Numerical Methods for Computing Angles Between Linear Subspaces

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Abstract. Assume that two subspaces $F$ and $G$ of a unitary space are defined as the ranges (or null spaces) of given rectangular matrices $A$ and $B$. Accurate numerical methods are developed for computing the principal angles $\theta_k(F, G)$ and orthogonal sets of principal vectors $u_k \in F$ and $v_k \in G$, $k = 1, 2, \ldots, q = \dim(G) \leq \dim(F)$. An important application in statistics is computing the canonical correlations $\theta_k = \cos \theta_k$ between two sets of variates. A perturbation analysis shows that the condition number for $\theta_k$ essentially is $\max \{k(A), k(B)\}$, where $k$ denotes the condition number of a matrix. The algorithms are based on a preliminary $QR$-factorization of $A$ and $B$ (or $A^H$ and $B^H$), for which either the method of Householder transformations (HT) or the modified Gram-Schmidt method (MGS) is used. Then $\cos \theta_k$ and $\sin \theta_k$ are computed as the singular values of certain related matrices. Experimental results are given, which indicates that MGS gives $\theta_k$ with equal precision and fewer arithmetic operations than HT. However, HT gives principal vectors, which are orthogonal to working accuracy, which is not generally true for MGS. Finally, the case when $A$ and/or $B$ are rank deficient is discussed.

1. Introduction. Let $F$ and $G$ be given subspaces of a unitary space $\mathbb{E}^n$, and assume that

$$p = \dim(F) \geq \dim(G) = q \geq 1.$$  

The smallest angle $\theta_1(F, G) = \theta_1 \in [0, \pi/2]$ between $F$ and $G$ is defined by

$$\cos \theta_1 = \max_{u \in F} \max_{v \in G} u^T v, \quad ||u||_2 = 1, \quad ||v||_2 = 1.$$  

Assume that the maximum is attained for $u = u_1$ and $v = v_1$. Then, $\theta_2(F, G)$ is defined as the smallest angle between the orthogonal complement of $F$ with respect to $u_1$ and that of $G$ with respect to $v_1$. Continuing in this way until one of the subspaces is empty, we are led to the following definition.

Definition. The principal angles $\theta_k \in [0, \pi/2]$ between $F$ and $G$ are recursively defined for $k = 1, 2, \ldots, q$ by

$$\cos \theta_k = \max_{u \in F} \max_{v \in G} u^H v, \quad ||u||_2 = 1, \quad ||v||_2 = 1,$$

subject to the constraints

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\[ u_j^T u = 0, \quad v_k^T v = 0, \quad j = 1, 2, \ldots, k - 1. \]

The vectors \((u_1, \ldots, u_k)\) and \((v_1, \ldots, v_k)\) are called principal vectors of the pair of spaces.

We note that the principal vectors need not be uniquely defined, but the principal angles always are. The vectors \(V = (v_1, \ldots, v_k)\) form a unitary basis for \(G\) and the vectors \(U = (u_1, \ldots, u_k)\) can be complemented with \((p - q)\) unitary vectors so that \((u_1, \ldots, u_p)\) form a unitary basis for \(F\). It can also be shown that
\[ u_j^T v_k = \begin{cases} 0, & j \neq k, j = 1, \ldots, p, k = 1, \ldots, q. \end{cases} \]

For an introduction to these concepts, we refer to [1]. An up to date list of references can be found in [9].

Principal angles and vectors have many important applications in statistics and numerical analysis. In [7], the statistical models of canonical correlations, factor analysis and stochastic equations are described in these terms. The eigenvalue problem \(Ax = \lambda Bx\) can have continuous eigenvalues if the nullspaces associated with \(A\) and \(B\) intersect [13]. By taking the vectors \(u_k\) corresponding to \(\cos \theta_k = 1\), we get a unitary basis for the intersection, which can be used to simultaneously deflate \(A\) and \(B\). Other applications are found in the theory of approximate least squares [8] and in the computation of invariant subspaces of a matrix [21].

The purpose of this paper is to develop new and more accurate methods for computing principal angles and vectors, when the subspaces are defined as the ranges (or nullspaces) of two given matrices \(A\) and \(B\). In Section 2, we describe the standard method of computing canonical correlations and show why this method may give rise to a serious loss of accuracy. Assuming that unitary bases for \(F\) and \(G\) are known, we derive, in Section 3, formulas for computing principal angles and vectors from the singular values and vectors for certain matrices. To find out how accurately the angles are defined in the presence of uncertainties in \(A\) and \(B\), first order perturbation results are given in Section 4. In Section 5, different numerical methods for computing the unitary bases, and the use of the formulas from Section 3, are discussed with respect to efficiency and accuracy. The special problems which arise when \(A\) and/or \(B\) are exactly or nearly rank deficient are discussed in Section 6. Finally, some numerical results are given in Section 7.

2. Canonical Correlations. For a matrix \(A\), we denote the range of \(A\) by \(R(A)\) and the nullspace of \(A\) by \(N(A)\):
\[
R(A) = \{ u \mid Ax = u \}, \quad N(A) = \{ x \mid Ax = 0 \}.
\]

In the problem of canonical correlations, we have \(F = R(A)\), \(G = R(B)\) where \(A\) and \(B\) are given rectangular matrices. Then, the canonical correlations are equal to \(\cos \theta_k\), and it can be shown that
\[
\cos \theta_k = \sigma_k, \quad u_k = A y_k, \quad v_k = B z_k, \quad k = 1, 2, \ldots, q,
\]
where \(\sigma_k \geq 0\) are eigenvalues and \(y_k, z_k\) properly normalized eigenvectors to the generalized eigenvalue problem
\[
\begin{bmatrix}
0 & A'' B \\
B'' A & 0
\end{bmatrix}
\begin{bmatrix}
y \\
z
\end{bmatrix} = \sigma
\begin{bmatrix}
A'' A & 0 \\
0 & B'' B
\end{bmatrix}
\begin{bmatrix}
y \\
z
\end{bmatrix}.
\]
Assume for convenience that $A$ and $B$ have full column rank. The standard method [6] of computing canonical correlations is to compute $A^H A$, $B^H B$, $A^H B$ and perform the Choleski decompositions

$$A^H A = R_A^H R_A, \quad B^H B = R_B^H R_B,$$

where $R_A$ and $R_B$ are upper triangular.

The eigenvalue problem (5) is then equivalent to the eigenvalue problems for a pair of Hermitian matrices

$$MM^H y_i = \sigma_i^2 y_i, \quad MM^H z_i = \sigma_i^2 z_i$$

where

$$M = (R_A^H)^{-1}(A^H B)R_B^{-1}, \quad \hat{y}_i = R_A y_i, \quad \hat{z}_i = R_B z_i.$$

These can be solved by standard numerical methods.

When $q = 1$ and $B = b$, the principal angles and vectors are closely related to the least squares problem of minimizing $\|b - Ax\|_2$. In fact, with the notations above (but dropping subscripts), we have

$$y = x/\|Ax\|_2, \quad z = 1/\|b\|_2, \quad \sigma = \|Ax\|_2/\|b\|_2,$$

and (5) is reduced to

$$A^H bz = \sigma A^H Ay, \quad b^H Ay = \sigma b^H bz.$$

But the first equation here is the normal equations for $x = \sigma y/z$. Thus, the classical algorithm reduces for $q = 1$ to solution of the normal equations by Choleski's method.

Lately it has been stressed by several authors that forming the normal equations in single precision involves a loss of information which cannot be retrieved. For linear least squares problems, other methods without this disadvantage have been developed ([2], [16] and [17]). Our aim in this paper is to generalize these methods to the case when $q > 1$.

3. Solution Using Singular Values. In most applications, each subspace is defined as the range, or the complement of the range, of a given matrix. In this case, a unitary basis for the subspace may be computed in a numerically stable way by well-known methods for the QR-decomposition of a matrix. These methods will produce for an $m \times n$ matrix $A$, with $m \geq n$, a decomposition

$$A = (Q' \mid Q'') \begin{pmatrix} S & \times \n \end{pmatrix} \begin{pmatrix} p & n \end{pmatrix} \times \begin{pmatrix} m - p & n \end{pmatrix}$$

where rank($S$) = $p$ and $Q = (Q' \mid Q''$) is unitary. Then $Q'$ gives a unitary basis for the range of $A$, $R(A)$, and $Q''$ a unitary basis for the complement $[R(A)]^\perp$. Notice that the case when a subspace is defined as the nullspace $N(A^H)$ of a matrix $A^H$ is included, since $N(A^H) = [R(A)]^\perp$. The computation of unitary bases will be discussed in more detail in Sections 5 and 6, and we assume here that such bases have been obtained.

Recently, an efficient and numerically stable algorithm for computing the singular value decomposition [11] (SVD) of a matrix has been developed [17]. This algorithm
will be our basic tool for computing principal angles and vectors. The relation between
singular values and our problem is clear from the following theorem.

**Theorem 1.** Assume that the columns of $Q_A$ and $Q_B$ form unitary bases for two
subspaces of a unitary space $E^n$. Put

\[(6) \quad M = Q_B^* Q_B,\]

and let the SVD of this $p \times q$ matrix be

\[(7) \quad M = YCZ^*, \quad C = \text{diag}(\sigma_1, \ldots, \sigma_r),\]

where $Y^T Y = Z^T Z = ZZ^* = I$. If we assume that $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r$, then the
principal angles and principal vectors associated with this pair of subspaces are given by

\[(8) \quad \cos \theta_k = \sigma_k(M), \quad U = Q_A Y, \quad V = Q_B Z.\]

**Proof.** It is known [18] that the singular values and singular vectors of a matrix
$M$ can be characterized by

\[(9) \quad \sigma_k = \max_{||y|| = 1, ||z|| = 1} (y^T M z) = y_k^T M z_k,\]

subject to

\[y^T y_j = z^T z_j = 0, \quad j = 1, \ldots, k - 1.\]

If we put

\[u = Q_A y \in R(Q_A), \quad v = Q_B z \in R(Q_B),\]

then it follows that $||u||_2 = ||y||_2, ||v||_2 = ||z||_2$ and

\[y^T y_j = u^T u_j, \quad z^T z_j = v^T v_j.\]

Since $y^T M z = y^T Q_A^* Q_B z = u^T v$, (9) is equivalent to

\[\sigma_k = \max_{||w|| = 1, ||v|| = 1} (u^T v) = u_k^T v_k,\]

subject to

\[u^T u_j = v^T v_j = 0, \quad j = 1, \ldots, k - 1.\]

Now (8) follows directly from the definition of principal angles and vectors (2),
which concludes the proof.

For small angles, $\theta_k$ is not well determined from $\cos \theta_k$ and we now develop
formulas for computing $\sin \theta_k$. Let $Q_A$ and $Q_B$ be defined as in Theorem 1. For
convenience, we change the notations slightly and write (7) and (8) as

\[(10) \quad M = Y_A C Y_B^*, \quad U_A = Q_A Y_A, \quad U_B = Q_B Y_B.\]

We split $Q_B$ according to

\[(11) \quad Q_B = P_A Q_B + (I - P_A) Q_B = P_A Q_B + P_A^* Q_B,\]

where $P_A = Q_A Q_A^*$ is the orthogonal projection onto $R(Q_A)$. Here

\[P_A Q_B = Q_A Q_A^* Q_B = Q_A M = Q_A Y_A C Y_B^*,\]

and hence the SVD of the matrix $P_A Q_B$ is given by
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\[ PAQ_B = U_A C Y_B^H, \quad C = \text{diag}(\cos \theta_k). \]

Since \( PA(I - P_A) = 0 \), we get, from squaring (11),
\[ Q_B^H(I - P_A)^2 Q_B = I - Q_B^H P_A Q_B = Y_B(I - C^2) Y_B^H. \]

It follows that the SVD of \((I - P_A)Q_B\) can be written
\[ (I - P_A)Q_B = W_A S Y_B^H, \quad S = \text{diag}(\sin \theta_k). \]

Comparing (13) with (12), it is evident that \( W_A \) gives the principal vectors in the complement \([R(Q_A)]^\perp\) associated with the pair of subspaces \([R(Q_A)], R(Q_B))\).

We will, for the rest of this section, assume that, in addition to (1), we have \( p + q \leq m \). (This is no real restriction, since, otherwise, we have \((m - p) + (m - q) \leq m\), and we can work with the complements of \(R(Q_A)\) and \(R(Q_B)\) instead.) Then, \( \dim([R(Q_A)]^\perp) = m - p \geq q \), and we can choose the \( m \times q \) matrix \( W_A \) in (13) so that \( W_A^H U_A = 0 \).

By analogy, we have formulas similar to (12) and (13) related to the splitting \( Q_A = P_B Q_A + (I - P_B)Q_A \),
\[ (14) \quad P_B Q_A = U_BC Y_A^H, \quad (I - P_B) Q_A = W_B S Y_A^H, \]

where again, since \( m - q \geq p \geq q \), we can choose the \( m \times q \) matrix \( W_B \) so that \( W_B^H U_B = 0 \). From (14), we get
\[ U_A = Q_A Y_A = (U_B C + W_B S) Y_A^H Y_A = (U_B W_B) \begin{pmatrix} C \\ S \end{pmatrix}. \]

If we put
\[ P_{B,A} = U_A U_B^H = (U_B W_B) \begin{pmatrix} C \\ S \end{pmatrix} U_B^H, \]
then, since \( R(Q_B) = R(U_B) \), we have for any \( x \in R(Q_B) \) that \( P_{B,A} x = U_A U_B^H (U_B y) = U_A y \), and thus
\[ P_{B,A} x \in R(Q_A), \quad ||x||_2 = ||P_{B,A} x||_2. \]

We can now always find an \( m \times (m - 2q) \) matrix \( Z_B \) such that \((U_B W_B Z_B)\) is a unitary basis in \( E^m \). Then
\[ P_{B,A} = (U_B W_B | Z_B) \begin{pmatrix} C & S \\ S & C \end{pmatrix} \begin{pmatrix} U_B^H \\ 0 \end{pmatrix} \begin{pmatrix} \begin{pmatrix} C \\ S \end{pmatrix} & 0 \\ 0 & I \end{pmatrix} \begin{pmatrix} W_B^H \\ Z_B^H \end{pmatrix}. \]

is the matrix of a unitary transformation, mapping \( R(Q_B) \) into \( R(Q_A) \). Its restriction to \( R(Q_B) \) is \( P_{B,A} \), and it leaves all vectors in \( R(Z_B) \) unchanged. This transformation is called a direct rotation \([9]\) from \( R(Q_B) \) into \( R(Q_A) \). It is distinguished from other unitary transformations \( P \) taking \( R(Q_B) \) into \( R(Q_A) \) by the property that it minimizes each unitarily invariant norm of \((I - P)^H(I - P)\). If \( R(Q_B) \cap [R(Q_A)]^\perp \) is empty, then all \( \theta_k < \pi/2 \) and the direct rotation is uniquely determined.

Similarly, we can construct a direct rotation taking \( R(U_A) \) into \( R(Q_B) \). It is obvious that the relations between the two subspaces are very completely characterized by the quantities \( C, S, U_A, W_A, U_B \) and \( W_B \).
4. Perturbation of Principal Angles. We consider here how the principal angles between $R(A)$ and $R(B)$ change when the elements in $A$ and $B$ are subject to perturbations. We assume in this analysis that the matrices $A$ and $B$ are $m \times p$ and $m \times q$, respectively, and have linearly independent columns. Consider first a perturbation of $A$ only,

$$A_\epsilon = A + \epsilon E = (A + \epsilon E_1) + \epsilon E_2,$$

where we have split the perturbation into components in and orthogonal to $R(A)$,

$$E_1 = P_A E, \quad E_2 = (I - P_A)E.$$

Let the polar decomposition of $A + \epsilon E_1$ be

$$A + \epsilon E_1 = Q_A H_A, \quad Q_A^* Q_A = I, \quad H_A \text{ positive definite.}$$

Then, since $R(A) = R(A + \epsilon E_1)$, $Q_A$ gives a unitary basis for $R(A)$.

To get a unitary basis for $R(A_\epsilon)$, we first note that for small absolute values of $\epsilon$, the matrix

$$(A + \epsilon E)H_A^{-1} = Q_A + \epsilon F_2, \quad F_2 = (I - P_A)F, \quad F = EH_A^{-1},$$

is nearly orthogonal. Indeed, since $Q_A^* F_2 = Q_A^* P_A F = 0$, we have

$$S = I - (Q_A + \epsilon F_2)^* (Q_A + \epsilon F_2) = -\epsilon^2 F_2^* F_2,$$

and

$$(16) \quad \sigma_i(S) = \epsilon^2 \cdot \sigma_i^2(F_2) \leq \epsilon^2 \sigma_i^2(F).$$

Then, using a series expansion from [4] for the unitary factor $Q_A$, in the polar decomposition of $A_\epsilon H_A^{-1}$, it follows that

$$(Q_A + \epsilon F_2) = Q_A (I - S)^{1/2}$$

$$(17) \quad = Q_A \left( I - \frac{1}{2}S - \frac{3}{8}S^2 - \cdots - \left( \frac{1}{p} \right)^p S^p - \cdots \right),$$

where the matrix series converges if $\rho(S) = \sigma_1(S) < 1$.

Also, asymptotically, when $\epsilon \to 0$, $Q_A,\epsilon$ is the unitary matrix with range $R(A_\epsilon)$ which is closest to $Q_A$.

From the well-known inequalities for singular values [15, p. 30],

$$\sigma_k(A + B) \leq \sigma_k(A) + \sigma_k(B), \quad \sigma_k(AB) \leq \sigma_k(A)\sigma_k(B), \quad k = 1, 2, \cdots,$$

we get

$$(18) \quad \sigma_i(F) \leq \sigma_i(E)\sigma_i(H_A^{-1}) \leq \sigma_i(E)/(\sigma_p(A) - \epsilon \sigma_1(E_1)).$$

Since certainly $\sigma_i(E) \geq \sigma_i(E_1)$, a sufficient condition for convergence of (17) is that

$$\epsilon \sigma_i(E)/\sigma_p(A) \leq \frac{1}{2}.$$

Premultiplying (17) by $P_B$, we get

$$P_B Q_A \epsilon = P_B Q_A + \epsilon P_B (I - P_A)F + P_B Q_A \left( \frac{1}{2}S + \frac{3}{8}S^2 + \cdots + \left( \frac{1}{p} \right)^p S^p + \cdots \right),$$

from which we derive the inequality

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\[ |\sigma_k(P_B Q_A) - \sigma_k(P_B Q_A)| \leq \epsilon \cdot \sigma_1(P_B(I - P_A)) + \tau, \]

where

\[ \tau = 2\sigma_1(S) + \frac{1}{2} \sigma_1^2(S) + \cdots \leq \frac{1}{4} \sigma_1(S)/(1 - \sigma_1(S)). \]

Now, we have \( \sigma_1(P_B(I - P_A)) = \sin \theta_{\max} \) and, estimating \( \sigma_1(S) \) and \( \sigma_1(F) \) by (16) and (18), it follows that

(19) \[ |\Delta \cos \theta_k| \leq \delta \cdot \sin \theta_{\max} + O(\delta^2), \quad \delta = \epsilon \sigma_1(E)/\sigma_1(A). \]

If instead we premultiply (17) by \( (I - P_B) \) and proceed in the same way, we arrive at

(20) \[ |\Delta \sin \theta_k| \leq \delta \cdot \cos \theta_{\min} + O(\delta^2), \quad \delta = \epsilon \sigma_1(E)/\sigma_1(A). \]

Now, assume that both \( A \) and \( B \) are perturbed by \( \delta A \) and \( \delta B \), respectively, where

\[ \|\delta A\|_2/\|A\|_2 \leq \epsilon_A, \quad \|\delta B\|_2/\|B\|_2 \leq \epsilon_B. \]

Then

\[ \cos \theta_k = [\sigma_k(P_B Q_A) - \sigma_k(P_B Q_A)] + [\sigma_k(P_B Q_A) - \sigma_k(P_B Q_A)] \]

and, from (19), we get

(21) \[ |\Delta \cos \theta_k| \leq \epsilon \kappa(A) \sin \theta_{\max}(A, B) + \epsilon \kappa(B) \sin \theta_{\max}(A, B) + O(\delta^2), \]

where

\[ \kappa(A) = \sigma_1(A)/\sigma_{\max}(A), \quad \kappa(B) = \sigma_1(B)/\sigma_{\max}(B), \quad \delta = \epsilon \kappa(A) + \kappa(B). \]

A corresponding estimate holds for \( |\Delta \sin \theta_k| \). Obviously, we have \( \theta(A, B) = \theta(A, B) + O(\delta) \), and, thus, these estimates can be simplified to

\[ \left| \Delta \begin{bmatrix} \cos \theta_k \\ \sin \theta_k \end{bmatrix} \right| \leq \delta \begin{bmatrix} \sin \theta_{\max} \\ \cos \theta_{\min} \end{bmatrix} + O(\delta^2). \]

Combining these two estimates yields

\[ |2 \cdot \sin \frac{1}{2} \Delta \theta_k| \leq \delta g(\hat{\theta}_k) + O(\delta^2) \]

where

\[ g(\theta) = \min \left( \frac{\sin \theta_{\max}}{\sin \theta}, \frac{\cos \theta_{\min}}{\cos \theta} \right), \quad \hat{\theta}_k = \theta_k + \frac{1}{2} \Delta \theta_k. \]

The maximum of \( g(\theta) \) for \( 0 \leq \theta \leq \pi/2 \) is attained for

\[ \theta = \arctan(\sin \theta_{\max}/\cos \theta_{\min}). \]

Since \( 2 \cdot \sin \frac{1}{2} \Delta \theta = \Delta \theta + O(\Delta \theta^3) \), it follows that

(22) \[ |\Delta \theta_k| \leq g_{\max}(\epsilon_A \kappa(A) + \epsilon_B \kappa(B)) + O(\delta^3), \]

where

\[ g_{\max} = (\sin^2 \theta_{\max} + \cos^2 \theta_{\min})^{1/2} \leq 2^{1/2}. \]

We conclude that when both \( \kappa(A) \) and \( \kappa(B) \) are small, then the angles \( \theta_k \) are well determined.
We note that, if the columns in $A$ are scaled, then $\kappa(A)$ will change but not $R(A)$. Also, the numerical algorithms for the $QR$-decomposition have the property that, unless column pivoting is used, they give the same numerical results independent of such a scaling. Therefore, it is often more relevant to take in (21) as condition number for $A$ the number

$$
\kappa'(A) = \min_{D} \kappa(AD), \quad D = \text{diag}(d_1, \ldots, d_p).
$$

It has been shown in [20] and [21] that $\kappa(AD)$ is not more than a factor of $p^{1/2}$ away from its minimum, if in $AD$ all columns have equal $L_2$-norm. This suggests that $A$ and $B$ should be assumed to be preconditioned so that

$$
\|a_i\|_2 = \|b_j\|_2 = 1, \quad i = 1, \ldots, p, \quad j = 1, \ldots, q.
$$

We remark that $\kappa'(A)$ is essentially the spanning precision of the basis in $R(A)$ provided by $A$ as defined in [21].

5. Numerical Methods. We assume in this section that the columns in $A$ and $B$ are linearly independent. The singular and near singular case will be briefly discussed in Section 6. For convenience, we also assume that $A$ and $B$ are real matrices, although all algorithms given here can easily be generalized to the complex case. Computed quantities will be marked by a bar.

In order to get the orthogonal bases for $F$ and $G$, we need the $QR$-decompositions of the matrices $A$ and $B$. We now describe two efficient methods for computing these. In the method of Householder triangularizations (HT) [16], orthogonal transformations of the type $Q_k = I - 2w_kw_k^T$ are used, where

$$
w_k = (0, \ldots, 0, w_{kk}, \ldots, w_{mk})^T, \quad \|w_k\|_2 = 1.
$$

The $m \times p$ matrix $A$ is reduced to triangular form using premultiplications

$$
Q_p \cdots Q_2 Q_1 A = \begin{pmatrix} R_A & \mid_{p}^p \mid_{m-p}^m \end{pmatrix}
$$

where $w_k$ is chosen so that $Q_k$ annihilates the appropriate elements in the $k$th column. Since $Q_k^{-1} = Q_k$, orthogonal bases $Q_A$ for $R(A)$ can then be computed by premultiplying the first $p$ columns in the unit matrix $I_m$ by the same transformations in reversed order,

$$
Q_A = Q_1 Q_2 \cdots Q_p \begin{pmatrix} I_p \\ 0 \end{pmatrix}.
$$

For this method, a very satisfactory error analysis is given in [23].

Assume that floating point arithmetic with a mantissa of $t$ binary digits is used, and that inner-products are accumulated in double precision wherever possible. Then, there exists an exactly orthogonal matrix $Q$ such that the computed matrices satisfy

$$
Q^T(A + E_A) = \begin{pmatrix} R_A \\ 0 \end{pmatrix}, \quad \bar{Q}_A = Q \begin{pmatrix} I_p \\ 0 \end{pmatrix} + F_A = Q_A + F_A,
$$

$$
\|E_A\|_F = 12.5p2^{-t} \|A\|_F, \quad \|F_A\|_F = 12.5p^{3/2}2^{-t},
$$

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where \( Q_A \) is an exactly orthogonal basis for \( R(A + E_A) \). From this and a similar estimate for \( Q_B \), we get

\[
|\sigma_k(M) - \sigma_k(\bar{M})| \leq \sigma_1(M - \bar{M}) \leq 13.0(p^{3/2} + q^{3/2})2^{-t},
\]

where \( \bar{M} = Q_A^T Q_B \) and the constant 13.0 accounts for the rounding errors in computing the product \( Q_A^T Q_B \). We have \( \sigma_k(\bar{M}) = \cos \bar{\theta}_k \), where \( \bar{\theta}_k \) are the exact angles between \( (A + E_A) \) and \( (B + E_B) \). Thus, the difference between \( \bar{\theta}_k \) and \( \theta_k \) can be estimated from (22).

\[
|\bar{\theta}_k - \theta_k| \leq 12.5 \cdot 2^{1/2} \cdot \delta + O(\delta^2), \quad \delta = (p(\kappa(A) + q\kappa(B)))2^{-t}.
\]

Finally, the errors \( \sigma_k(\bar{M}) - \sigma_k(M) \) in computing the singular values of \( \bar{M} \), using the procedure in [17], will be of the same order of magnitude as those in (24).

The error estimate given above is satisfactory, except when \( \theta_k \ll 1 \). In this case, the errors in \( \cos \theta_k \) from (24) will give rise to errors in \( \theta_k \) which may be much larger than those in (25). We return later to the problem of accurately computing small angles.

An orthogonal basis \( Q_A' \) for \( [R(A)]^\perp = N(A^T) \) can be obtained by applying the transformations \( Q_k, k = p, \ldots, 1 \), to the last \( (n - p) \) columns in \( T_n \),

\[
Q_A' = Q_1 Q_2 \cdots Q_p \left( \begin{array}{c} 0 \\ 1_{n-p} \end{array} \right).
\]

Also, in this case, the estimate (23) for \( Q_A' \), (24) and (25) still hold if the factor \( p^{3/2} \) is everywhere replaced by \( p(m - p)^{3/2} \).

The QR-decomposition of a matrix \( A \) can also be computed using the modified Gram-Schmidt method (MGS) [2]. The matrix \( A \) is then transformed in \( p \) steps, \( A = A_1, A_2, \ldots, A_{p+1} = Q_A \) where

\[
A_k = (q_1, \ldots, q_{k-1}, a_k^{(k)}, \ldots, a_p^{(k)}).
\]

The matrix \( A_{k+1}, k = 1, 2, \ldots, p \), is computed by

\[
q_k = a_k^{(k)}/||a_k^{(k)}||_2, \quad a_j^{(k+1)} = (I - q_k q_k^T)a_j^{(k)}, \quad j > k,
\]

and the elements in the \( k \)th row of \( R_A \) are

\[
r_{kk} = ||a_k^{(k)}||_2, \quad r_{kj} = q_k^T a_j^{(k)}, \quad j > k.
\]

It has been shown in [2, pp. 10, 15] that the computed matrices \( \bar{R}_A \) and \( Q_A \) satisfy

\[
A + E_A = \bar{Q}_A \bar{R}_A, \quad ||E_A||_F \leq 1.5(p - 1)2^{-t} ||A||_F,
\]

\[
||Q_A - \bar{Q}_A||_2 \leq p(p + 1)k(A)2^{-t},
\]

where \( Q_A \) is an exactly orthogonal basis for \( R(A + E_A) \) and quantities of order \( \kappa(A)2^{-2t} \) have been neglected. With MGS, \( Q_A \) will in general not be orthogonal to working accuracy, and, therefore, we cannot hope to get principal vectors which are nearly orthogonal. Also, the condition numbers \( \kappa(A) \) and \( \kappa(B) \) will enter in the estimate corresponding to (24). However, since \( \kappa(A) \) and \( \kappa(B) \) already appear in (25), we can hope to get the principal angles as accurately as with HT. Experimental results reported in Section 7 indicate that this actually is the case.
An advantage with MGS is that the total number of multiplications required to compute $R_A$ and $Q_A$ is less than for HT, i.e.,

\[ \text{MGS: } p^2m, \quad \text{HT: } 2p^2(m - p/3). \]

If only the principal angles are wanted, then the number of multiplications in the SVD-algorithm is approximately $2q^2(p - q/3)$. Thus, when $m \gg p$, the dominating work is in computing $Q_A$ and $Q_B$ and, in this case, MGS requires only half as much work as HT. If also the principal vectors are wanted, we must compute the full SVD of $M = Y_A C y_B^T$. Assuming two iterations per singular value, this requires approximately $7q^2(p + 10q/21)$ multiplications. To compute $U_A = Q_A Y_A$ and $U_B = Q_B Y_B$ a further $mq(p + q)$ multiplications are needed.

To get a basis for $[R(A)]^\top$ using MGS, we have to apply the method to the bordered matrix $(A | I_n)$, and, after $zzz$ steps, pick out $(zzz - p)$ appropriate columns. Especially when $(zzz - p) \ll zzz$, the number of multiplications compares unfavourably with HT,

\[ \text{MGS: } n^2(m + 2p), \quad \text{HT: } 2mp(m - p) + \frac{3}{2}p^3. \]

In some applications, e.g. canonical correlations, we want to express the principal vectors as linear combinations of the columns in $A$ and $B$, respectively. We have $U_A = Q_A Y_A = A(R_A^{-1} Y_A)$, and hence

\[ U_A = A X_A, \quad U_B = B X_B, \]

where

\[ X_A = R_A^{-1} Y_A, \quad X_B = R_B^{-1} Y_B. \]

We remark that if we let $\bar{X}_A$ and $\bar{X}_B$ denote the computed matrices, then $AX_A$ and $BX_B$ will not in general be orthogonal to working accuracy even when HT is used.

We now turn to the problem of accurately determining small angles. One method is to compute $\sin \theta_e$ from the SVD (13) of the matrix

\[ G = (I - P_A)Q_B = Q_B - Q_A M. \]

If we put $\bar{G} = Q_B - Q_A \bar{M}$, then, using $\bar{Q}_A = Q_A + F_A$, we get

\[ \bar{Q}_B + \bar{Q}_A (\bar{Q}_A^T Q_B) = \bar{G} + (I - Q_A Q_A^T) F_B + (Q_A F_A^T + F_A Q_A^T)(Q_B + F_B). \]

Neglecting second order quantities,

\[ ||\bar{Q} - \bar{G}||_2 \leq ||F_B||_2 + 2||F_A||_2 + 2q^{1/2}2^{-\epsilon}, \]

where the last term accounts for the final rounding of the elements in $\bar{M}$ and $\bar{G}$. Thus, if $\bar{Q}_A$ and $\bar{Q}_B$ are computed by HT, we have, from (23),

\[ |\sigma_k(\bar{G}) - \sigma_k(\bar{G})| \leq 13.2(q^{3/2} + 2p^{3/2})2^{-\epsilon}. \]

It follows that the singular values of the computed matrix $\bar{G}$ will differ little from $\sin \theta_e$, and, thus, small angles will be as accurately determined as is allowed by (25). From (26), the corresponding error estimate for MGS is obtained. In the spirit of the modified Gram-Schmidt method, the matrix $G$ should be computed as

\[ G = (I - q_1 q_1^T) \cdots (I - q_m q_m^T) Q_B. \]
Computational experience indicates that this gives much improved accuracy in \( \sin \theta \) when \( \kappa(A) \gg \kappa(B) \).

Since the matrix \( G \) is \( m \times q \), computing the singular values of \( G \) when \( m \gg q \) will require about \( 2mq^2 \) multiplications. If \( Y_A \) has been computed, then the SVD of \( G \) may be computed with only \( mq^2 \) multiplications from

\[
G Y_B = (I - P_A)Q_B Y_B = W_A S.
\]

Moreover, if \( U_A \) and \( U_B \) are available, we can obtain \( \sin \theta \) from

\[
(U_B - U_A C)^{T}(U_B - U_A C) = S^2
\]

or, alternatively,

\[
(U_B - U_A)^{T}(U_B - U_A) = 2(I - C).
\]

From the last equation, we can compute \( 2 \sin \frac{1}{2} \theta_k = (2(1 - \cos \theta_k))^{1/2} \), which, since \( 0 \leq \frac{1}{2} \theta_k \leq \pi/4 \), accurately determines both \( \sin \theta_k \) and \( \cos \theta_k \).

We finally remark about an apparent imperfection of MGS. When \( A = B \) (exactly), we will obviously get \( \tilde{Q}_A = \tilde{Q}_B \). The exact angle equals zero, and HT will always give computed angles near zero. This is not true for MGS, however, since we only have the estimate

\[
||I - \tilde{Q}^{T}_A \tilde{Q}_A||_2 \leq 2p(p + 1)\kappa(A)2^{-1}.
\]

Therefore, the singular values of \( \tilde{M} = \tilde{Q}^{T}_A \tilde{Q}_A \) may not be near one when \( \kappa(A) \) is large. If, however, only \( A \simeq B \), then the rounding errors in computing \( Q_A \) and \( Q_B \) will not be correlated, and in an ill-conditioned case, we will probably not get all angles near zero either with HT or MGS.

When \( A = B \), then \( \tilde{M} = \tilde{Q}^{T}_A \tilde{Q}_A \) will be symmetric and, thus, SVD will give \( \tilde{Y}_A \simeq \tilde{Y}_B \) and, therefore, \( \tilde{U}_A \simeq \tilde{U}_B \) also with MGS. It follows that, if (32) is used, MGS will always yield angles near zero in this case.

We have not tried to determine error estimates for the methods based on (30)-(32). On the test matrices described in Section 7, the method based on (28) gave significantly more accurate results, especially for the more well-conditioned angles.

6. The Singular Case. We now consider the case when \( A \) and/or \( B \) does not have full column rank. In this case, the problem of computing principal angles and vectors is not well posed, since arbitrarily small perturbations in \( A \) and \( B \) will change the rank of \( A \) and/or \( B \). The main computational difficulty then lies in assigning the correct rank to \( A \) and \( B \). The most satisfactory way of doing this generally is the following [10]. Let the \( m \times p \) matrix \( A \) have the SVD

\[
A = Q_A D_A V_A^{T}, \quad D_A = \text{diag}(\sigma_1(A)),
\]

Let \( \epsilon \) be a suitable tolerance and determine \( p' \leq p \) from

\[
\sum_{j=\mu}^{n} \sigma_{j}(A) \leq \epsilon^2 < \sum_{j=\mu'}^{n} \sigma_{j}(A).
\]

We then approximate \( A \) with an \( m \times p \) matrix \( A' \) such that \( \text{rank}(A') = p' \),

\[
A' = (Q'_A Q'_B) \begin{pmatrix} D'_A & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} V'_A & V'_B \end{pmatrix}^{T}, \quad D'_A = \text{diag}(\sigma_1, \ldots , \sigma_{p'}),
\]

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where \( Q_A = (Q_A' Q_A'') \), \( V_A = (V_A' V_A'') \) have been partitioned consistently with the diagonal matrix. The matrix \( B \) is approximated in the same way.

If, instead of (1), we assume that
\[
p' = \text{rank}(A') \geq \text{rank}(B') = q' \geq 1,
\]
then we can compute the principal angles and vectors associated with \( R(A') \) and \( R(B') \) by the previously derived algorithms, where now \( Q_A' \) and \( Q_B' \) should replace \( Q_A \) and \( Q_B \).

In order to express the principal vectors of \( R(A') \) as linear combinations of columns in \( A' \), we must solve the compatible system
\[
A'X_A = U_A = Q_A' Y_A.
\]
Since \( V_A'' \) is an orthogonal basis for \( N(A) \), the general solution can be written
\[
X_A = V_A' D_A'^{-1} Y_A + V_A'' C_A,
\]
where \( C_A \) is an arbitrary matrix. It follows that, by taking \( C_A = 0 \), we get the unique solution which minimizes \( \|X_A\|_F \); cf. [17]. Thus, we should take
\[
(34) \quad X_A = V_A' D_A'^{-1} Y_A, \quad X_B = V_B' D_B'^{-1} Y_B,
\]
where \( X_A \) is \( p \times p' \) and \( X_B \) is \( q \times q' \).

The approach taken above also has the advantage that only one decomposition, the SVD, is used throughout. It can, of course, also be used in the nonsingular case. However, computing the SVD of \( A \) and \( B \) requires much more work than computing the corresponding \( QR \)-decompositions. In order to make the \( QR \)-methods work also in the singular case, column pivoting must be used. This is usually done in such a way ([2], [12] and [16]) that the triangular matrix \( R = (r_{ij}) \) satisfies
\[
\sum_{i=1}^{j} |r_{ii}| < j \leq n.
\]
Such a triangular matrix is called normalized, and, in particular, the sequence \( |r_{11}|, |r_{22}|, \ldots, |r_{pp}| \) is nonincreasing. In practice, it is often satisfactory to take the numerical rank of \( A \) to be \( p' \) if for a suitable tolerance \( \varepsilon \) we have
\[
(35) \quad |r_{p'p'}| > \varepsilon \geq |r_{p'+1,p'+1}|.
\]
We then approximate \( A = Q_AR_A \) by a matrix \( A' = Q_AR_A' \) of rank \( p' \) by putting
\[
r_{i'i} = r_{i'i}, \quad i \leq p', \quad r_{i'i} = 0, \quad i > p'.
\]
It has been shown in [14] how to obtain the solution (32) of minimum length from this decomposition.

If we use the criterion (33), there is a risk of choosing \( p' \) too large. Indeed, it seems difficult to improve on the inequalities [12]
\[
(36) \quad 3(4^k + 6k - 1)^{-1/2} |r_{kk}| \leq \sigma_k(A) \leq (n + k + 1)^{1/2} |r_{kk}|
\]
from which it is seen that \( \sigma_k(A) \) may be smaller than \( |r_{kk}| \) by a factor of magnitude \( 2^{-k} \).

However, this rarely occurs in practice. Often the inequality
\[
\kappa(A) \geq |r_{11}|/|r_{pp}|,
\]
where \( \kappa(A) \) is the condition number of \( A \), is much larger than \( |r_{kk}| \).
represents a pretty good approximation to the condition number for the nonsingular case.

7. Test Results. The algorithms in Section 5 have been tested on the UNIVAC 1108 of Lund University. Single precision floating-point numbers are represented by a normalized 27 bit mantissa, whence the machine precision is equal to $2^{-26} \approx 1.5 \cdot 10^{-8}$.

For the tests, we have taken $F = R(A)$, where $A$ is the $m \times p$ matrix

$$A = \frac{1}{k^{1/2}} \begin{pmatrix} e & 0 & \cdots & 0 \\ 0 & e & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & e \end{pmatrix} \; \frac{1}{m/p}, \quad e = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}$$

and $m/p$ is an integer. Thus, $A$ is already orthogonal, and we can take $Q_A = A$. Further, $G = R(B)$ where $B$ is the $m \times p$ Vandermonde matrix

$$B = \begin{pmatrix} 1 & x_0 & \cdots & x_0^{p-1} \\ 1 & x_1 & \cdots & x_1^{p-1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{m-1} & \cdots & x_{m-1}^{p-1} \end{pmatrix}, \quad x_i = -1 + 2i/(m + 1).$$

The condition number $\kappa(B)$ is known to grow exponentially with $p$, when the ratio $m/p$ is kept constant. These matrices $A$ and $B$ are the ones appearing in [6]. There is exactly one vector, $u = (1, 1, \cdots, 1)^T$, which belongs to both $F$ and $G$, so there will be one minimum angle $\theta = 0$.

For the tests, the matrix $B$ was generated in double precision and then rounded to single precision. The procedures used for the $QR$-decompositions are apart from minor details identical with procedures published in [3] and [5]. The columns were implicitly scaled to have equal $L_2$-norm and column pivoting was performed. Inner products were not accumulated in double precision. For checking purposes, a three term recurrence relation [8] was used in double precision to compute an exact single precision orthogonal basis for $R(B)$.

For $m/p = 2$ and $p = 5(2)17$, $Q_A$ was computed both by the method of Householder and the modified Gram-Schmidt method. Then $\cos \theta_i$, $Y_A$ and $Y_B$ were com-

| Table 1 |
|---|---|---|---|---|---|---|
| $m$ | $p$ | $F(U_A)$ | $F(U_B)$ | $m(\cos \bar{\theta}_i)$ | $F(U_A)$ | $F(U_B)$ | $m(\cos \bar{\theta}_i)$ |
| 10 | 5 | 15 | 21 | 5 | 20 | 18 | 4 |
| 14 | 7 | 22 | 35 | 8 | 27 | 33 | 10 |
| 18 | 9 | 40 | 27 | 10 | 37 | 437 | 41 |
| 22 | 11 | 42 | 29 | 38 | 40 | 1130 | 49 |
| 26 | 13 | 58 | 48 | 1416 | 47 | 9013 | 621 |
| 30 | 15 | 62 | 51 | 2535 | 60 | 55322 | 1758 |
| 34 | 17 | 68 | 60 | 7582 | 76 | 788466 | 32650 |
Table 2

<table>
<thead>
<tr>
<th>$k$</th>
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<th>$p = 13$</th>
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<th>Gram-Schmidt</th>
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Table 3

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<th>$m(\sin \hat{\theta}_k)$</th>
<th>$m(\sin \tilde{\theta}_k)$</th>
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1 $\sin \tilde{\theta}_k$ computed as $\sigma_k(I - P_A)Q_A$, $\sin \hat{\theta}_k$ as $\sigma_k(I - P_B)Q_A$.

...computed by the procedure in [17], and finally $U_A$ and $U_B$ from (11). The results are shown in Table 1, where

$$m(\sigma_k) = \max_k |\sigma_k - \hat{\sigma}_k| \cdot 10^8, \quad F(U) = \|I - U^TU\|_F \cdot 10^8.$$  

Notice, that because of rounding errors in the computation of the SVD, the values $\sigma_k$ are not exact to single precision.

For the Gram-Schmidt method, the predicted lack of orthogonality in $U_B$, when $\kappa(B)$ is large, is evident. However, there is no significant difference in the accuracy of $\cos \tilde{\theta}_k$ between the two methods. In Table 2, we show for $m = 26$ and $p = 13$ the errors in $\cos \tilde{\theta}_k$ for each $k$.

For the same values of $m$ and $p$, $\sin \theta_k$ were computed from the singular values of both the matrix $(I - P_A)Q_B$ and the matrix $(I - P_B)Q_A$. The results in Table 3 again show no significant difference in accuracy between the two methods. For the Gram-Schmidt method, the values of $\sin \hat{\theta}_k$ differ somewhat between the two matrices,
Table 4

<table>
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\(^1\) sin \(\hat{\theta}_k\) computed as \(\sigma_d((I - P_A)Q_B)\), sin \(\hat{\theta}_k\) as \(\sigma_d((I - P_B)Q_A)\).

whereas the corresponding values for the Householder method are almost identical. This is confirmed by Table 4, where, again for \(m = 26, p = 13\), results for each \(k\) are shown. For the Gram-Schmidt method the matrix \((I - P_B)Q_A\) was computed both from (28) as \(Q_A = Q_d(Q_b^T Q_d)\) and from (29) as \(\prod (I - q_i q_i^T)Q_B\). The results in Table 3 clearly show that (29) should be used.

The authors are very pleased to acknowledge the help of Mr. Jan Svensson, who carried out most of the tests described in this section.

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