2 P_1, \tag{2}$$

where each P_j is a symmetric orthogonal matrix of the form

$$P_j = \begin{bmatrix} 1 & & & & & & & \\ & \cdot & & & & & & \\ & & \cdot & & & & & \\ & & & 1 & & & & \\ & & & & -c_j & & & s_j \\ & & & & & 1 & & \\ & & & & & & \cdot & \\ & & & & & & & \cdot \\ & & & & & & & & 1 \\ & & & & s_j & & & & c_j \end{bmatrix} \quad (\textit{row } j).$$

Equation (1) *holds if the elements c_j and s_j are such that*

$$\begin{bmatrix} -c_j & s_j \\ s_j & c_j \end{bmatrix} \begin{bmatrix} z_j \\ \rho_{j-1} \end{bmatrix} = \begin{bmatrix} 0 \\ \rho_j \end{bmatrix}, \tag{3a}$$

where

$$\rho_j^2 = \rho_{j-1}^2 + z_j^2, \tag{3b}$$

$$c_j = \rho_{j-1}/\rho_j, \tag{3c}$$

$$s_j = z_j/\rho_j, \tag{3d}$$

for $j = 1, 2, \ldots, n-1$. (When $j = 1$ we define $\rho_0 = z_n$.) If the last component of z is nonzero, P can be formed into the matrix

$$P = \begin{bmatrix} \gamma_1 & & & & & \sigma_1 z_n \\ \sigma_2 z_1 & \gamma_2 & & & & \sigma_2 z_n \\ \sigma_3 z_1 & \sigma_3 z_2 & \gamma_3 & & & \sigma_3 z_n \\ \cdot & \cdot & \cdot\ \cdot & & & \cdot \\ \cdot & \cdot & \cdot\ \cdot\ \cdot & & & \cdot \\ \cdot & \cdot & \cdot\ \cdot\ \cdot\ \cdot & & & \cdot \\ \sigma_{n-1} z_1 & \sigma_{n-1} z_2 & \cdot\ \cdot\ \cdot\ \cdot & & \gamma_{n-1} & \sigma_{n-1} z_n \\ \sigma_n z_1 & \sigma_n z_2 & \cdot\ \cdot\ \cdot\ \cdot & & \sigma_n z_{n-1} & \sigma_n z_n \end{bmatrix},$$

where the elements σ_j and γ_j are defined by the recurrence relations

$$\left.\begin{array}{l} 4(\text{i})\ \textit{for } j = 1, 2, \ldots, n-1 \textit{ define} \\ \qquad \sigma_j = s_j/\rho_{j-1}, \quad \gamma_j = -c_j; \\ 4(\text{ii})\ \textit{define } \sigma_n = 1/\rho_{n-1} \quad (= 1/\|z\|). \end{array}\right\} \tag{4}$$

[*Note*: We require $z_n \neq 0$, but in general there may be $z_j = 0$ for $j < n$. For such j we define $P_j = I$, $\sigma_j = 0$, $\gamma_j = 1$, so the jth row and column of P will be unit vectors. Without loss of generality we may assume $z_1 \neq 0$.]

Proof. We shall define

$$P = P_{n-1}P_{n-2} \cdots P_2P_1 \equiv \begin{bmatrix} p_1^T \\ p_2^T \\ \cdot \\ \cdot \\ \cdot \\ p_n^T \end{bmatrix},$$

and the partial product

$$P_tP_{t-1} \cdots P_2P_1 \equiv Q_t.$$

The first t rows of Q_t are unaffected by subsequent rotations $P_{t+1}, \ldots, P_{n-1}$ and so we can write

(5) $$Q_t = \begin{bmatrix} p_1^T \\ \cdot \\ \cdot \\ \cdot \\ p_t^T \\ e_{t+1}^T \\ \cdot \\ \cdot \\ \cdot \\ e_{n-1}^T \\ q_t^T \end{bmatrix}.$$

Using Eq. (1), the vector $Q_tz \equiv v_t$ is of the form

(6) $$v_t^T = (0, \ldots, 0, z_{t+1}, \ldots, z_{n-1}, \rho_t),$$

and since Q_t is orthogonal

(7) $$z = Q_t^Tv_t.$$

Substituting (5) and (6) into (7), we have

$$\begin{bmatrix} z_1 \\ \cdot \\ \cdot \\ \cdot \\ z_t \\ z_{t+1} \\ \cdot \\ \cdot \\ \cdot \\ z_{n-1} \\ z_n \end{bmatrix} = \begin{bmatrix} 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \\ z_{t+1} \\ \cdot \\ \cdot \\ \cdot \\ z_{n-1} \\ 0 \end{bmatrix} + \rho_tq_t$$

giving

$$q_t^T = \left(\frac{z_1}{\rho_t}, \frac{z_2}{\rho_t}, \dots, \frac{z_t}{\rho_t}, 0, \dots, 0, \frac{z_n}{\rho_t}\right).$$

At the $(t + 1)$th stage, Q_t is premultiplied by P_{t+1} giving the row p_{t+1}^T as a linear combination of the two rows

$$(0, 0, \dots, 0, 1, 0, \dots, 0, 0)$$
$$\left(\frac{z_1}{\rho_t}, \frac{z_2}{\rho_t}, \dots, \frac{z_t}{\rho_t}, 0, 0, \dots, 0, \frac{z_n}{\rho_t}\right).$$

Thus

$$p_{t+1}^T = \left(\frac{z_1 s_{t+1}}{\rho_t}, \frac{z_2 s_{t+1}}{\rho_t}, \dots, \frac{z_t s_{t+1}}{\rho_t}, -c_{t+1}, 0, \dots, \frac{z_n s_{t+1}}{\rho_t}\right),$$

and if we define $\sigma_{t+1} = s_{t+1}/\rho_t$ and $\gamma_{t+1} = -c_{t+1}$, we have the required result. □

THEOREM A1 (LQ FACTORIZATION OF AN ELEMENTARY MATRIX). *Let $\widetilde{A}$ be a matrix of the form*

$$\widetilde{A} = \begin{bmatrix} I & q \\ & 1 \end{bmatrix} \equiv I_{m+1} + \begin{bmatrix} q \\ 0 \end{bmatrix} e_{m+1}^T,$$

where q is an m-vector. The matrix $\widetilde{A}$ has the LQ factorization $\widetilde{A} = \widetilde{L}\widetilde{Q}$, where $\widetilde{L}$ is a special lower-triangular matrix and $\widetilde{Q}$ is an orthogonal matrix of the form

$$\widetilde{L} = \begin{bmatrix} \widetilde{M} & \\ \sigma^T & \alpha \end{bmatrix}, \qquad \widetilde{Q} = \begin{bmatrix} \widetilde{N} & \sigma \\ -\alpha q^T & \alpha \end{bmatrix}.$$

Both $\widetilde{M}$ and $\widetilde{N}$ are special lower-triangular matrices defined by

$$\widetilde{M} = \widetilde{M}(q, \sigma, \delta), \qquad \widetilde{N} = \widetilde{N}(\sigma, -q, \gamma) = \widetilde{M}^{-1} = \widetilde{M}^T - \sigma q^T,$$

where the vectors σ, γ, δ and the scalar α are generated by the following recurrence relations:

$$\left.\begin{aligned} &8(\text{i}) \ \textit{define } \rho_0 = 1; \\ &8(\text{ii}) \ \textit{for } j = 1, 2, \dots, m \textit{ set} \\ &\qquad \rho_j^2 = \rho_{j-1}^2 + q_j^2, \\ &\qquad \sigma_j = -q_j/(\rho_j \rho_{j-1}), \\ &\qquad \gamma_j = -\rho_{j-1}/\rho_j, \\ &\qquad \delta_j = 1/\gamma_j; \\ &8(\text{iii}) \ \textit{define } \alpha = 1/\rho_m. \end{aligned}\right\} \tag{8}$$

Proof (*of Theorem* A1). The LQ factors of $\widetilde{A}$ could be computed directly from the relation

$$\widetilde{A}\widetilde{Q}^T \equiv \begin{bmatrix} I & q \\ & 1 \end{bmatrix} \widetilde{Q}^T = \widetilde{L},$$

where $\tilde{Q}$ is a product of plane rotations designed to eliminate the elements of q one by one. However, we show now that $\tilde{Q}$ may instead be constructed as a product of plane rotations such that

$$\tilde{Q}\begin{bmatrix}-q\\1\end{bmatrix} \equiv P_m \cdots P_2P_1\begin{bmatrix}-q\\1\end{bmatrix} = \omega e_{m+1}, \tag{9}$$

with

$$\omega = (q^Tq + 1)^{1/2}. \tag{10}$$

(It turns out that this method is slightly more efficient, and it allows us to use Lemma A1 to develop the structure of $\tilde{Q}$.) Let $\tilde{L}$ be partitioned in the form

$$\tilde{L} = \begin{bmatrix}\tilde{M} & \\ y^T & \alpha\end{bmatrix},$$

and suppose that in place of (9) and (10) we have

$$\tilde{Q}\begin{bmatrix}-q\\1\end{bmatrix} = \begin{bmatrix}w\\ \omega\end{bmatrix}, \qquad w^Tw + \omega^2 = q^Tq + 1.$$

Multiplying the relation $\tilde{L}\tilde{Q} = \tilde{A}$ by $[{}^{-q}_{\ 1}]$ gives

$$\begin{bmatrix}\tilde{M} & \\ y^T & \alpha\end{bmatrix}\begin{bmatrix}w\\ \omega\end{bmatrix} = \begin{bmatrix}I & q\\ & 1\end{bmatrix}\begin{bmatrix}-q\\1\end{bmatrix},$$

i.e.

$$\begin{bmatrix}\tilde{M}w\\ y^Tw + \alpha\omega\end{bmatrix} = \begin{bmatrix}0\\1\end{bmatrix}.$$

Since $\tilde{M}$ must be nonsingular this gives $w = 0$, $\alpha\omega = 1$ and $\omega^2 = q^Tq + 1$.

We have thus proved that Eqs. (9) and (10) are true.

From Lemma A1 we can therefore say that $\tilde{Q} = P_m \cdots P_2P_1$ is of the form

$$\tilde{Q} = \begin{bmatrix}\tilde{N} & \sigma\\ -\alpha q^T & \alpha\end{bmatrix},$$

where

(i) $\tilde{N} = \tilde{N}(\sigma, -q, \gamma)$ is a special lower-triangular matrix;

(ii) the quantities σ, γ and α are obtained from the recurrence relations (3) and (4) by replacing z, σ and n by $[{}^{-q}_{\ 1}]$, $[{}^{\sigma}_{\alpha}]$ and $m + 1$, respectively;

(iii) in particular,

$$\alpha \equiv \sigma_{m+1} = 1\Big/\left\|\begin{bmatrix}-q\\1\end{bmatrix}\right\| = (q^Tq + 1)^{-1/2} = 1/\omega,$$

which is consistent with the use of α in $\tilde{L}$ above.

Using (3) to eliminate c_j and s_j in (4) now gives the recurrence relations (8) for generating σ, γ and α, and the structure of $\tilde{Q}$ and $\tilde{N}$ is determined.

It remains to determine the structure of $\tilde{L}$ and $\tilde{M}$. From the equation $\tilde{A} = \tilde{L}\tilde{Q}$ it follows immediately that $\tilde{M}\tilde{N} = I$, and hence the diagonals of $\tilde{M}$ are the reciprocals of those of $\tilde{N}$, i.e. $\tilde{M}_{ii} = 1/\gamma_j = \delta_j$. Next, the equation $\tilde{A}\tilde{Q}^T = \tilde{L}$ readily gives the relation $\tilde{M} = \tilde{N}^T + q\sigma^T$, and from the structure of $\tilde{N}$ it follows that $\tilde{M}_{ij} = q_i\sigma_j$ for $i > j$, and hence $\tilde{M}$ is the special lower-triangular matrix $\tilde{M}(q, \sigma, \delta)$. Finally, the equation $\tilde{A}\tilde{Q}^T = \tilde{L}$ also gives $y = \sigma$, which completes the structure of $\tilde{L}$. The theorem is now proved. □

THEOREM A2 (*LDV* FACTORIZATION OF AN ELEMENTARY MATRIX). *Let A be a matrix of the form*

$$A = D + pe_s^T,$$

where p is an m-vector such that $p_s \neq 0$ and $D = \mathrm{diag}(d_1, d_2, \ldots, d_m)$ with $d_s = 0$ and $d_j \geqslant 0$ for $j = 1, 2, \ldots, s-1, s+1, \ldots, m$. If p_s is the first element of p such that $|p_s| > 0$ and $d_s = 0$, then A has an LDV factorization $A = \tilde{L}\tilde{D}\tilde{V}$ where

$$\tilde{L} = \begin{bmatrix}
1 \\
p_2\beta_1 & 1 \\
p_3\beta_1 & p_3\beta_2 & 1 \\
\vdots & \vdots & \vdots & \ddots \\
p_s\beta_1 & p_s\beta_2 & p_s\beta_3 & \cdots & 1 \\
p_{s+1}\beta_1 & p_{s+1}\beta_2 & p_{s+1}\beta_3 & \cdots & p_{s+1}\beta_s & 1 \\
p_{s+2}\beta_1 & p_{s+2}\beta_2 & p_{s+2}\beta_3 & \cdots & p_{s+2}\beta_s & 0 & 1 \\
\vdots & \vdots & \vdots & \cdots & \vdots & \vdots & \vdots & 1 \\
\vdots & \vdots & \vdots & \cdots & \vdots & \vdots & \vdots & \vdots & \ddots \\
p_m\beta_1 & p_m\beta_2 & p_m\beta_3 & \cdots & p_m\beta_s & 0 & 0 & \cdots & 1
\end{bmatrix},$$

$$\tilde{V} = \begin{bmatrix}
1 - p_1\beta_1 & & & & \beta_1 \\
-\beta_2 p_1 & 1 - p_2\beta_2 & & & \beta_2 \\
-\beta_3 p_1 & -\beta_3 p_2 & 1 - p_3\beta_3 & & \beta_3 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
\vdots & \vdots & \vdots & \cdots & \beta_{s-1} \\
-\beta_s p_1 & -\beta_s p_2 & -\beta_s p_3 & \cdots & \beta_s \\
0 & 0 & 0 & \cdots & \cdots & 1 \\
\vdots & \vdots & \vdots & \cdots & \cdots & \cdots & \ddots \\
0 & 0 & 0 & \cdots & \cdots & \cdots & 0 & 1
\end{bmatrix},$$

$$\tilde{D} = \operatorname{diag}(\tilde{d}_1, \tilde{d}_2, \ldots, \tilde{d}_m) = \operatorname{diag}(\hat{d}_1, \hat{d}_2, \ldots, \hat{d}_{s-1}, \hat{d}_s, d_{s+1}, \ldots, d_m)$$

and the matrix $(\tilde{D}^+)^{1/2}\tilde{V}(D^+)^{-1/2}$ *is orthogonal. The vectors* $\hat{d}$ *and* β *are generated by the following recurrence relations*:

$$\text{(11)}\qquad \left.\begin{array}{ll} \text{11(i)} & \textit{define } t_0 = 1; \\ \text{11(ii)} & \textit{for } k = 1, 2, \ldots, s-1 \textit{ compute the following}: \\ & \textit{if } d_k = 0 \textit{ then set } v_k = 0 \textit{ otherwise set } v_k = p_k/d_k, \\ & t_k = t_{k-1} + v_k p_k, \\ & \hat{d}_k = d_k t_k / t_{k-1}, \\ & \beta_k = v_k / t_k; \\ \text{11(iii)} & \textit{define } \hat{d}_s = p_s^2/t_{s-1} \textit{ and } \beta_s = 1/p_s. \end{array}\right\}$$

Proof. We shall prove this theorem in two stages. Firstly, we shall assume that d_s is the only zero element of D and then consider the case where other d_j are zero (together with their associated p_j).

Consider the matrix A_s made up of the first s rows and columns of A. If A is partitioned as

$$A = \begin{bmatrix} D_1 & p^{(1)} & \\ & p_s & \\ & p^{(2)} & D_2 \end{bmatrix},$$

then A_s can be written as

$$A_s = \begin{bmatrix} D_1 & p^{(1)} \\ & p_s \end{bmatrix} = \begin{bmatrix} I & \\ & p_s \end{bmatrix} \begin{bmatrix} D_1^{1/2} & \\ & 1 \end{bmatrix} \begin{bmatrix} I & q \\ & 1 \end{bmatrix} \begin{bmatrix} D_1^{1/2} & \\ & 1 \end{bmatrix}$$

$$= \begin{bmatrix} I & \\ & p_s \end{bmatrix} (D_s^+)^{1/2} \tilde{A}_s (D_s^+)^{1/2},$$

where

$$\text{(12)}\qquad \tilde{A}_s = \begin{bmatrix} I & q \\ & 1 \end{bmatrix}, \quad D_s^+ = \begin{bmatrix} D_1 & \\ & 1 \end{bmatrix} \quad \text{and} \quad q = D_1^{-1/2} p.$$

From Theorem A1 we know that $\tilde{A}_s$ has the orthogonal factorization $\tilde{A}_s = \tilde{L}_s \tilde{Q}_s$ where $\tilde{L}_s$ and $\tilde{Q}_s$ are constructed from the quantities q, σ, γ, δ and α as shown. Let us define

$$\text{(13)}\qquad \left.\begin{array}{ll} \bar{d}_j = d_j \delta_j^2, & \beta_j = \sigma_j/(\delta_j d_j^{1/2}), \\ \theta_j = \gamma_j/\delta_j = 1/\delta_j^2, & \Delta = \operatorname{diag}(\delta_1, \delta_2, \ldots, \delta_{s-1}, \alpha), \end{array}\right\}$$

and $e = (1, 1, \ldots, 1)^T$. Using the notation of Theorem A1, we now have

$$A_s = \begin{bmatrix} I & \\ & p_s \end{bmatrix} (D_s^+)^{1/2} \widetilde{A}_s (D_s^+)^{1/2} = \begin{bmatrix} I & \\ & p_s \end{bmatrix} (D_s^+)^{1/2} \widetilde{L}_s \widetilde{Q}_s (D_s^+)^{1/2},$$

where

$$\begin{bmatrix} I & \\ & p_s \end{bmatrix} (D_s^+)^{1/2} \widetilde{L}_s = \begin{bmatrix} I & \\ & p_s \end{bmatrix} (D_s^+)^{1/2} \begin{bmatrix} \widetilde{M}(q, \sigma, \delta) & \\ \sigma^T & \alpha \end{bmatrix}$$

$$(14a) \qquad = \begin{bmatrix} \widetilde{M}(p, \beta, e) & \\ p_s \beta^T & 1 \end{bmatrix} (D_s^+)^{1/2} \Delta \begin{bmatrix} I & \\ & p_s \end{bmatrix} = \hat{L} (D_s^+)^{1/2} \Delta \begin{bmatrix} I & \\ & p_s \end{bmatrix},$$

and

$$\widetilde{Q}_s (D_s^+)^{1/2} = \begin{bmatrix} \widetilde{N}(\sigma, -q, \gamma) & \sigma \\ -\alpha q^T & \alpha \end{bmatrix} (D_s^+)^{1/2}$$

$$(14b) \qquad = \begin{bmatrix} I & \\ & p_s \end{bmatrix} \Delta (D_s^+)^{1/2} \begin{bmatrix} \widetilde{N}(\beta, -p^{(1)}, \theta) & \beta \\ -\left(\frac{1}{p_s}\right) p^{(1)T} & 1/p_s \end{bmatrix} = \begin{bmatrix} I & \\ & p_s \end{bmatrix} \Delta (D_s^+)^{1/2} \hat{V}.$$

Combining (14a) and (14b) gives $A_s = \hat{L}\hat{D}\hat{V}$, where

$$\hat{L} = \begin{bmatrix} \widetilde{M} & \\ p_s \beta^T & 1 \end{bmatrix}, \qquad \hat{V} = \begin{bmatrix} \widetilde{N} & \beta \\ -\left(\frac{1}{p_s}\right) p^{(1)T} & 1/p_s \end{bmatrix}$$

and

$$(15) \qquad \hat{D} = (D_s^+)^{1/2} \Delta^2 (D_s^+)^{1/2} \begin{bmatrix} I & \\ & p_s^2 \end{bmatrix} = \Delta^2 D_s^+ \begin{bmatrix} I & \\ & p_s^2 \end{bmatrix}$$

$$= \operatorname{diag}(d_1 \delta_1^2, d_2 \delta_2^2, \ldots, d_{s-1} \delta_{s-1}^2, p_s^2 \alpha^2).$$

Equations (14b) and (15) also give the orthogonal matrix $\widetilde{Q}_s$ as

$$\widetilde{Q}_s = \begin{bmatrix} I & \\ & p_s \end{bmatrix} \Delta (D_s^+)^{1/2} \hat{V} (D_s^+)^{-1/2} = \hat{D}^{1/2} \hat{V} (D_s^+)^{-1/2}.$$

We can now simplify the expressions for $\bar{d}_j$, β_j and θ_j in (13). From the definitions of ρ_j, σ_j, δ_j and q_j in (8) and (12) we have

$$\rho_j^2 = \rho_{j-1}^2 + q_j^2 = \rho_{j-1}^2 + p_j^2/d_j;$$

$$\bar{d}_j = d_j/\gamma_j^2 = d_j \rho_j^2 / \rho_{j-1}^2;$$

$$\beta_j = \sigma_j\gamma_j/d_j^{1/2} = q_j/(\rho_j^2 d_j^{1/2}) = p_j/(\rho_j^2 d_j);$$

$$\theta_j = \gamma_j^2 = \rho_{j-1}^2/\rho_j^2 = (\rho_j^2 - p_j^2/d_j)/\rho_j^2 = 1 - p_j^2/(\rho_j^2 d_j) = 1 - p_j\beta_j.$$

From 8(iii) we also have $\alpha^2 = 1/\rho_{s-1}^2$. Since all these expressions require ρ_j^2 rather than ρ_j, we can define $t_j = \rho_j^2$ and avoid the computation of all square roots.

If we now consider the factorization of the complete matrix $D + pe_s^T$, we must have

$$A = \begin{bmatrix} \hat{L} & \\ Y & I \end{bmatrix} \begin{bmatrix} \hat{D} & \\ & D_2 \end{bmatrix} \begin{bmatrix} \hat{V} & \\ & I \end{bmatrix},$$

where Y is a matrix to be determined. If the factors of the last expression are multiplied out and right- and left-hand sides are equated, we have $p^{(2)}e_s^T = Y\hat{D}\hat{V}$, where e_s^T is the last row of the sth-order identity matrix. Multiplying both sides by $(D_s^+)^{-1}\hat{V}^T$ and noting that $\hat{V}(D_s^+)^{-1}\hat{V}^T = \hat{D}^{-1}$, since $\hat{D}^{1/2}\hat{V}(D_s^+)^{-1/2}$ is orthogonal, we have

$$p^{(2)}e_s^T(D_s^+)^{-1}\hat{V}^T = Y\hat{D}\hat{V}(D_s^+)^{-1}\hat{V}^T = Y.$$

Consequently, since

$$e_s^T(D_s^+)^{-1} = e_s^T \text{ and } e_s^T\hat{V}^T = \begin{bmatrix} \beta^T & \dfrac{1}{p_s} \end{bmatrix},$$

we have

$$Y = p^{(2)}\begin{bmatrix} \beta^T & \dfrac{1}{p_s} \end{bmatrix}.$$

If we define $\beta_s = 1/p_s$, this completes the proof in the case where $d_j > 0$ for $j = 1, 2, \ldots, s-1, s+1, \ldots, m$.

If A has k rows and columns equal to zero (that is $d_j = 0$ corresponding to $p_j = 0$), we can apply the method just described to the matrix of $m - k$ remaining rows and columns and regard the *LDV* factors so obtained as being of order m by inserting suitable rows and columns of the identity matrix. This gives the recurrence relations (11). □

COROLLARY. *Let A be a matrix of the form*

$$A = D + \begin{bmatrix} p \\ 0 \end{bmatrix} e_{m+1}^T \equiv \begin{bmatrix} D_1 & p \\ & 1 \end{bmatrix},$$

where p is an m-vector and

$$D = \operatorname{diag}(d_1, d_2, \ldots, d_m, 1) \equiv \begin{bmatrix} D_1 & \\ & 1 \end{bmatrix},$$

with D_1 positive definite. The matrix A has an LDV factorization $A = \hat{L}\hat{D}\hat{V}$ where

$$\hat{L} = \begin{bmatrix} \widetilde{M} & \\ \beta^T & 1 \end{bmatrix}, \qquad \hat{D} = \operatorname{diag}(\bar{d}_1, \bar{d}_2, \ldots, \bar{d}_m, \alpha^2), \qquad \hat{V} = \begin{bmatrix} \widetilde{N} & \beta \\ -p^T & 1 \end{bmatrix},$$

and the matrix $\hat{D}^{1/2}\hat{V}D^{-1/2}$ *is orthogonal. Both* $\widetilde{M}$ *and* $\widetilde{N}$ *are special lower-triangular matrices defined by*

$$\widetilde{M} = \widetilde{M}(p, \beta), \qquad \widetilde{N} = \widetilde{N}(\beta, -p, \theta) = \widetilde{M}^T - \beta p^T,$$

where the vectors $\bar{d}$, β, θ *and the scalar* α^2 *are generated by the following recurrence relations*:

$$(16)\qquad \left.\begin{array}{l} \text{16(i) } \textit{define } t_0 = 1; \\ \text{16(ii) } \textit{for } j = 1, 2, \ldots, m \textit{ set} \\ \qquad t_j = t_{j-1} + p_j^2/d_j, \\ \qquad \bar{d}_j = d_j t_j / t_{j-1}, \\ \qquad \beta_j = p_j/(d_j t_j), \\ \qquad \theta_j = 1 - p_j\beta_j; \\ \text{16(iii) } \textit{define } \alpha^2 = 1/t_m. \ \square \end{array}\right\}$$

LEMMA A2. *Let z be an n-vector and P an orthogonal matrix such that*

$$(17)\qquad Pz = \|z\| e_n.$$

In particular, let P be the product of plane rotations $P = P_1 P_2 \cdots P_{n-1}$, *where each* P_j *is the form given in Lemma* A1. *Equation* (17) *holds if the element* c_j *and* s_j *defining* P_j *are such that*

$$\begin{bmatrix} -c_j & s_j \\ s_j & c_j \end{bmatrix} \begin{bmatrix} z_j \\ \rho_{j+1} \end{bmatrix} = \begin{bmatrix} 0 \\ \rho_j \end{bmatrix},$$

where

$$(18)\qquad \rho_j^2 = \rho_{j+1}^2 + z_j^2, \qquad c_j = \rho_{j+1}/\rho_j, \qquad s_j = z_j/\rho_j,$$

for $j = n-1, n-2, \ldots, 1$. (*When* $j = n-1$ *we define* $\rho_n = z_n$.) *If the last component of z is nonzero, P can be formed into the matrix*

$$P = \begin{bmatrix} \gamma_1 & \sigma_1 z_2 & \sigma_1 z_3 & \cdots & \cdot & \cdot & \sigma_1 z_n \\ & \gamma_2 & \sigma_2 z_3 & \cdots & \cdot & \cdot & \sigma_2 z_n \\ & & \gamma_3 & \cdots & \cdot & \cdot & \sigma_3 z_n \\ & & & \cdots & \cdot & \cdot & \cdot \\ & & & \cdots & \cdot & \cdot & \cdot \\ & & & \cdot & \cdot & \cdot & \cdot \\ & & & & \gamma_{n-2} & \sigma_{n-2} z_{n-1} & \sigma_{n-2} z_n \\ & & & & & \gamma_{n-1} & \sigma_{n-1} z_n \\ \sigma_n z_1 & \sigma_n z_2 & \sigma_n z_3 & \cdots & \cdot & \sigma_n z_{n-1} & \sigma_n z_n \end{bmatrix},$$

where the elements σ_j *and* γ_j *are defined by the recurrence relations*

$$\left.\begin{array}{ll} \text{19(i)} & \textit{for } j = n-1, n-2, \ldots, 1 \textit{ define} \\ & \sigma_j = s_j/\rho_{j+1}, \quad \gamma_j = -c_j; \\ \text{19(ii)} & \textit{define } \sigma_n = 1/\rho_1 \quad (= 1/\|z\|). \end{array}\right\} \tag{19}$$

[*Note*: As in Lemma A1, we require $z_n \neq 0$; but if $z_j = 0$ for $j < n$, we define $P_j = I$, $\sigma_j = 0$, $\gamma_j = 1$.]

Proof. This lemma is proved in a similar way to Lemma A1. □

THEOREM A3 (*LQ* FACTORIZATION OF AN ELEMENTARY MATRIX). *Let $\widetilde{A}$ be an $(m+1) \times (m+1)$ matrix of the form $\widetilde{A} = I_{m+1} - \hat{q}\hat{q}^T$, where $\hat{q} = \left[\begin{smallmatrix} q \\ \alpha \end{smallmatrix}\right]$, with α a scalar ($\alpha \neq 0$) and $\|\hat{q}\| = 1$. The matrix $\widetilde{A}$ has the LQ factorization $\widetilde{A} = \widetilde{L}\widetilde{Q}$, where $\widetilde{L}$ is a special lower-triangular matrix and $\widetilde{Q}$ is an orthogonal matrix of the form*

$$\widetilde{L} = \begin{bmatrix} \widetilde{M} & \\ \alpha\sigma^T & 0 \end{bmatrix}, \quad \widetilde{Q} = \begin{bmatrix} \widetilde{M}^T & \alpha\sigma \\ q^T & \alpha \end{bmatrix}.$$

The matrix $\widetilde{M} = \widetilde{M}(q, \sigma, \gamma)$ is a special lower-triangular matrix with the vectors σ and γ defined by the following recurrence relations:

$$\left.\begin{array}{ll} \text{20(i)} & \textit{define } \rho_{m+1} = \alpha; \\ \text{20(ii)} & \textit{for } j = m, m-1, \ldots, 1 \textit{ set} \\ & \rho_j^2 = \rho_{j+1}^2 + q_j^2, \\ & \sigma_j = q_j/(\rho_{j+1}\rho_j), \\ & \gamma_j = -\rho_{j+1}/\rho_j. \end{array}\right\} \tag{20}$$

Proof. We shall obtain the *LQ* factorization of $\widetilde{A}$ by construction. Let $\widetilde{Q}$ be the orthogonal matrix $\widetilde{Q} = P_1 P_2 \cdots P_m$ constructed as in Lemma A2 such that

$$\widetilde{Q}\hat{q} = \|\hat{q}\| e_{m+1} = e_{m+1}. \tag{21}$$

Replacing z, σ and n by $\left[\begin{smallmatrix} q \\ \alpha \end{smallmatrix}\right]$, $\left[\begin{smallmatrix} \sigma \\ \sigma_{m+1} \end{smallmatrix}\right]$ and $m+1$, respectively, we see from Lemma A2 that $\widetilde{Q}$ may be partitioned in the form

$$\widetilde{Q} = \begin{bmatrix} \widetilde{M}^T & \alpha\sigma \\ \sigma_{m+1} q^T & \sigma_{m+1}\alpha \end{bmatrix},$$

where $\widetilde{M} = \widetilde{M}(q, \sigma, \gamma)$. From 19(ii) we have $\sigma_{m+1} = 1/\|\hat{q}\| = 1$, and using (18) to eliminate c_j and s_j from (19) gives the recurrence relations stated in (20).

To obtain $\widetilde{L}$ we use Eq. (21) and the fact that $\widetilde{Q}$ is orthogonal. Thus

$$\widetilde{A} = \widetilde{A}\widetilde{Q}^T\widetilde{Q} = (I_{m+1} - \hat{q}\hat{q}^T)\widetilde{Q}^T\widetilde{Q} = (\widetilde{Q}^T - \hat{q}e_{m+1}^T)\widetilde{Q}$$

$$= \left(\begin{bmatrix} \widetilde{M} & q \\ \alpha\sigma^T & \alpha \end{bmatrix} - \hat{q}e_{m+1}^T \right) \widetilde{Q} = \begin{bmatrix} \widetilde{M} & 0 \\ \alpha\sigma^T & 0 \end{bmatrix} \widetilde{Q} \equiv \widetilde{L}\widetilde{Q},$$

as required. □

THEOREM A4 (LDV FACTORIZATION OF AN ELEMENTARY MATRIX). *Let A be a matrix of the form*

$$A = D - \begin{bmatrix} p \\ \alpha_2 \end{bmatrix} [p^T \quad \alpha_2],$$

where p is an m-vector, α_1 and α_2 are nonzero scalars,

$$D = \operatorname{diag}(d_1, d_2, \ldots, d_m, \alpha_1^2) \equiv \begin{bmatrix} D_1 & \\ & \alpha_1^2 \end{bmatrix},$$

and

$$\left\| D^{-1/2} \begin{bmatrix} p \\ \alpha_1 \end{bmatrix} \right\|^2 = p^T D_1^{-1} p + \frac{\alpha_2^2}{\alpha_1^2} = 1.$$

The matrix A has an LDV factorization $A = \hat{L}\hat{D}\hat{V}$ where

$$\hat{L} = \begin{bmatrix} \widetilde{M} & 0 \\ \alpha_2 \beta^T & 0 \end{bmatrix}, \quad \hat{D} = \operatorname{diag}(\bar{d}_1, \bar{d}_2, \ldots, \bar{d}_m, 1), \quad \hat{V} = \begin{bmatrix} \widetilde{M}^T & \alpha_2 \beta \\ p^T & \alpha_2 \end{bmatrix}, \tag{22}$$

and the matrix $\hat{D}^{1/2} \hat{V} D^{-1/2}$ is orthogonal. The matrix $\widetilde{M} = \widetilde{M}(p, \beta)$ is a special lower-triangular matrix and the vectors $\bar{d}$, and β are generated by the following recurrence relations:

$$\left.\begin{aligned} &23(\text{i}) \quad \textit{define } t_{m+1} = \alpha_2^2/\alpha_1^2; \\ &23(\text{ii}) \quad \textit{for } j = m, m-1, \ldots, 1 \textit{ set} \\ &\qquad t_j = t_{j+1} + p_j^2/d_j, \\ &\qquad \bar{d}_j = d_j t_{j+1}/t_j, \\ &\qquad \beta_j = -p_j/(d_j t_{j+1}). \end{aligned}\right\} \tag{23}$$

Proof. The matrix to be factorized can be written as

$$A = D - \begin{bmatrix} p \\ \alpha_2 \end{bmatrix} [p^T \quad \alpha_2] = D^{1/2}(I_{m+1} - \hat{q}\hat{q}^T)D^{1/2} = D^{1/2}\widetilde{A}D^{1/2},$$

where

$$q = D_1^{-1/2} p, \qquad \alpha = \alpha_2/\alpha_1, \qquad \hat{q} = \begin{bmatrix} q \\ \alpha \end{bmatrix}, \qquad \widetilde{A} = I_{m+1} - \hat{q}\hat{q}^T. \tag{24}$$

The requirement $p^T D_1^{-1} p + \alpha_2^2/\alpha_1^2 = 1$ ensures that $q^T q + \alpha^2 = \|\hat{q}\|^2 = 1$; and hence we know from Theorem A3 that $\widetilde{A}$ has the orthogonal factorization $\widetilde{A} = \widetilde{L}\widetilde{Q}$, where $\widetilde{L}$ and $\widetilde{Q}$ are constructed from the quantities q, σ, γ and α as shown. Let us define

$$\left.\begin{aligned} &\delta_j = d_j^{1/2}\gamma_j, \quad \bar{d}_j = \delta_j^2, \quad \beta_j = \sigma_j/\delta_j, \\ &\Delta = \operatorname{diag}(\delta_1, \delta_2, \ldots, \delta_m, 1), \quad e = (1, 1, \ldots, 1)^T. \end{aligned}\right\} \tag{25}$$

Using the notation of Theorem A3 we now have

$$A = D^{1/2}\widetilde{A}D^{1/2} = (D^{1/2}\widetilde{L})(\widetilde{Q}D^{1/2}),$$

where

$$D^{1/2}\widetilde{L} = \begin{bmatrix} D_1^{1/2} & 0 \\ & \alpha_1 \end{bmatrix}\begin{bmatrix} \widetilde{M}(q, \sigma, \gamma) & 0 \\ \alpha\sigma^T & 0 \end{bmatrix} = \begin{bmatrix} \widetilde{M}(p, \sigma, \delta) & 0 \\ \alpha_1\alpha\sigma^T & 0 \end{bmatrix}$$

(26a) $$= \begin{bmatrix} \widetilde{M}(p, \beta, e) & 0 \\ \alpha_2\beta^T & 0 \end{bmatrix}\Delta = \hat{L}\Delta$$

and

$$\widetilde{Q}D^{1/2} = \begin{bmatrix} \widetilde{M}(q, \sigma, \gamma)^T & \alpha\sigma \\ q^T & \alpha \end{bmatrix}\begin{bmatrix} D_1^{1/2} & \\ & \alpha_1 \end{bmatrix} = \begin{bmatrix} \widetilde{M}(p, \sigma, \delta)^T & \alpha_1\alpha\sigma \\ p^T & \alpha_1\alpha \end{bmatrix}$$

(26b) $$= \Delta\begin{bmatrix} \widetilde{M}(p, \beta, e)^T & \alpha_2\beta \\ p^T & \alpha_2 \end{bmatrix} = \Delta\hat{V}.$$

Combining (26a) and (26b) gives $A = \hat{L}\hat{D}\hat{V}$ where $\hat{L}$ and $\hat{V}$ are the matrices defined in (22), and

$$\hat{D} = \Delta^2 = \mathrm{diag}(\delta_1^2, \delta_2^2, \dots, \delta_m^2, 1) = \mathrm{diag}(\bar{d}_1, \bar{d}_2, \dots, \bar{d}_m, 1).$$

Equation (26b) also gives the orthogonal matrix $\widetilde{Q}$ as

$$\widetilde{Q} = \Delta\hat{V}D^{-1/2} = \hat{D}^{1/2}\hat{V}D^{-1/2},$$

as required.

Using the definitions of ρ_j, σ_j, γ_j and q_j in (20) and (24), we can now simplify the expressions for $\bar{d}_j$ and β_j in (25) as follows:

$$\bar{d}_j = d_j\gamma_j^2 = d_j\rho_{j+1}^2/\rho_j^2;$$
$$\beta_j = \sigma_j/(\gamma_j d_j^{1/2}) = -q_j/(\rho_{j+1}^2 d_j^{1/2}) = -p_j/(\rho_{j+1}^2 d_j).$$

From 20(i) we also have $\rho_{m+1}^2 = \alpha^2 = \alpha_2^2/\alpha_1^2$. Finally, as in Theorem A2, we define $t_j = \rho_j^2$ to avoid the computation of square roots. The recurrence relations (23) now follow and the theorem is proved. □

LEMMA A3 (CHOLESKY FACTORS OF $D_1 + pp^T$). *If p is an m-vector and $D_1 = \mathrm{diag}(d_1, d_2, \dots, d_m)$ where $d_i > 0$, the Cholesky factorization of $D_1 + pp^T$ is*

(27a) $$D_1 + pp^T = \widetilde{M}D_2\widetilde{M}^T,$$

where

$$D_2 = \mathrm{diag}(\bar{d}_1, \bar{d}_2, \dots, \bar{d}_m), \qquad \widetilde{M} = \widetilde{M}(p, \beta),$$

with

(27b) $$\widetilde{M}D_2\beta = p,$$

(27c) $$\beta^T D_2 \beta = 1 - \alpha^2 > 0.$$

The quantities $\bar{d}_j$, β_j *and* α^2 *are given by the recurrence relations* (12).

Proof. Using the notation and results of Theorem A2, we can write down the LDV factorization

(28) $$\begin{bmatrix} D_1 & p \\ & 1 \end{bmatrix} = \hat{L}\hat{D}\hat{V}.$$

If

$$D = \begin{bmatrix} D_1 & \\ & 1 \end{bmatrix}, \quad \hat{D} = \begin{bmatrix} D_2 & \\ & \alpha^2 \end{bmatrix}, \quad \widetilde{Q} = \hat{D}^{1/2}\hat{V}D^{-1/2},$$

then the matrix $\widetilde{Q}$ is orthogonal. Post-multiplying (28) by $D^{-1/2}$ gives

$$\begin{bmatrix} D_1^{1/2} & p \\ & 1 \end{bmatrix} = \hat{L}\hat{D}\hat{V}D^{-1/2} = \hat{L}\hat{D}^{1/2}\widetilde{Q},$$

and since $\widetilde{Q}\widetilde{Q}^T = I$ we have

$$\begin{bmatrix} D_1^{1/2} & p \\ & 1 \end{bmatrix}\begin{bmatrix} D_1^{1/2} & \\ p^T & 1 \end{bmatrix} = \hat{L}\hat{D}\hat{L}^T = \begin{bmatrix} \widetilde{M} & \\ \beta & 1 \end{bmatrix}\begin{bmatrix} D_2 & \\ & \alpha^2 \end{bmatrix}\begin{bmatrix} \widetilde{M}^T & \beta \\ & 1 \end{bmatrix}.$$

Hence

$$\begin{bmatrix} D_1 + pp^T & p \\ p^T & 1 \end{bmatrix} = \begin{bmatrix} \widetilde{M}D_2\widetilde{M}^T & \widetilde{M}D_2\beta \\ \beta^T D_2 \widetilde{M}^T & \beta^T D_2 \beta + \alpha^2 \end{bmatrix}$$

and relations (27) follow immediately. □

LEMMA A4 (CHOLESKY FACTORS OF $D_1 - pp^T$). *If p is an m-vector, D_1 = diag$(d_1, d_2, \ldots, d_m)$ where $d_i > 0$ and $\alpha^2 = 1 - p^T D_1^{-1} p > 0$, the Cholesky factorization of $D_1 - pp^T$ is*

(29a) $$D_1 - pp^T = \widetilde{M}\widetilde{D}_2\widetilde{M}^T,$$

where

$$D_2 = \text{diag}(\bar{d}_1, \bar{d}_2, \ldots, \bar{d}_m), \qquad \widetilde{M} = \widetilde{M}(p, \beta),$$

with

(29b) $$\widetilde{M}D_2\beta = -p,$$

(29c) $$\beta^T D_2 \beta = 1/\alpha^2 - 1 > 0.$$

The quantities $\bar{d}_j$ *and* β_j *are defined by the recurrence relations* (23), *with* 23(i) *replaced by* $t_{m+1} = \alpha^2$.

Proof. Using the notation and results of Theorem A4, we have $\alpha^2 = \alpha_2^2/\alpha_1^2$ and the LDV factorization

$$\begin{bmatrix} D_1 & \\ & \alpha_1^2 \end{bmatrix} - \begin{bmatrix} p \\ \alpha_2 \end{bmatrix} [p^T \quad \alpha_2] = \hat{L}\hat{D}\hat{V} \, (= \hat{L}\hat{D}\hat{L}^T) = \begin{bmatrix} \widetilde{M} & \\ \alpha_2 \beta^T & 0 \end{bmatrix} \begin{bmatrix} D_2 & \\ & 1 \end{bmatrix} \begin{bmatrix} \widetilde{M}^T & \alpha_2 \beta \\ p^T & \alpha_2 \end{bmatrix}.$$

Hence

$$\begin{bmatrix} D_1 - pp^T & -\alpha_2 p \\ -\alpha_2 p^T & \alpha_1^2 - \alpha_2^2 \end{bmatrix} = \begin{bmatrix} \widetilde{M} D_2 \widetilde{M}^T & \alpha_2 \widetilde{M} D_2 \beta \\ \alpha_2 \beta^T D_2 \widetilde{M}^T & \alpha_2^2 \beta^T D_2 \beta \end{bmatrix}$$

and relations (29) follow immediately. □

Division of Numerical Analysis and Computing
National Physical Laboratory
Teddington, Middlesex, England

Division of Numerical Analysis and Computing
National Physical Laboratory
Teddington, Middlesex, England

Applied Mathematics Division
DSIR, Wellington, New Zealand

1. R. FLETCHER & M. J. D. POWELL (1973), *On the Modification of LDL^T Factorizations*, AERE report, TP 519.

2. W. M. GENTLEMAN (1973), "Least squares computations by Givens transformations without square roots," *J. Inst. Math. Appl.*, v. 12, pp. 329–336. MR 48 #7575.

3. P. E. GILL, G. H. GOLUB, W. MURRAY & M. A. SAUNDERS (1974), "Methods for modifying matrix factorizations," *Math. Comp.*, v. 28, pp. 505–535.

4. E. HELLERMAN & D. RARICK (1971), "Reinversion with the preassigned pivot procedure," *Math. Programming*, v. 1, pp. 195–216. MR 45 #2895

5. E. HELLERMAN & D. RARICK (1972), "The partitioned preassigned pivot procedure (P^4)," *Sparse Matrices and Their Applications*, D. J. Rose and R. A. Willoughby (Editors), Plenum Press, New York, pp. 67–76. MR 48 #10075.

6. M. A. SAUNDERS (1972), *Product Form of the Cholesky Factorization for Large-Scale Linear Programming*, Report STAN–CS–72–301, Computer Science Department, Stanford University, Stanford, California.