

# Computing the CS Decomposition of a Partitioned Orthonormal Matrix

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**Summary.** This paper describes an algorithm for simultaneously diagonalizing by orthogonal transformations the blocks of a partitioned matrix having orthonormal columns.

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## 1. Introduction

The purpose of this paper is to describe an algorithm for computing the decomposition described in the following theorem.

**Theorem 1.1.** Let  $Q \in \mathbb{R}^{n \times p}$  have orthonormal columns. Partition  $Q$  in the form

$$Q = \begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix} \begin{matrix} k \\ \ell \end{matrix} \quad (k + \ell = n). \quad (1.1)$$

Then there are orthonormal matrices  $U_1 \in \mathbb{R}^{k \times k}$ ,  $U_2 \in \mathbb{R}^{(n-k) \times (n-k)}$ , and  $V \in \mathbb{R}^{p \times p}$ , such that

$$\begin{bmatrix} U_1^T & 0 \\ 0 & U_2^T \end{bmatrix} \begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix} V = \begin{bmatrix} U_1^T Q_1 V \\ U_2^T Q_2 V \end{bmatrix}$$

assumes one of the following forms

$$1. \ k \geq p, \ell \geq p$$

$$\begin{array}{c|c} \begin{bmatrix} C \\ 0 \\ S \\ 0 \end{bmatrix} & \begin{matrix} p \\ k-p \\ p \\ \ell-p \end{matrix} \end{array}$$

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$$\begin{array}{cc}
 2. \ k \geq p, \ell \leq p & 3. \ k \leq p, \ell \geq p \\
 \begin{array}{c} \ell \quad p-\ell \\ \left[ \begin{array}{cc} C & 0 \\ 0 & I \\ 0 & 0 \end{array} \right] \begin{array}{l} \ell \\ p-\ell \\ k-p \end{array} \\ \hline \left[ \begin{array}{cc} S & 0 \end{array} \right] \ell \end{array} & \begin{array}{c} k \quad p-k \\ \left[ \begin{array}{cc} C & 0 \\ S & 0 \\ 0 & I \\ 0 & 0 \end{array} \right] \begin{array}{l} k \\ k \\ p-k \\ \ell-p \end{array} \end{array} \\
 4. \ k \leq p, \ell \leq p & \\
 \begin{array}{c} n-p \quad p-\ell \quad p-k \\ \left[ \begin{array}{ccc} C & 0 & 0 \\ 0 & I & 0 \\ S & 0 & 0 \\ 0 & 0 & I \end{array} \right] \begin{array}{l} n-p \\ p-\ell \\ n-p \\ p-k \end{array} \end{array} & 
 \end{array}$$

Here  $C$  and  $S$  are nonnegative diagonal matrices satisfying

$$C^2 + S^2 = I. \tag{1.2}$$

This decomposition can be used to compute the generalized singular value decomposition [5, 10, 11] and a variety of decompositions relating to canonical angles between subspaces [1, 9]. A proof of a generalization of Theorem 1.1 is given in [5]. If the diagonal entries of  $C$  and  $S$  are denoted by  $\gamma_i$  and  $\sigma_i$ , then it follows from (1.2) that

$$\gamma_i^2 + \sigma_i^2 = 1.$$

Hence for some angle  $\theta_i$ , we have  $\gamma_i = \cos \theta_i$  and  $\sigma_i = \sin \theta_i$ . This accounts for the choice of letters  $C$  (cosine) and  $S$  (sine), and for the name “ $CS$  decomposition.”

The decomposition is not as complicated as the four forms listed above might suggest. The central idea – that  $Q_1$  and  $Q_2$  can be simultaneously diagonalized – is expressed by the first form. The remaining forms treat the special cases where  $Q_1$  or  $Q_2$  have too few rows to accommodate a full diagonal matrix.

This paper is organized as follows. In §2 we prove Theorem 1.1 for the special case  $k = \ell = p$ . The proof is constructive and suggests an algorithm; however, this algorithm is numerically unstable. In §3 we show how Jacobi’s method for the symmetric eigenvalue problem may be used to make the algorithm stable. In §4, it is shown how the special case  $k = \ell = p$  can be extended to the general theorem.

### 2. The Case $k = \ell = p$

In this section we assume that the matrices  $Q_1$  and  $Q_2$  in (1.1) are square and establish the existence of the  $CS$  decomposition, which in this case takes the form

$$\begin{bmatrix} U_1^T Q_1 \\ U_2^T Q_2 \end{bmatrix} V = \begin{bmatrix} C \\ S \end{bmatrix}. \quad (2.1)$$

To construct  $U_1$ ,  $V$ , and  $C$ , note that from (2.1)

$$U_1^T Q_1 V = C. \quad (2.2)$$

Since  $U_1$  and  $V$  are orthogonal and  $C$  is a nonnegative, diagonal matrix, (2.2) is the singular value decomposition of  $Q_1$ . Thus  $U_1$  is the matrix of left singular vectors of  $Q_1$  and  $V$  is the matrix of right singular vectors. The matrix  $C$  is the diagonal matrix of singular values of  $Q_1$ .

The matrix

$$\begin{bmatrix} C \\ \bar{Q}_2 \end{bmatrix} \equiv \begin{bmatrix} U_1^T & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix} V$$

has orthonormal columns. Hence,

$$C^2 + \bar{Q}_2^T \bar{Q}_2 = I, \quad (2.3)$$

which implies that

$$\bar{Q}_2^T \bar{Q}_2 = I - C^2$$

is diagonal. This means that the columns of  $\bar{Q}_2$  are orthogonal.

The matrix  $U_2$  is constructed as follows.

1. If  $\bar{q}_j^{(2)} \neq 0$  set  $u_j^{(2)} = \bar{q}_j^{(2)} / \|\bar{q}_j^{(2)}\|$ , where  $\|\cdot\|$  is the Euclidean norm. (2.4)
2. Fill in the remaining columns of  $U_2$  with an orthonormal basis for the orthogonal complement of the column space of  $\bar{Q}_2$ .

It then follows from the orthogonality of the columns of  $\bar{Q}_2$  that

1.  $U_2$  is orthogonal,
2.  $U_2^T \bar{Q}_2 = S$ , where  $S = \text{diag}(\sigma_1, \sigma_2, \dots, \sigma_p)$  with  $\sigma_j = \begin{cases} \|\bar{q}_j^{(2)}\| & q_j \neq 0 \\ 0 & q_j = 0 \end{cases}$ .

This completes the proof of Theorem 1.1 for  $k = \ell = p$ .

### 3. The algorithm

The construction described in §2 is effectively an algorithm for computing the CS decomposition of  $Q$ . Specifically, the singular value decomposition of  $Q_1$  may be calculated by standard techniques [3, 4, 7]. The formation of  $\bar{Q}_2 = Q_2 V$  requires only a matrix multiplication. The normalization of the nonzero columns of  $\bar{Q}_2$  in (2.4) is easy to accomplish. Finally, the orthonormal basis required in (2.4) may be computed in a number of ways (e.g. see [2, 3, 8]).

Unfortunately, this algorithm is unstable in the presence of rounding error. The problem occurs when some column  $\bar{q}_j^{(2)}$  of  $\bar{Q}_2$  has a norm smaller than  $\varepsilon_M^{\frac{1}{2}}$ , where  $\varepsilon_M$  is the rounding unit for the arithmetic used in the computation (e.g.,  $\varepsilon_M \cong 10^{-t}$  for  $t$ -digit, decimal, floating-point arithmetic). In this case it is possible for (2.3) to be satisfied up to rounding error, but for the columns of  $\bar{Q}_2$  to

be far from orthogonal. For example, with  $\varepsilon_M = 10^{-6}$  the use of the singular value decomposition of  $Q_1$  to reduce  $Q$  might give

$$\begin{bmatrix} C \\ \bar{Q}_2 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 3 \cdot 10^{-4} & 4 \cdot 10^{-6} \\ 4 \cdot 10^{-4} & 3 \cdot 10^{-6} \end{bmatrix}.$$

In this case, the transformed  $Q$  is orthogonal to working accuracy, since

$$I - C^2 - \bar{Q}_2^T \bar{Q}_2 = -10^{-7} \begin{bmatrix} 2.5 & 2.4 \cdot 10^{-2} \\ 2.4 \cdot 10^{-2} & 2.5 \cdot 10^{-4} \end{bmatrix}.$$

But if  $U_2$  is constructed according to (2.4), the result is

$$U_2 = \begin{bmatrix} 0.6 & 0.8 \\ 0.8 & 0.6 \end{bmatrix},$$

a matrix which is far from orthogonal.

To circumvent this problem, we suggest the following procedure.

1. Determine an orthogonal matrix  $J$  such that  $\bar{Q}_2 J$  can be normalized to give a matrix  $U_2$  that is orthogonal to working accuracy.
2. Determine an orthogonal matrix  $K$  such that  $K^T C J$  is diagonal.

If we then replace  $V$  by  $VJ$ , replace  $U_1$  by  $U_1 K$ , and form  $U_2$  from  $\bar{Q}_2 J$  as in (2.4), the result is

$$\begin{bmatrix} U_1^T Q_1 \\ U_2^T \bar{Q}_2 \end{bmatrix} V = \begin{bmatrix} K^T C J \\ U_2^T \bar{Q}_2 \end{bmatrix}. \quad (3.1)$$

Since  $K^T C J$  and  $U_2^T \bar{Q}_2$  are diagonal, (3.1) is the *CS* decomposition of  $Q$ .

Turning now to the determination of  $J$ , we first make the assumption that the columns of  $\bar{Q}_2$  are linearly independent. In practice, rounding error will almost certainly insure that this is true. The most likely exception occurs when a column of  $\bar{Q}_2$  is exactly zero, and this may be treated by replacing the column with a random vector of order  $\varepsilon_M$ . Alternatively, zero columns may be ignored while  $J$  is determined and then treated as in step 2 of (2.4).

We shall now make a precise statement of what is required of  $J$ . Let

$$(\bar{Q}_2 J)^T (\bar{Q}_2 J) = D^2 + E, \quad (3.2)$$

where  $D^2$  is a diagonal matrix consisting of the diagonal entries of  $(\bar{Q}_2 J)^T (\bar{Q}_2 J)$ . The matrix  $U_2$  formed by normalizing the columns of  $\bar{Q}_2 J$  is  $\bar{Q}_2 J D^{-1}$ . Hence from (3.2)

$$U_2^T U_2 = I + D^{-1} E D^{-1}, \quad (3.3)$$

and for  $U_2$  to be orthogonal to working accuracy it is required that the elements of  $D^{-1} E D^{-1}$  all be less than  $\varepsilon_M$ . In other words, if we set

$$A = \bar{Q}_2^T \bar{Q}_2, \quad (3.4)$$

then we wish to determine an orthogonal  $J$  such that  $J^T A J$  is nearly diagonal in the sense that

$$|e_{ij}| \leq \varepsilon_M d_i d_j, \quad (3.6)$$

where  $d_i$ ,  $d_j$ , and  $e_{ij}$  are elements in the decomposition (3.2).

From the foregoing, it is seen that  $J$  must be determined as an approximate set of eigenvectors of the matrix  $A$ , the goodness of the approximation being judged by (3.6). The most widely used method for solving symmetric eigenvalue problems is Householder tridiagonalization followed by the  $QR$  algorithm [7, 8]. However, this method behaves erratically when the elements of the matrix vary widely in size, as they may be expected to do in our application. Here the algorithm of choice is Jacobi's method. Ruitishauser [6] has published an elegant implementation of the algorithm, and we refer the reader to his paper for details. What follows is a brief description of the method, leading to an identity we shall need later.

The Jacobi method is an iteration in which zeros are introduced into the off-diagonal elements of  $A$  by plane rotations. Later transformations may destroy zeros introduced earlier; but if the order of the transformations is arranged properly the net effect is to cause all the off-diagonal elements to converge to zero – ultimately quadratically.

One step of the iteration goes as follows. First an off-diagonal element  $a_{ij}$  is selected for annihilation. The transformation  $J_{ij}$  that accomplishes this task has the form

$$J_{ij} = \begin{bmatrix} I_{i-1} & 0 & 0 & 0 & 0 \\ 0 & c & 0 & s & 0 \\ 0 & 0 & I_{j-i-1} & 0 & 0 \\ 0 & -s & 0 & c & 0 \\ 0 & 0 & 0 & 0 & I_{p-j} \end{bmatrix},$$

where

$$c^2 + s^2 = 1. \quad (3.7)$$

It is readily verified that the  $(i, j)$ -element of  $J_{ij}^T A J_{ij}$  is given by

$$a_{ii}cs + a_{ij}c^2 - a_{ij}s^2 - a_{jj}cs,$$

and setting this to zero gives the identity mentioned above:

$$(a_{jj} - a_{ii})cs = a_{ij}(c^2 - s^2). \quad (3.8)$$

It is always possible to find  $c$  and  $s$  satisfying (3.7) and (3.8) such that

$$s \leq c. \quad (3.9)$$

Whenever an element  $a_{ij}$  satisfies

$$|a_{ij}| \leq \varepsilon_M \sqrt{a_{ii}a_{jj}}$$

[cf. (3.6)], it is set to zero and the transformation is skipped. The rotations  $J_{ij}$  are accumulated in  $V$  and  $\bar{Q}_2$ ; i.e.  $V$  is replaced by  $VJ_{ij}$  and  $\bar{Q}_2$  by  $\bar{Q}_2J_{ij}$ .

It is important to remember that although we are diagonalizing  $A$ , it is the orthogonality of the columns of  $\bar{Q}_2$  that is the object of the process. These are equivalent provided the equality  $A = \bar{Q}_2^T \bar{Q}_2$  is maintained; however, there is a possibility that this relation will degrade as rotations are accumulated in  $A$  and  $\bar{Q}_2$ . Such a degradation will be signaled by cancellation in some diagonal element of  $A$ . We therefore recommend that the initial values  $\alpha_i$  of the  $a_{ii}$  be stored, and whenever a new value of  $a_{ii}$  is found to satisfy

$$a_{ii} \leq 0.1 \alpha_i \quad (\text{say}),$$

the  $i$ -th row and column of  $A$  be recomputed from the current value of  $\bar{Q}_2$ .

We have now completed the first part of our program: namely we have found a matrix  $J$ , consisting of the product of the rotations  $J_{ij}$ , for which  $\bar{Q}_2J$  can be normalized. We must now find a matrix  $K$  such that  $K^T CJ$  is diagonal. The surprising fact is that *we may take  $K=J$ , provided we do not perform certain unnecessary rotations.*

To see this, consider what happens when a Jacobi rotation  $J_{ij}$  is used to orthogonalize  $\bar{q}_i^{(2)}$  and  $\bar{q}_j^{(2)}$ . The result will be established if it can be shown that  $J_{ij}^T CJ_{ij}$  is nearly diagonal. The only elements of  $C$  affected by this transformation are those in the  $2 \times 2$  submatrix in rows and columns  $i$  and  $j$  of  $C$ . The transformed  $2 \times 2$  submatrix is given by

$$\begin{bmatrix} c & -s \\ s & c \end{bmatrix} \begin{bmatrix} \gamma_i & 0 \\ 0 & \gamma_j \end{bmatrix} \begin{bmatrix} c & s \\ -s & c \end{bmatrix} = \begin{bmatrix} \gamma_i c^2 + \gamma_j s^2 & (\gamma_i - \gamma_j) cs \\ (\gamma_i - \gamma_j) cs & \gamma_i s^2 + \gamma_j c^2 \end{bmatrix}. \quad (3.10)$$

Thus we must show that  $(\gamma_i - \gamma_j)cs$  is small.

Because the original matrix  $Q$  is assumed to be nearly orthogonal, the columns of

$$\begin{bmatrix} \gamma_i & 0 \\ 0 & \gamma_j \\ \bar{q}_i^{(2)} & \bar{q}_j^{(2)} \end{bmatrix}$$

are nearly orthogonal. Since  $a_{ij} = \bar{q}_i^{(2)T} \bar{q}_j^{(2)}$ , there are numbers  $\varepsilon_i$ , small compared with one, such that

$$\gamma_i^2 + a_{ii} = 1 + \varepsilon_i, \quad (3.11)$$

$$\gamma_j^2 + a_{jj} = 1 + \varepsilon_j. \quad (3.12)$$

Moreover, the cross-product

$$a_{ij} = \bar{q}_i^{(2)T} \bar{q}_j^{(2)} = (\gamma_i \ 0 \ \bar{q}_i^{(2)T}) \begin{bmatrix} 0 \\ \gamma_j \\ \bar{q}_j^{(2)} \end{bmatrix}$$

must also be small compared with one. From (3.11) and (3.12), it follows that

$$a_{jj} - a_{ii} = \varepsilon_j - \varepsilon_i + \gamma_i^2 - \gamma_j^2$$

Hence from (3.8)

$$(\gamma_i^2 - \gamma_j^2)cs = a_{ij}(c^2 - s^2) + (\varepsilon_i - \varepsilon_j)cs,$$

or

$$(\gamma_i - \gamma_j)cs = \frac{a_{ij}(c^2 - s^2) + (\varepsilon_i - \varepsilon_j)cs}{\gamma_i + \gamma_j}. \quad (3.13)$$

This shows that if  $\gamma_i + \gamma_j$  is bounded below, say

$$\gamma_i + \gamma_j \geq \tau,$$

then the off-diagonal element of  $J_{ij}^T C J_{ij}$  is proportional to the deviation of  $Q$  from orthogonality, as measured by  $\varepsilon_i$ ,  $\varepsilon_j$ , and  $a_{ij}$ .

Equation (3.13) suggests that  $J^T C J$  can be far from diagonal if  $\gamma_i + \gamma_j$  is small. However, in this case it is unnecessary to perform the rotation. To see this, ignore  $\varepsilon_i$  and  $\varepsilon_j$  in (3.11) and (3.12) to get, approximately,

$$a_{ii} \cong 1 - \gamma_i^2 \quad \text{and} \quad a_{jj} \cong 1 - \gamma_j^2.$$

It then follows from (3.3) and (3.4), that if  $q_i$  and  $q_j$  are normalized to give  $u_i$  and  $u_j$ ,

$$u_i^T u_j \cong \frac{a_{ij}}{\sqrt{(1 - \gamma_i^2)(1 - \gamma_j^2)}}.$$

Now when  $\gamma_i, \gamma_j \geq 0$  are restricted to satisfy  $\gamma_i + \gamma_j \leq \tau < 1$ , the function  $(1 - \gamma_i^2)(1 - \gamma_j^2)$  assumes minimum for  $\gamma_i = \tau, \gamma_j = 0$  or  $\gamma_j = \tau, \gamma_i = 0$ . Hence, approximately,

$$|u_i^{(2)T} u_j^{(2)}| \leq \frac{a_{ij}}{\sqrt{1 - \tau^2}}. \quad (3.14)$$

Thus the deviation from orthogonality of  $u_i^{(2)}$  and  $u_j^{(2)}$  is also proportional to the deviation of  $Q$  from orthogonality.

Thus we modify the Jacobi iteration by suppressing the rotation whenever

$$\gamma_i + \gamma_j \leq \tau.$$

A value of 0.7 for  $\tau$ , which makes the denominators in (3.13) and (3.14) approximately equal, would appear reasonable. As each rotation is computed, it must be accumulated in  $U_1$  as well as in  $\bar{Q}_2$  and  $V$ .

There remains the question of how to treat the diagonal elements of  $C$ . From (3.10), it is seen that the new  $i$ -th diagonal element is given by

$$\gamma_i c^2 + \gamma_j s^2 = \gamma_i + (\gamma_j - \gamma_i) s^2$$

From (3.8), (3.11) and (3.12) it follows that

$$(\gamma_j - \gamma_i) s^2 = \frac{a_{ij}(c^2 - s^2) + (\varepsilon_i - \varepsilon_j)cs}{\gamma_i + \gamma_j} t,$$

where by (3.9)  $t = s/c \leq 1$ . Since  $\gamma_i + \gamma_j \geq 0.7$ , we see that the diagonal entries of  $C$  are effectively unchanged in the passage to  $J_{ij}^T C J_{ij}$ .

It is instructive to note that the above analysis is not cast in terms of rounding error but in terms of the deviation of  $Q$  from orthogonality as measured by the size of  $I - Q^T Q$ . This is a consequence of the fact that the existence of the CS decomposition requires exact orthogonality. Any deviation from orthogonality must affect the attempt to compute the decomposition, even in exact arithmetic.

The following is a summary of the algorithm.

- 1: Compute the singular value decomposition  $U_1^T Q_1 V = C$  of  $Q_1$ ;
- 2:  $Q_2 := Q_2 V$ ;
- 3:  $A := Q_2^T Q_2$ ;
- 4: **loop** until  $|a_{ij}| \leq \sqrt{a_{ii} a_{jj}} \epsilon_M$  for all  $i, j$ ,  $i \neq j$ ;
- 4.1: select pivot indices  $i$  and  $j$ ;
- 4.2: **if**  $\gamma_i + \gamma_j \geq 0.7$  **then**
- 4.2.1: form the Jacobi rotation  $J$ ;
- 4.2.2:  $V := VJ$ ;
- 4.2.3:  $Q_2 := Q_2 J$ ;
- 4.2.4:  $U_2 := U_2 J$ ;
- 4.2.5:  $A := J^T A J$ ;
- 4.2.6: If  $a_{ii}$  or  $a_{jj}$  has decreased too much recompute the corresponding rows and columns of  $A$ ;
- 4.2: **end if**;
- 4: **end loop**;
- 5: normalize  $Q_2$  to give  $U_2$  and  $S$ ;

#### 4. The General Case

We shall now show how the general problem of computing the CS decomposition of a partitioning of  $Q$  can be reduced to that of computing a CS decomposition when  $Q_1$  and  $Q_2$  are square. There are four cases, corresponding to the four forms in Theorem 1.1; however, the first and the last forms illustrate the techniques sufficiently well, and only these will be treated here.

Assume that  $k, \ell \geq p$  in (1.1). Let  $\bar{U}_1$  and  $\bar{U}_2$  be orthogonal matrices with the property that the first  $p$  columns of  $\bar{U}_i$  contains the column space of  $Q_i$ . Such matrices may be effectively constructed by computing the  $QR$  decompositions of the  $Q_i$  [3, 8].

If  $\bar{U}_i$  is partitioned in the form

$$\bar{U}_i = \begin{bmatrix} \bar{U}_1^{(i)} & \bar{U}_2^{(i)} \end{bmatrix},$$

then  $\bar{U}_2^{(i)T} Q_i = 0$ . Hence

$$\begin{bmatrix} U_1^T & 0 \\ 0 & U_2^T \end{bmatrix} \begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix} = \begin{bmatrix} U_1^{(1)T} Q_1 \\ 0 \\ U_1^{(2)T} Q_2 \\ 0 \end{bmatrix},$$



and the problem reduces to that of computing the CS decomposition of a matrix

$$\begin{bmatrix} \bar{U}_1^{(1)T} Q_1 \\ \bar{U}_1^{(2)T} Q_2 \end{bmatrix},$$

whose submatrices are square.

Turning to the fourth form in Theorem 1.1, let

$$V_1 = \begin{pmatrix} k & p-k \\ V_1^{(1)} & V_2^{(1)} \end{pmatrix}$$

be an orthogonal matrix with the property that the column space of  $V_1^{(1)}$  contains the column space of  $Q_1^T$ . Then

$$QV_1 = \begin{bmatrix} Q_1 V_1^{(1)} & Q_1 V_2^{(1)} \\ Q_2 V_1^{(1)} & Q_2 V_2^{(1)} \end{bmatrix} = \begin{bmatrix} \bar{Q}_1 & 0 \\ \bar{Q}_2^{(2)} & \bar{Q}_2^{(2)} \end{bmatrix} \begin{matrix} k \\ p-k \\ \ell \end{matrix}$$

By orthogonality  $\bar{Q}_2^{(2)T} \bar{Q}_1^{(2)} = 0$  and  $\bar{Q}_2^{(2)} \bar{Q}_2^{(2)T} = I$ . Hence if

$$\bar{U}_2 = \begin{pmatrix} n-p & p-k \\ \bar{U}_1^{(2)} & \bar{Q}_2^{(2)} \end{pmatrix},$$

is orthogonal, then

$$\begin{bmatrix} I & 0 \\ 0 & \bar{U}_2^T \end{bmatrix} \begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix} V_1 = \begin{bmatrix} \bar{Q}_1 & 0 \\ \bar{Q}_2 & 0 \\ 0 & I \end{bmatrix} \begin{matrix} k \\ p-k \\ n-p \\ p-k \end{matrix}. \quad (4.1)$$

Now consider the matrix

$$\begin{bmatrix} \bar{Q}_1 \\ \bar{Q}_2 \end{bmatrix} \begin{matrix} k \\ n-p \end{matrix}$$

Since  $n-p = k - (p-\ell) \leq k$ ,  $\bar{Q}_2$  has more columns than rows. We may therefore apply a variant of the reduction just described to obtain an orthogonal matrix  $V_2$  and an orthogonal matrix

$$\bar{U}_1 = \begin{pmatrix} n-p & p-\ell \\ \bar{U}_1^{(1)} & \bar{U}_2^{(1)} \end{pmatrix},$$

such that

$$\begin{bmatrix} U_1^T & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} \bar{Q}_1 \\ \bar{Q}_2 \end{bmatrix} V_2 = \begin{bmatrix} \tilde{Q}_1 & 0 \\ 0 & I \\ \tilde{Q}_2 & 0 \end{bmatrix} \begin{matrix} n-p \\ p-\ell \\ n-p \end{matrix}. \quad (4.2)$$

If we combine (4.1) and (4.2), the result is a transform of  $Q$  that has the form

$$\begin{bmatrix} n-p & p-\ell & p-k \\ \tilde{Q}_1 & 0 & 0 \\ 0 & I & 0 \\ \tilde{Q}_2 & 0 & 0 \\ 0 & 0 & I \end{bmatrix} \begin{matrix} n-p \\ p-\ell \\ n-p \\ p-k \end{matrix},$$

in which the unreduced matrices  $\tilde{Q}_1$  and  $\tilde{Q}_2$  are square.

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