AN EFFECTIVE AND ROBUST ALGORITHM FOR FINDING PRINCIPAL ANGLES BETWEEN SUBSPACES USING AN A-BASED SCALAR PRODUCT

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Abstract. Computation of principal angles between subspaces is important in many applications, e.g., in statistics and information retrieval. In statistics, the angles are closely related to measures of dependency and covariance of random variables. When applied to column-spaces of matrices, the principal angles describe canonical correlations of a matrix pair. We highlight that all popular software codes for canonical correlations compute only cosine of principal angles, thus, making impossible, because of round-off errors, finding small angles accurately. We review a combination of sine and cosine based algorithms that provides accurate results for all angles. We generalize the method to the computation of principal angles in an A-based scalar product, for a symmetric and positive definite matrix A. We prove basic perturbation theorems for absolute errors for sine and cosine of principal angles with improved constants. Numerical examples and a detailed description of our code are given.

Key words. principal angles, canonical correlations, subspaces, scalar product, orthogonal projection, algorithm, accuracy, round-off errors, perturbation analysis

1. Introduction.

Let us consider two real-valued matrices F and G, each with n rows, and their corresponding column-spaces $\mathcal{F}$ and $\mathcal{G}$, which are subspaces in R^n, assuming that

$$p = \dim \mathcal{F} \geq \dim \mathcal{G} = q \geq 1.$$

Then the *principal angles*

$$\theta_1, \ldots, \theta_q \in [0, \pi/2]$$

between $\mathcal{F}$ and $\mathcal{G}$ may be defined, e.g., [12, 9], recursively for $k = 1, \ldots, q$ by

$$\cos(\theta_k) = \max_{u \in \mathcal{F}} \max_{v \in \mathcal{G}} u^T v = u_k^T v_k$$

subject to

$$\|u\| = \|v\| = 1, \; u^T u_i = 0, \; v^T v_i = 0, \; i = 1, \ldots, k-1.$$

The vectors $u_1, \ldots, u_q$ and $v_1, \ldots, v_q$ are called principal vectors. Here and below $\| \cdot \|$ denotes the standard Euclidian norm of a vector or, when applied to a matrix, the corresponding induced operator norm, also called the spectral norm, of the matrix.

According to [19], the notion of canonical angles between subspaces goes back to Jordan, 1875. Principal angles between subspaces, first of all, the smallest and the largest angles, serve as important tools in functional analysis, see books [1, 8, 13] and a survey [6], and in perturbation theory of invariant subspaces, e.g., [5, 19, 17, 14, 16]. Computation of principal angles between subspaces is needed in many applications. For example, in statistics, the angles are closely related to measures of dependency and covariance of random variables, see a canonical analysis of [4]. When applied to column-spaces $\mathcal{F}$ and $\mathcal{G}$ of matrices F and G, the principal angles describe canonical correlations $\sigma_k(F, G)$ of a matrix pair, e.g. [12, 11], which is important in such applications as system identification and information retrieval. Principal angles between subspaces also appear naturally in computations of eigenspaces, e.g., [15], where angles provide information about solution quality and need to be computed with high accuracy.

A Singular Value Decomposition (SVD)-based algorithm [7, 2, 3, 9, 11] for computing cosines of principal angles can be formulated as follows. Let columns of matrices $Q_F \in R^{n \times p}$ and $Q_G \in R^{n \times q}$ form orthonormal bases for the subspaces $\mathcal{F}$ and $\mathcal{G}$ respectively. The reduced SVD of $Q_F^T Q_G$ is

$$Y^T Q_F^T Q_G Z = \operatorname{diag}(\sigma_1, \sigma_2, \ldots, \sigma_q), \tag{1.1}$$

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where $Y \in R^{p\times q}$, $Z \in R^{q\times q}$ both have orthonormal columns. Then the principal angles can be computed as

$$\theta_k = \arccos(\sigma_k),\ k = 1,\dots,q, \tag{1.2}$$

where

$$0 \le \theta_1 \le \dots \le \theta_q \le \frac{\pi}{2},$$

while principal vectors are given by

$$u_k = Q_F y_k,\ v_k = Q_G z_k,\ k = 1,\dots,q.$$

The equivalence [2, 9] of the original geometric definition of principal angles and the SVD-based approach is based on the following general theorem on an equivalent representation of singular values.

THEOREM 1.1. *If $M \in R^{m\times n}$ then the singular values of M are defined recursively for by*

$$\sigma_k = \max_{y\ \in R^m}\ \max_{z\ \in R^n}\ y^T M z\ =\ y_k^T M z_k,\ k = 1,\dots,\min\{m,n\}, \tag{1.3}$$

subject to

$$\|y\| = \|z\| = 1,\ y^T y_i = 0,\ z^T z_i = 0,\ i = 1,\dots,k-1. \tag{1.4}$$

The vectors y_i and z_i are, respectively, left and right singular vectors.

The proof of the theorem is straightforward if based on Allakhverdiev's representation, see [8], of singular numbers:

$$\sigma_k = \left\| M - \sum_{i=1}^{k-1} v_i u_i^T \sigma_i \right\|,$$

and using the well-known formula of the induced Euclidian norm of a matrix as the norm of the corresponding bilinear form.

To apply the theorem to principal angles, one takes $M = Q_F^T Q_G$.

The SVD-based algorithm for cosine is considered as the standard one at present, and is implemented in software packages, e.g., in MATLAB, version 5.3, 2000, code SUBSPACE.m, revision 5.5, where $Q_F \in R^{n\times p}$ and $Q_G \in R^{n\times q}$ are computed using the QR factorization.

However, this algorithm cannot provide accurate results for small angles in the presence of round-off errors. Namely, when using the standard double-precision arithmetic $EPS \approx 10^{-16}$ the algorithm fails to compute accurately angles smaller than 10^{-8}, see Section 2. While the problem has been highlighted in the now classical paper [2] as well as the cure has been suggested, it apparently went unnoticed.

In statistics, most software packages include a code for computing $\sigma_k = cos(\theta_k)$, which are called *canonical correlations*, see, e.g., CANCOR Fortran code in FIRST MDS Package of AT&T, CANCR (DCANCR) Fortran subroutine in IMSL STAT/LIBRARY G03ADF Fortran code in NAG package, CANCOR subroutine in Splus, and CANCORR procedure in SAS/STAT Software. While computing accurately cosine of principle angles in corresponding precision, these codes do not compute sine. But the cosine simply equals to one in double precision for all angles smaller than 10^{-8}, see next section. Therefore, it's impossible in principle to observe an improvement in canonical correlations for angles smaller than 10^{-8} in double precision. It might not be typically important when processing experimental statistical data, because the expected measurement error may be so great that a statistician would deem the highly correlated variable essentially redundant and therefore not useful as a further explanatory variable in their model. Statistical computer experiments are different, however, – no measurement error – so accurate computation of very high correlations may be important in such applications.

The largest principal angle is related to the notion of distance, or a gap, between equidimensional subspaces. If $p = q$, the distance is defined [1, 8, 9, 13] as

$$\text{gap}(\mathcal{F},\mathcal{G}) = \|P_F - P_G\| = \sin(\theta_q) = \sqrt{1 - (\cos(\theta_q))^2}, \tag{1.5}$$

where P_F and P_G are orthogonal projectors onto $\mathcal{F}$ and $\mathcal{G}$ respectively.

This formulation provides insight into a possible alternative algorithm for computing principle angles. The corresponding algorithm, described in [2], while being mathematically equivalent to the previous one in exact arithmetic, is accurate for small angles in computer arithmetic as it computes the sine of principle angles directly, without using SVD (1.1) leading to the cosine. We review the algorithm of [2] based on a general form of (1.5) in Section 3. Let us also mention here an alternative approach for computing sine and cosine of principle angles, using the CS decomposition [18, 21].

In some applications, e.g., when solving symmetric generalized eigenvalue problems [15], the default scalar product $u^T v$ cannot be used and needs to be replaced with an A-based scalar product $(u,v)_A = u^T A v$, where A is a symmetric positive definite matrix. In statistics, a general scalar product for computing canonical correlations gives a user an opportunity, for example, to take into account an *a priori* information that some vector components are more meaningful than other.

In Section 4, we propose extension of the algorithms to an A-based scalar product and provide the corresponding theoretical justification.

In Section 5, we prove new absolute perturbation estimates for sine and cosine of principal angles computed in the A-based scalar product. When $A = I$ our estimates are, of course, similar to those of [2, 22, 20, 11, 10], but the technique we use is different and our constants are somewhat better.

We consider particular implementation of algorithms used in our MATLAB code SUBSPACEA.m in Section 6, with emphasis to the large-scale case, $n \gg p$, and sparse ill-conditioned matrix A. As our code performs orthogonalization of columns of matrices F and G, it is not quite suitable for sparse matrices F and G, cf. [11]. Finally, numerical results are presented in Section 7.

For simplicity, we only discuss real spaces and real scalar products; however, all results can be trivially generalized to cover complex spaces as well. In fact, our code SUBSPACEA.m is written for the general complex case.

2. A Bug In The Cosine-based Algorithm.

Let d be a constant and

$$\mathcal{F} = \text{Span}\ \left\{(1\ 0)^T\right\},\ \mathcal{G} = \text{Span}\ \left\{(1\ d)^T\right\}.$$

Then the angle between the one-dimensional subspaces $\mathcal{F}$ and $\mathcal{G}$ can be computed as

$$\theta = \arcsin\left(\frac{d}{\sqrt{1+d^2}}\right). \tag{2.1}$$

In the table below d varies from one to small values. Formula (2.1) is accurate for small angles, so we use it as an "exact" answer in the second column of the table. We use the MATLAB built-in function SUBSPACE.m (revision 5.5) which implements (1.1) to compute values for the third column of the table.

It is apparent that SUBSPACE.m returns inaccurate results for $d \le 10^{-8}$, which is approximately $\sqrt{EPS}$ for double precision.

d	Formula (2.1)	SUBSPACE.m
1.0	7.853981633974483e-001	7.853981633974483e-001
1.0e-04	9.999999966666666e-005	9.999999986273192e-005
1.0e-06	9.999999999996666e-007	1.000044449242271e-006
1.0e-08	1.000000000000000e-008	-6.125742274543099e-017
1.0e-10	1.000000000000000e-010	-6.125742274543099e-017
1.0e-16	9.999999999999998e-017	-6.125742274543099e-017
1.0e-20	9.999999999999998e-021	-6.125742274543099e-017
1.0e-30	1.000000000000000e-030	-6.125742274543099e-017

In this simple one-dimensional example the algorithm of SUBSPACE.m is reduced to computing

$$\theta = \arccos\left(\frac{1}{\sqrt{1+d^2}}\right).$$

This formula clearly shows that the inability to compute accurately small angles is integrated in the standard algorithm, and cannot be fixed without changing the algorithm itself. The cosine, that is a canonical correlation, is computed accurately and simply equals to one for all positive $d \leq 10^{-8}$. However, one cannot determine small angles from a cosine accurately in the presence of round-off errors. In statistical terms, it illustrates the problem we already mentioned above that the canonical correlation itself does not show any improvement in correlation when d is smaller than 10^{-8} in double precision.

In the next section, we consider a formula [2] that computes directly sine of principle angles as in (2.1).

3. A Sine-Based Algorithm. We first review known sine-based formulas for the largest principle angle. Results of [1, 13] concerning the aperture of two linear manifolds give

$$\|P_F - P_G\| = \max\left\{\max_{x\in\mathcal{G},\|x\|=1} \|(I-P_F)x\|,\ \max_{y\in\mathcal{F},\|y\|=1} \|(I-P_G)y\|\right\}. \tag{3.1}$$

Let columns of matrices $Q_F \in R^{n\times p}$ and $Q_G \in R^{n\times q}$ form orthonormal bases for the subspaces $\mathcal{F}$ and $\mathcal{G}$ respectively. Then orthogonal projectors on $\mathcal{F}$ and $\mathcal{G}$ are $P_F = Q_F Q_F^T$ and $P_G = Q_G Q_G^T$, correspondingly. Our norm $\|\cdot\|$ is invariant under left multiplication by Q_F, or Q_G, thus, we obtain

$$\|P_F - P_G\| = \max\{\|(I - Q_F Q_F^T)Q_G\|, \|(I - Q_G Q_G^T)Q_F\|\}. \tag{3.2}$$

If $p \neq q$ then expression of (3.2) is always equal to one, e.g., if $p > q$ then the second term under maximum is one. If $p = q$, then both terms are the same and yield $\sin(\theta_q)$ by (1.5). Thus, under our assumption $p \geq q$, only the first term is interesting to analyze. We note that the first term is the largest singular value of $(I - Q_F Q_F^T)Q_G$. What if we consider other singular values of the matrix?

This provides an insight into how to find a sine-based formulation to obtain the principal angles, which is embodied in the following theorem [2]:

THEOREM 3.1. *Singular values of matrix* $(I - Q_F Q_F^T)Q_G$ *are* $\mu_k = \sqrt{1-\sigma_{q-k+1}^2},\ k = 1,\ldots,q,$ *where* σ_k *are defined in (1.1). Moreover, the principle angles satisfy the equalities* $\theta_k = \arcsin(\mu_{q-k+1})$.

The right principal vectors can be computed as

$$v_k = Q_G z_k,\ k = 1,\ldots,q,$$

where z_k *are corresponding orthonormal right singular vectors of matrix* $(I - Q_F Q_F^T)Q_G$. *The left principal vectors are then computed by*

$$u_k = Q_F Q_F^T v_k/\sigma_k,\ k = 1,\ldots,q.$$

Proof. Our proof is essentially the same as that of [2]. We reproduce it here for completeness as we use a similar proof later for a general scalar product.

Let $B = (I - P_F)Q_G = (I - Q_F Q_F^T)Q_G$. Using the fact that $I - P_F$ is a projector and that $Q_G^T Q_G = I$, we have

$$\begin{aligned} B^T B &= Q_G^T(I-P_F)(I-P_F)Q_G = Q_G^T(I-P_F)Q_G \\ &= I - Q_G^T Q_F Q_F^T Q_G. \end{aligned}$$

Utilizing the SVD (1.1), we obtain $Q_F^T Q_G = Y\Sigma Z^T$, where $\Sigma = \text{diag}\,(\sigma_1, \sigma_2, \ldots, \sigma_q)$, then

$$Z^T B^T B Z = I - \Sigma^2 = \text{diag}\,(1-\sigma_1^2, 1-\sigma_2^2, \ldots, 1-\sigma_q^2).$$

Thus, the singular values of B are given by $\mu_k = \sqrt{1-\sigma_{q-k+1}^2},\ k = 1,\ldots,q$, and the formula for the principal angles $\theta_k = \arcsin(\mu_{q-k+1})$ follows directly from (1.2). □

We can now use the theorem to formulate an algorithm for computing all the principal angles. This approach meets our goal of a sine-based formulation, which should provide accurate computation of small angles. However, for large angles we keep the cosine-based algorithm.

ALGORITHM 3.1 : **Modified SUBSPACE.m.**

Input: *real matrices F and G with the same number of rows.*

1. *Compute orthogonal bases* $Q_F = \mathrm{orth}(F)$, $Q_G = \mathrm{orth}(G)$ *of column-spaces of F and G.*
2. *Compute SVD for cosine:* $[Y, \mathrm{diag}\,(\sigma_1, \ldots, \sigma_q), Z] = \mathrm{svd}(Q_F^T Q_G)$.
3. *Compute matrices of left* $U_{\cos} = Q_F Y$ *and right* $V_{\cos} = Q_G Z$ *principal vectors.*
4. *Compute matrix* $B = \begin{cases} Q_G - Q_F(Q_F^T Q_G), & \text{if } \mathrm{rank}(Q_F) \ge \mathrm{rank}(Q_G); \\ Q_F - Q_G(Q_G^T Q_F), & \text{otherwise.} \end{cases}$
5. *Compute SVD for sine:* $[Y, \mathrm{diag}\,(\mu_1, \ldots, \mu_q), Z] = \mathrm{svd}(B)$.
6. *Compute matrices $U_{\sin}$ and $V_{\sin}$ of left and right principal vectors:*
   $V_{\sin} = Q_G Z$, $U_{\sin} = Q_F(Q_F^T V_{\sin})$, *if* $\mathrm{rank}(Q_F) \ge \mathrm{rank}(Q_G)$;
   $U_{\sin} = Q_F Z$, $V_{\sin} = Q_G(Q_G^T U_{\sin})$, *otherwise.*
7. *Compute the principle angles, for* $k = 1, \ldots, q$:
   $\theta_k = \begin{cases} \arccos(\sigma_k), & \text{if } \sigma_k^2 \ge 1/2; \\ \arcsin(\mu_{q-k+1}), & \text{if } \mu_{q-k+1}^2 \le 1/2. \end{cases}$
8. *Form matrices U and V by picking up corresponding columns of $U_{\sin}$, $V_{\sin}$ and $U_{\cos}$, $V_{\cos}$, according to the choice for θ_k above.*

Output: *Principal angles $\theta_1, \ldots, \theta_q$ between column-spaces of matrices F and G, and corresponding matrices U and V of left and right principal vectors, correspondingly.*

Let us highlight again that in exact arithmetic the sine and cosine based approaches give the same results, e.g., columns of $U_{\sin}$ and $V_{\sin}$ must be the same as those of $U_{\cos}$, $V_{\cos}$, without round-off errors.

REMARK 3.1. *On Step 1 of the algorithm, the orthogonalization can be performed using the QR method, or the SVD, where the latter is apparently more robust for almost linearly dependent columns.*

REMARK 3.2. *A check* $\mathrm{rank}(Q_F) \ge \mathrm{rank}(Q_G)$ *on Steps 4 and 6 of the algorithm removes the need for our assumption* $p = \mathrm{rank}(Q_F) \ge \mathrm{rank}(Q_G) = q$.

REMARK 3.3. *We replace here*

$$(I - Q_F Q_F^T) Q_G = Q_G - Q_F(Q_F^T Q_G)$$

to avoid having any matrices of the size n-by-n in the algorithm, which allows us to compute principle angles efficiently for large n as well.

REMARK 3.4. *A different sine-based approach, using eigenvalues of $P_F - P_G$, is described in [3], see a similar statement of Theorem 3.4. It is less attractive numerically as it requires computing an n-by-n matrix and finding all its nonzero eigenvalues.*

To summarize, the algorithm uses the cosine-based formulation (1.1), (1.2) for large angles and the sine-based formulation of Theorem 3.1 for small angles, which allows accurate computation of all angles.

Theorem 3.1 characterizes singular values of the product $(I - P_F)Q_G$, which are sine of the principal angles. What are singular values of matrix $P_F Q_G$? A trivial modification of the previous proof leads to the following not really surprising result that these are cosine of the principal angles.

THEOREM 3.2. *Singular values of matrix $Q_F Q_F^T Q_G$ are exactly the same as σ_k, defined in (1.1).*

We conclude this subsection with another simple and known, e.g., [19, 23], sine and cosine representations of principal angles, this time using orthogonal projectors P_F and P_G on subspaces $\mathcal{F}$ and $\mathcal{G}$, correspondingly.

THEOREM 3.3. *Let assumptions of Theorem 3.1 be satisfied. Then $\sigma_1 \ge \sigma_2 \ge \ldots \ge \sigma_q$ are q largest singular values of matrix $P_F P_G$, in particular,*

$$\sigma_1 = \|P_F P_G\|.$$

Other $n - q$ singular values are all equal to zero.

REMARK 3.5. *As singular values of $P_F P_G$ are the same as those of $P_G P_F$, subspaces $\mathcal{F}$ and $\mathcal{G}$ play symmetric roles in Theorem 3.3, thus, our assumption that $p = \dim\, \mathcal{F} \ge \dim\, \mathcal{G} = q$ is irrelevant here.*

THEOREM 3.4. *Let assumptions of Theorem 3.1 be satisfied. Then* $\mu_1 \geq \mu_2 \geq \ldots \geq \mu_q$ *are* q *largest singular values of matrix* $(I - P_F)P_G$*, in particular,*

$$\mu_1 = \|(I - P_F)P_G\|.$$

Other $n - q$ *singular values are all equal to zero.*

REMARK 3.6. *Comparing Theorems 3.3 and 3.4 shows trivially that sine of principal angles between* $\mathcal{F}$ *and* $\mathcal{G}$ *are the same as cosine of principal angles between* $\mathcal{F}^\perp$ *and* $\mathcal{G}$*, because* $I - P_F$ *is an orthogonal projector on* $\mathcal{F}^\perp$*.*

REMARK 3.7. *What can we say about singular values of matrix* $(I - P_G)P_F$*, in other words, how do cosine of principal angles between subspaces* $\mathcal{F}^\perp$ *and* $\mathcal{G}$ *compare to cosine of principal angles between their orthogonal complements* $\mathcal{F}$ *and* $\mathcal{G}^\perp$*? If* $p = q$*, they are absolutely the same, in particular, the minimal angle between subspaces* $\mathcal{F}^\perp$ *and* $\mathcal{G}$ *is in this case the same as the minimal angle between their orthogonal complements* $\mathcal{F}$ *and* $\mathcal{G}^\perp$*, e.g. [6], and, in fact, is equal to* $\text{gap}(\mathcal{F}, \mathcal{G}) = \|P_F - P_G\|$ *as we already discussed. When* $p > q$*, subspaces* $\mathcal{F}$ *and* $\mathcal{G}^\perp$ *must have a nontrivial intersection, because the sum of their dimensions is too big; thus, the minimal angle between subspaces* $\mathcal{F}$ *and* $\mathcal{G}^\perp$ *must be zero in this case, which corresponds to* $\|(I - P_G)P_F\| = 1$*, while* $\|(I - P_F)P_G\|$ *may be less than one. To be more specific,* $\dim(\mathcal{F} \cap \mathcal{G}^\perp) \geq p - q$*, thus, at least* $p - q$ *singular values of matrix* $(I - P_G)P_F$ *are equal to one. Then, we have the following statement, cf. Ex. 1.2.6 of [3]: the set of singular values of* $(I - P_G)P_F$*, when* $p > q$*, consists of* $p - q$ *ones,* q *singular values of* $(I - P_F)P_G$ *and* $n - p$ *zeros, which completely clarifies the issue of principal angles between orthogonal complements. In particular, this shows that the smallest positive sine of principal angles between* $\mathcal{F}$ *and* $\mathcal{G}$*, called the* minimum gap*, is the same as that between* $\mathcal{F}^\perp$ *and* $\mathcal{G}^\perp$ *[13].*

In the next section, we deal with an arbitrary scalar product.

4. Generalization to an A-based Scalar Product. Let $A \in R^{n\times n}$ be a fixed symmetric positive definite matrix. Let $(x, y)_A = (x, Ay) = y^T Ax$ be an A-based scalar product, $x, y \in R^n$. Let $\|x\|_A = \sqrt{(x, x)_A}$ be the corresponding vector norm and let $\|B\|_A$ be the corresponding induced matrix norm of a matrix $B \in R^{n\times n}$. We note that $\|x\|_A = \|A^{1/2}x\|$ and $\|B\|_A = \|A^{1/2}BA^{-1/2}\|$.

In order to define principal angles based on this scalar product, we will follow arguments of [2, 9], but in an A-based scalar product instead of the standard Euclidean scalar product. Again, we will assume for simplicity of notation that $p \geq q$.

Principal angles

$$\theta_1, \ldots, \theta_q \in [0, \pi/2]$$

between subspaces $\mathcal{F}$ and $\mathcal{G}$ in the A-based scalar product $(\cdot, \cdot)_A$ are defined recursively for $k = 1, \ldots, q$ by analogy with the previous definition for $A = I$ as

$$\cos(\theta_k) = \max_{u \in \mathcal{F}} \max_{v \in \mathcal{G}} (u, v)_A = (u_k, v_k)_A \tag{4.1}$$

subject to

$$\|u\|_A = \|v\|_A = 1, \; (u, u_i)_A = 0, \; (v, v_i)_A = 0, \; i = 1, \ldots, k - 1. \tag{4.2}$$

The vectors $u_1, \ldots, u_q$ and $v_1, \ldots, v_q$ are called principal vectors relative to the A-based scalar product.

The following Theorem justifies the consistency of the definition above and provides a cosine-based algorithm for computing the principle angles in the A-based scalar product. It is a direct generalization of the cosine-based approach of [2, 9].

THEOREM 4.1. *Let columns of* $Q_F \in R^{n\times p}$ *and* $Q_G \in R^{n\times q}$ *be now* A*-orthonormal bases for the subspaces* F *and* G *respectively. Let* $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_q$ *be singular values of* $Q_F^T A Q_G$ *with corresponding left and right singular vectors* y_k *and* z_k*,* $k = 1, \ldots, q$*. Then the principal angles relative to the scalar product* $(\cdot, \cdot)_A$ *as defined in (4.1) and (4.2) are computed as*

$$\theta_k = \arccos(\sigma_k), \; k = 1, \ldots, q, \tag{4.3}$$

where

$$0 \leq \theta_1 \leq \ldots \leq \theta_q \leq \frac{\pi}{2},$$

while principal vectors are given by

$$u_k = Q_F y_k,\ v_k = Q_G z_k,\ k = 1, \ldots, q.$$

Proof. We first rewrite definition (4.1) and (4.2) of principal angles in the following equivalent form. For $k = 1, \ldots, q$,

$$\cos(\theta_k) = \max_{y\ \in R^p} \max_{z\ \in R^q} y^T Q_F^T A Q_G z \ = \ y_k^T Q_F^T A Q_G z_k$$

subject to

$$\|y\| = \|z\| = 1,\ y^T y_i = 0,\ z^T z_i = 0,\ i = 1, \ldots, k-1,$$

where $u = Q_F y \in \mathcal{F}$, $v = Q_G z \in \mathcal{G}$ and $u_k = Q_F y_k \in \mathcal{F}$, $v_k = Q_G z_k \in \mathcal{G}$.

Since Q_F and Q_G have A-orthonormal columns, $Q_F^T A Q_F = I$ and $Q_G^T A Q_G = I$. This implies

$$\|u\|_A^2 = y^T Q_F^T A Q_F y = y^T y = \|y\|^2 = 1$$

and

$$\|v\|_A^2 = z^T Q_G^T A Q_G z = z^T z = \|z\|^2 = 1.$$

For $i \neq j$, we derive

$$(u_i, u_j)_A = y_i^T Q_F^T A Q_F y_j = y_i^T y_j = 0$$

and

$$(v_i, v_j)_A = z_i^T Q_G^T A Q_G z_j = z_i^T z_j = 0.$$

Now, let the reduced SVD of $Q_F^T A Q_G$ be

$$Y^T Q_F^T A Q_G Z \ = \ \operatorname{diag}(\sigma_1, \sigma_2, \ldots, \sigma_q), \tag{4.4}$$

where $Y \in R^{p \times q}$, $Z \in R^{q \times q}$ both have orthonormal columns.

Then, by Theorem 1.1 with $M = Q_F^T A Q_G$, the equality $\cos(\theta_k) = \sigma_k,\ k = 1, \ldots, q$ just provides two equivalent representations of the singular values of $Q_F^T A Q_G$, and y_z and z_k can be chosen as columns of matrices Y and Z, correspondingly. The statement of the theorem follows. □

Let us now make a trivial, but helpful observation that links principal angles in the A-based scalar product with principal angles in the original standard scalar product. We formulate it as

THEOREM 4.2. *Under assumptions of Theorem 4.1 the principal angles between subspaces $\mathcal{F}$ and $\mathcal{G}$ relative to the scalar product $(\cdot, \cdot)_A$, coincide with the principal angles between subspaces $A^{1/2}\mathcal{F}$ and $A^{1/2}\mathcal{G}$ relative to the original scalar product $(\cdot, \cdot)$.*

Proof. One way to prove it is just to notice that our definition of the principal angles between subspaces $\mathcal{F}$ and $\mathcal{G}$ relative to the scalar product $(\cdot, \cdot)_A$ turns into a definition of the principal angles between subspaces $A^{1/2}\mathcal{F}$ and $A^{1/2}\mathcal{G}$ relative to the original scalar product $(\cdot, \cdot)$, if we make a substitution $A^{1/2}u \mapsto u$ and $A^{1/2}v \mapsto v$.

Another proof is to use the representation

$$Q_F^T A Q_G = \left(A^{1/2} Q_F\right)^T A^{1/2} Q_G,$$

where columns of matrices $A^{1/2}Q_F$ and $A^{1/2}Q_G$ are orthonormal with respect to the original scalar product $(\cdot,\cdot)$ and span subspaces $A^{1/2}\mathcal{F}$ and $A^{1/2}\mathcal{G}$, correspondingly. Now our Theorem 4.1 is equivalent to the traditional SVD theorem on cosine of principal angles between subspaces $A^{1/2}\mathcal{F}$ and $A^{1/2}\mathcal{G}$ relative to the original scalar product $(\cdot,\cdot)$, formulated in the Introduction. □

The A-orthogonal projectors on subspaces $\mathcal{F}$ and $\mathcal{G}$ are now defined by formulas

$$P_F = Q_F Q_F^{*_A} = Q_F Q_F^T A \text{ and } P_G = Q_G Q_G^{*_A} = Q_G Q_G^T A,$$

where $*_A$ denotes the A-adjoint.

To obtain a sine-based formulation in the A-based scalar product that is accurate for small angles, we first adjust (1.5) and (3.1) to the new A-based scalar product:

$$\begin{aligned}\text{gap}_A(\mathcal{F},\mathcal{G}) &= \|P_F - P_G\|_A \\ &= \max\left\{\max_{x\in\mathcal{G},\|x\|_A=1} \|(I-P_F)x\|_A,\ \max_{y\in\mathcal{F},\|y\|_A=1} \|(I-P_G)y\|_A\right\}.\end{aligned} \tag{4.5}$$

If $p=q$, this equation will yield $\sin(\theta_q)$, consistently with Theorem 4.1. Similarly to the previous case $A=I$, only the first term under maximum is of interest under our assumption that $p \geq q$. Using the fact that

$$\|x\|_A = \|Q_G z\|_A = \|z\|,\ \forall x\in\mathcal{G},\ x = Q_G z,\ z\in R^q,$$

the term of interest can be rewritten as

$$\max_{x\in\mathcal{G},\|x\|_A=1} \|(I-P_F)x\|_A = \|A^{1/2}(I - Q_F Q_F^T A)Q_G\|. \tag{4.6}$$

Here we use the standard induced Euclidian norm $\|\cdot\|$ for computational purposes. Similar to our arguments in the previous section, we obtain a more general formula for all principal angles in the following:

THEOREM 4.3. *Eigenvalues $\nu_k,\ k=1,\ldots,q$, of matrix S^TAS, where $S=(I-Q_FQ_F^TA)Q_G$, are equal to $\nu_k = 1-\sigma_{q-k+1}^2$, where σ_k are defined in (4.4). Moreover, the principle angles satisfy the equalities*

$$\theta_k = \arcsin\left(\sqrt{\nu_{q-k+1}}\right).$$

The right principal vectors can be computed as

$$v_k = Q_G z_k,\ k=1,\ldots,q,$$

where z_k are corresponding orthonormal right eigenvectors of matrix S^TAS. The left principal vectors are then computed by

$$u_k = Q_F Q_F^T A v_k/\sigma_k,\ k=1,\ldots,q.$$

Proof. We first notice that squares of singular values $\mu_k,\ k=1$ of matrix $A^{1/2}(I-Q_FQ_F^TA)Q_G$, which appear in (4.6), coincide with eigenvalues $\nu_k=\mu_k^2$ of the product S^TAS. Using the fact that $Q_F^TAQ_F=I$ and $Q_G^TAQ_G=I$, we have

$$\begin{aligned}S^TAS &= Q_G^T(I - AQ_FQ_F^T)A(I-Q_FQ_F^TA)Q_G \\ &= I - Q_G^TAQ_FQ_F^TAQ_G.\end{aligned}$$

Utilizing the SVD (4.4), we obtain $Q_F^TAQ_G = Y\Sigma Z^T$, where $\Sigma = \text{diag}\,(\sigma_1,\sigma_2,\ldots,\sigma_q)$, then

$$Z^TS^TASZ = I - \Sigma^2 = \text{diag}\,(1-\sigma_1^2, 1-\sigma_2^2,\ldots,1-\sigma_q^2).$$

Thus, the eigenvalues of S^TAS are given by $\nu_k = 1-\sigma_{q-k+1}^2,\ k=1,\ldots,q$, and the formula for the principal angles follows directly from (4.3). □

We can easily modify the previous proof to obtain the following analog of Theorem 3.2:

THEOREM 4.4. *Singular values of matrix $A^{1/2}Q_FQ_F^TAQ_G = A^{1/2}P_FQ_G$ coincide with σ_k, defined in (4.4).*

It is also useful to represent principal angles using exclusively A-orthogonal projectors P_F and P_G on subspaces $\mathcal{F}$ and $\mathcal{G}$, correspondingly, similarly to Theorems 3.3 and 3.4.

THEOREM 4.5. *Under assumptions of Theorem 4.1, $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_q$ are q largest singular values of matrix $A^{1/2}P_FP_GA^{-1/2}$, in particular,*

$$\sigma_1 = \|P_FP_G\|_A.$$

Other $n-q$ singular values are all equal to zero.

Proof. First, we rewrite

$$A^{1/2}P_FP_GA^{-1/2} = A^{1/2}Q_FQ_F^TAQ_GQ_G^TAA^{-1/2} = A^{1/2}Q_F\left(A^{1/2}Q_F\right)^TA^{1/2}Q_G\left(A^{1/2}Q_G\right)^T.$$

As columns of matrices $A^{1/2}Q_F$ and $A^{1/2}Q_G$ form orthonormal with respect to the original scalar product $(\cdot,\cdot)$ bases of subspaces $A^{1/2}\mathcal{F}$ and $A^{1/2}\mathcal{G}$, correspondingly, the last product equals to the product of orthogonal (not A-orthogonal!) projectors $P_{A^{1/2}\mathcal{F}}$ and $P_{A^{1/2}\mathcal{G}}$, on subspaces $A^{1/2}\mathcal{F}$ and $A^{1/2}\mathcal{G}$.

Second, we can now use Theorem 3.3 to state that cosine of principle angles between subspaces $A^{1/2}\mathcal{F}$ and $A^{1/2}\mathcal{G}$ with respect to the original scalar product $(\cdot,\cdot)$ are given by q largest singular values of the product $P_{A^{1/2}\mathcal{F}}P_{A^{1/2}\mathcal{G}} = A^{1/2}P_FP_GA^{-1/2}$.

Finally, we use Theorem 4.2 to conclude that these singular values are, in fact, $\sigma_k,\ k=1,\ldots,q$ – the cosine of principle angles between subspaces $\mathcal{F}$ and $\mathcal{G}$ with respect to the A-based scalar product. □

THEOREM 4.6. *Let assumptions of Theorem 4.3 be satisfied. Then $\mu_1 \geq \mu_2 \geq \ldots \geq \mu_q$ are q largest singular values of matrix $A^{1/2}(I-P_F)P_GA^{-1/2}$, in particular,*

$$\mu_1 = \|(I-P_F)P_G\|_A.$$

Other $n-q$ singular values are all equal to zero.

Proof. We rewrite

$$A^{1/2}(I-P_F)P_GA^{-1/2} = \left(I - A^{1/2}Q_F\left(A^{1/2}Q_F\right)^T\right)A^{1/2}Q_G\left(A^{1/2}Q_G\right)^T = \left(I-P_{A^{1/2}\mathcal{F}}\right)P_{A^{1/2}\mathcal{G}},$$

and then follow arguments similar to those of the previous proof, but now using Theorem 3.4 instead of Theorem 3.3. □

Remarks 3.5–3.7 for the case $A = I$ hold in the general case, too, with evident modifications.

Our final theoretical results are perturbation theorems in the next section.

5. Perturbation of Principal Angles in the A-based scalar product. In the present section, for simplicity, we *always assume* that matrices F, G and their perturbations $\widetilde{F}$, $\widetilde{G}$ have the same rank, thus, in particular, $p = q$.

We notice that F and G appear symmetrically in the definition of the principal angles, under our assumption that they and their perturbations have the same rank. This means that we do not have to analyze the perturbation of F and G together at the same time. Instead, we first study only a perturbation in G.

Before we start with an estimate for cosine, let us introduce a new notation $\ominus$ using an example:

$$(\mathcal{G}+\widetilde{\mathcal{G}}) \ominus \mathcal{G} = (\mathcal{G}+\widetilde{\mathcal{G}}) \cap \mathcal{G}^{\perp},$$

where $\ominus$ and the orthogonal complement to $\mathcal{G}$ are understood in the A-based scalar product.

LEMMA 5.1. *Let $\sigma_1,\sigma_2,\ldots,\sigma_q$, and $\widehat{\sigma}_1,\widehat{\sigma}_2,\ldots,\widehat{\sigma}_q$, be cosine of principle angles between subspaces $\mathcal{F}$, $\mathcal{G}$ and $\mathcal{F}$, $\widetilde{\mathcal{G}}$, correspondingly, computed in the A-based scalar product. Then, for $k=1,\ldots,q$:*

$$(5.1)\quad |\sigma_k - \widehat{\sigma}_k| \leq \max\left\{\cos\left(\theta_{\min}\{(\mathcal{G}+\widetilde{\mathcal{G}})\ominus\mathcal{G},\ \mathcal{F}\}\right);\ \cos\left(\theta_{\min}\{(\mathcal{G}+\widetilde{\mathcal{G}})\ominus\widetilde{\mathcal{G}},\ \mathcal{F}\}\right)\right\}\mathrm{gap}_A(\mathcal{G},\widetilde{\mathcal{G}}),$$

where $\theta_{\min}$ *is the smallest angle between corresponding subspaces, measured in the* A*-based scalar product.*

Proof. The proof is based on the following identity:

$$A^{1/2}Q_FQ_F^TAQ_{\widetilde{G}} = A^{1/2}Q_FQ_F^TAQ_GQ_G^TAQ_{\widetilde{G}} + A^{1/2}Q_FQ_F^TA(I - Q_GQ_G^TA)Q_{\widetilde{G}}, \tag{5.2}$$

which is a multidimensional analog of the trigonometric formula for the cosine of the sum of two angles. Now we use two classical theorems on perturbation of singular values with respect to addition:

$$s_k(T+S) \le s_k(T) + \|S\|, \tag{5.3}$$

and with respect to multiplication:

$$s_k(TS^T) \le s_k(T)\|S^T\|, \tag{5.4}$$

where T and S are matrices of corresponding sizes. We first take $T = A^{1/2}Q_FQ_F^TAQ_GQ_G^TAQ_{\widetilde{G}}$ and $S = A^{1/2}Q_FQ_F^TA(I - Q_GQ_G^TA)Q_{\widetilde{G}}$ in (5.3) to get:

$$\widehat{\sigma}_k = s_k(A^{1/2}Q_FQ_F^TAQ_{\widetilde{G}}) \le s_k(A^{1/2}Q_FQ_F^TAQ_GQ_G^TAQ_{\widetilde{G}}) + \|A^{1/2}Q_FQ_F^TA(I - Q_GQ_G^TA)Q_{\widetilde{G}}\|,$$

where the first equality follows from Theorem 4.4. In the second term in the sum on the right, we need to estimate a product, similar to a product of *three* orthoprojectors. We notice that column vectors of $(I - Q_GQ_G^TA)Q_{\widetilde{G}}$ belong to the subspace $(\mathcal{G} + \widetilde{\mathcal{G}}) \ominus \mathcal{G}$. Let $P_{(\mathcal{G}+\widetilde{\mathcal{G}})\ominus\mathcal{G}}$ be an A-orthogonal projector on the subspace. Then the second term can be rewritten, using also projector $Q_FQ_F^TA = P_F$ as

$$A^{1/2}Q_FQ_F^TA(I - Q_GQ_G^TA)Q_{\widetilde{G}} = A^{1/2}Q_FQ_F^TAP_{(\mathcal{G}+\widetilde{\mathcal{G}})\ominus\mathcal{G}}(I - Q_GQ_G^TA)Q_{\widetilde{G}} =$$

$$\left(A^{1/2}P_FP_{(\mathcal{G}+\widetilde{\mathcal{G}})\ominus\mathcal{G}}A^{-1/2}\right)A^{1/2}(I - Q_GQ_G^TA)Q_{\widetilde{G}};$$

therefore, it can be estimated as

$$\|A^{1/2}Q_FQ_F^TA(I - Q_GQ_G^TA)Q_{\widetilde{G}}\| \le \|A^{1/2}P_FP_{(\mathcal{G}+\widetilde{\mathcal{G}})\ominus\mathcal{G}}A^{-1/2}\|\|A^{1/2}(I - Q_GQ_G^TA)Q_{\widetilde{G}}\|.$$

The first multiplier in the last product equals

$$\|A^{1/2}P_FP_{(\mathcal{G}+\widetilde{\mathcal{G}})\ominus\mathcal{G}}A^{-1/2}\| = \|P_FP_{(\mathcal{G}+\widetilde{\mathcal{G}})\ominus\mathcal{G}}\|_A = \cos\left(\theta_{\min}\{(\mathcal{G}+\widetilde{\mathcal{G}})\ominus\mathcal{G},\, \mathcal{F}\}\right),$$

similar to (4.6) and using Theorem 4.5 for subspaces $(\mathcal{G}+\widetilde{\mathcal{G}})\ominus\mathcal{G}$ and $\mathcal{F}$; while the second multiplier is $\operatorname{gap}_A(\mathcal{G},\widetilde{\mathcal{G}})$, because of our assumption $\dim \mathcal{F} = \dim \mathcal{G} = \dim \widetilde{\mathcal{G}}$. To estimate the first term in the sum, we apply (5.4) with $T = A^{1/2}Q_FQ_F^TAQ_G$ and $S^T = Q_G^TAQ_{\widetilde{G}}$:

$$s_k(A^{1/2}Q_FQ_F^TAQ_GQ_G^TAQ_{\widetilde{G}}) \le s_k(A^{1/2}Q_FQ_F^TAQ_G)\|Q_G^TAQ_{\widetilde{G}}\| \le s_k(A^{1/2}Q_FQ_F^TAQ_G) = \sigma_k,$$

simply because the second multiplier here is the cosine of an angle between $\mathcal{G}$ and $\widetilde{\mathcal{G}}$ in A-based scalar product, which is, of course, bounded by one from above. Thus, we proved

$$\widehat{\sigma}_k \le \sigma_k + \cos\left(\theta_{\min}\{(\mathcal{G}+\widetilde{\mathcal{G}})\ominus\mathcal{G},\, \mathcal{F}\}\right)\operatorname{gap}_A(\mathcal{G},\widetilde{\mathcal{G}}).$$

Changing places of $Q_{\widetilde{G}}$ and Q_G, we obtain

$$\sigma_k \le \widehat{\sigma}_k + \cos\left(\theta_{\min}\{(\mathcal{G}+\widetilde{\mathcal{G}})\ominus\widetilde{\mathcal{G}},\, \mathcal{F}\}\right)\operatorname{gap}_A(\mathcal{G},\widetilde{\mathcal{G}}),$$

and come to the statement of the lemma. □

REMARK 5.1. *Let us try to clarify a meaning of constants appearing in the statement of Lemma 5.1. Let us consider, e.g.,* $\cos\left(\theta_{\min}\{(\mathcal{G}+\widetilde{\mathcal{G}})\ominus\mathcal{G},\,\mathcal{F}\}\right)$. *The cosine takes its maximal value, one, when at least one direction of the perturbation of* $\mathcal{G}$ *is* A*-orthogonal to* $\mathcal{G}$ *and parallel to* $\mathcal{F}$ *at the same time. It is small, on the contrary, when a part of the perturbation,* A*-orthogonal to* $\mathcal{G}$*, is also* A*-orthogonal to* $\mathcal{F}$*. As* $(\mathcal{G}+\widetilde{\mathcal{G}})\ominus\mathcal{G}\subseteq\mathcal{G}^{\perp}$*, we have*

$$\cos\left(\theta_{\min}\{(\mathcal{G}+\widetilde{\mathcal{G}})\ominus\mathcal{G},\,\mathcal{F}\}\right)\leq\cos\left(\theta_{\min}\{\mathcal{G}^{\perp},\,\mathcal{F}\}\right)=\sin\left(\theta_{\max}\{\mathcal{G},\,\mathcal{F}\}\right)=\mathrm{gap}_A(\mathcal{G},\mathcal{F})$$

- the constant of the asymptotic perturbation estimate of [2] (where $A=I$*). The latter term is small, if subspaces* $\mathcal{G}$ *and* $\mathcal{F}$ *are close to each other, which can be considered more as a cancellation prize as in this case cosine of all principal angles is almost one and a perturbation estimate for the cosine does not help much, because of the cancellation effect.*

REMARK 5.2. *A natural approach similar to that of [11] with* $A=I$ *involves a simpler identity:*

$$Q_F^TAQ_{\widetilde{G}}=Q_F^TAQ_G+Q_F^TA(Q_{\widetilde{G}}-Q_G),$$

where a norm of the second term is then estimated. Then (5.3) gives an estimate of singular values using $\|A^{1/2}(Q_{\widetilde{G}}-Q_G)\|$*. As singular values are invariant with respect to particular choices of matrices* $Q_{\widetilde{G}}$ *and* Q_G *with* A*-orthonormal columns, as far as they provide ranges* $\widetilde{\mathcal{G}}$ *and* $\mathcal{G}$*, correspondingly, we can choose them to minimize the norm of the difference, which gives:*

$$\inf_Q\|A^{1/2}(Q_G-Q_{\widetilde{G}}Q)\|, \tag{5.5}$$

where Q *is an arbitrary* q*-by-*q *orthogonal matrix. This quantity appears in [11] with* $A=I$ *as a special type of the Procrustes problem. In [11], it is estimated in terms of the gap between subspaces* $\widetilde{\mathcal{G}}$ *and* $\mathcal{G}$ *(using an extra assumption that* $2q\leq n$*). Repeating similar arguments, we derive:*

$$|\sigma_k-\widehat{\sigma}_k|\leq\inf_Q\|A^{1/2}(Q_G-Q_{\widetilde{G}}Q)\|_A\leq\sqrt{2}\,\mathrm{gap}_A(\mathcal{G},\widetilde{\mathcal{G}}),\ \ k=1,\ldots,q. \tag{5.6}$$

Our Lemma 5.1 furnishes estimates of the perturbation of singular values in terms of the gap directly, which gives a much better constant, consistent with that of the asymptotic estimate of [2] for $A=I$*, see the previous remark.*

Now we prove a separate estimate for sine.

LEMMA 5.2. *Let* $\mu_1,\mu_2,\ldots,\mu_q$*, and* $\widehat{\mu}_1,\widehat{\mu}_2,\ldots,\widehat{\mu}_q$*, be sine of principle angles between subspaces* $\mathcal{F}$*,* $\mathcal{G}$*, and* $\mathcal{F}$*,* $\widetilde{\mathcal{G}}$*, correspondingly, computed in the* A*-based scalar product. Then, for* $k=1,\ldots,q$*:*

$$|\mu_k-\widehat{\mu}_k|\leq\max\left\{\sin\left(\theta_{\max}\{(\mathcal{G}+\widetilde{\mathcal{G}})\ominus\mathcal{G},\,\mathcal{F}\}\right);\,\sin\left(\theta_{\max}\{(\mathcal{G}+\widetilde{\mathcal{G}})\ominus\widetilde{\mathcal{G}},\,\mathcal{F}\}\right)\right\}\mathrm{gap}_A(\mathcal{G},\widetilde{\mathcal{G}}), \tag{5.7}$$

where $\theta_{\max}$ *is the largest angle between corresponding subspaces, measured in the* A*-based scalar product.*

Proof. The proof is based on the following identity:

$$A^{1/2}(I-Q_FQ_F^TA)Q_{\widetilde{G}}=A^{1/2}(I-Q_FQ_F^TA)Q_GQ_G^TAQ_{\widetilde{G}}+A^{1/2}(I-Q_FQ_F^TA)(I-Q_GQ_G^TA)Q_{\widetilde{G}},$$

which is a multidimensional analog of the trigonometric formula for the sine of the sum of two angles. The rest of the proof is similar to that of Lemma 5.1.

We take $T=A^{1/2}(I-Q_FQ_F^TA)Q_GQ_G^TAQ_{\widetilde{G}}$ and $S=A^{1/2}(I-Q_FQ_F^TA)(I-Q_GQ_G^TA)Q_{\widetilde{G}}$ and use (5.3) to get

$$s_k(A^{1/2}(I-Q_FQ_F^TA)Q_{\widetilde{G}})\leq s_k(A^{1/2}(I-Q_FQ_F^TA)Q_GQ_G^TAQ_{\widetilde{G}})+\|A^{1/2}(I-Q_FQ_F^TA)(I-Q_GQ_G^TA)Q_{\widetilde{G}}\|.$$

In the second term in the sum on the right, $Q_FQ_F^TA=P_F$ and we deduce

$$A^{1/2}(I-Q_FQ_F^TA)(I-Q_GQ_G^TA)Q_{\widetilde{G}}=A^{1/2}(I-P_F)P_{(\mathcal{G}+\widetilde{\mathcal{G}})\ominus\mathcal{G}}(I-Q_GQ_G^TA)Q_{\widetilde{G}}=$$

$$\left(A^{1/2}(I-P_F)P_{(\mathcal{G}+\widetilde{\mathcal{G}})\ominus\mathcal{G}}A^{-1/2}\right)\left(A^{1/2}(I-Q_GQ_G^TA)Q_{\widetilde{G}}\right),$$

using notation $P_{(\mathcal{G}+\widetilde{\mathcal{G}})\ominus\mathcal{G}}$ for the A-orthogonal projector on the subspace $(\mathcal{G}+\widetilde{\mathcal{G}})\ominus\mathcal{G}$, introduced in the proof of Lemma 5.1. Therefore, the second term can be estimated as

$$\|A^{1/2}(I-Q_FQ_F^TA)(I-Q_GQ_G^TA)Q_{\widetilde{G}}\| \le \|A^{1/2}(I-P_F)P_{(\mathcal{G}+\widetilde{\mathcal{G}})\ominus\mathcal{G}}A^{-1/2}\|\|A^{1/2}(I-Q_GQ_G^TA)Q_{\widetilde{G}}\|.$$

The first multiplier,

$$\|A^{1/2}(I-P_F)P_{(\mathcal{G}+\widetilde{\mathcal{G}})\ominus\mathcal{G}}A^{-1/2}\| = \|(I-P_F)P_{(\mathcal{G}+\widetilde{\mathcal{G}})\ominus\mathcal{G}}\|_A = \sin\left(\theta_{\max}\{(\mathcal{G}+\widetilde{\mathcal{G}})\ominus\mathcal{G},\,\mathcal{F}\}\right)$$

by Theorem 4.6 as dim $\mathcal{F} \ge$ dim $((\mathcal{G}+\widetilde{\mathcal{G}})\ominus\mathcal{G})$, while the second multiplier is simply $\mathrm{gap}_A(\mathcal{G},\widetilde{\mathcal{G}})$, because of our assumption dim $\mathcal{G}=$ dim $\widetilde{\mathcal{G}}$.

To estimate the first term in the sum, we take with $T = A^{1/2}(I-Q_FQ_F^TA)Q_G$ and $S^T = Q_G^TAQ_{\widetilde{G}}$ and apply (5.4) :

$$s_k(A^{1/2}(I-Q_FQ_F^TA)Q_GQ_G^TAQ_{\widetilde{G}}) \le s_k(A^{1/2}(I-Q_FQ_F^TA)Q_G)\|Q_G^TAQ_{\widetilde{G}}\| \le s_k(A^{1/2}(I-Q_FQ_F^TA)Q_G),$$

using exactly the same arguments as in the proof of Lemma 5.1.

Thus, we have proved

$$\widehat{\mu}_k \le \mu_k + \sin\left(\theta_{\max}\{(\mathcal{G}+\widetilde{\mathcal{G}})\ominus\mathcal{G},\,\mathcal{F}\}\right)\mathrm{gap}_A(\mathcal{G},\widetilde{\mathcal{G}}).$$

Changing places of $Q_{\widetilde{G}}$ and Q_G, we get

$$\mu_k \le \widehat{\mu}_k + \sin\left(\theta_{\max}\{(\mathcal{G}+\widetilde{\mathcal{G}})\ominus\widetilde{\mathcal{G}},\,\mathcal{F}\}\right)\mathrm{gap}_A(\mathcal{G},\widetilde{\mathcal{G}}).$$

The statement of the lemma follows. □

Remark 5.3. *Let us also highlight that simpler estimates:*

$$|\mu_k-\widehat{\mu}_k| \le \mathrm{gap}_A(\mathcal{G},\widetilde{\mathcal{G}}),\ |\sigma_k-\widehat{\sigma}_k| \le \mathrm{gap}_A(\mathcal{G},\widetilde{\mathcal{G}}),\ k=1,\dots,q,$$

which are not as sharp as those we prove in Lemmas 5.1 and 5.2, can be derived almost trivially using orthoprojectors, see [22, 20, 10], where this approach is used for the case $A=I$. Indeed, we start with identities

$$A^{1/2}P_FP_{\widetilde{G}}A^{-1/2} = A^{1/2}P_FP_GA^{-1/2} + \left(A^{1/2}P_FA^{-1/2}\right)\left(A^{1/2}(P_{\widetilde{G}}-P_G)A^{-1/2}\right)$$

for the cosine and

$$A^{1/2}(I-P_F)P_{\widetilde{G}}A^{-1/2} = A^{1/2}(I-P_F)P_GA^{-1/2} + \left(A^{1/2}(I-P_F)A^{-1/2}\right)\left(A^{1/2}(P_{\widetilde{G}}-P_G)A^{-1/2}\right)$$

for the sine, and use (5.3) and Theorems 4.5 and 4.6. A norm of the second term is then estimated from above by $\mathrm{gap}_A(\mathcal{G},\widetilde{\mathcal{G}})$, using the fact that for an A-orthoprojector P_F we have $\|P_F\|_A = \|I-P_F\|_A = 1$.

Instead of the latter, we can use a bit more sophisticated approach, as in [10], if we introduce the A-orthogonal projector $P_{\mathcal{G}+\widetilde{\mathcal{G}}}$ on the subspace $\mathcal{G}+\widetilde{\mathcal{G}}$. Then the norm of second term is bounded by $\mathrm{gap}_A(\mathcal{G},\widetilde{\mathcal{G}})$ times $\|P_FP_{\mathcal{G}+\widetilde{\mathcal{G}}}\|_A$ for the cosine and times $\|(I-P_F)P_{\mathcal{G}+\widetilde{\mathcal{G}}}\|_A$ for the sine, where we can now use Theorem 4.5 to provide a geometric interpretation of these two constants. This leads to estimates similar to those of [10] for $A=I$:

$$|\mu_k-\widehat{\mu}_k| \le \cos\left(\theta_{\min}\{\mathcal{F},\,\mathcal{G}+\widetilde{\mathcal{G}}\}\right)\mathrm{gap}_A(\mathcal{G},\widetilde{\mathcal{G}}),\ k=1,\dots,q,$$

and

$$|\sigma_k-\widehat{\sigma}_k| \le \cos\left(\theta_{\min}\{\mathcal{F}^{\perp},\,\mathcal{G}+\widetilde{\mathcal{G}}\}\right)\mathrm{gap}_A(\mathcal{G},\widetilde{\mathcal{G}}),\ k=1,\dots,q.$$

However, the apparent constant "improvement" in the second estimate, for the sine, is truly misleading as

$$\cos\left(\theta_{\min}\{\mathcal{F}^{\perp},\, \mathcal{G}+\widetilde{\mathcal{G}}\}\right) = 1$$

simply because $\dim\,\mathcal{F} < \dim\,(\mathcal{G}+\widetilde{\mathcal{G}})$ *in all cases except for the trivial possibility* $\mathcal{G}=\widetilde{\mathcal{G}}$*, so subspaces* $\mathcal{F}^{\perp}$ *and* $\mathcal{G}+\widetilde{\mathcal{G}}$ *must have a nontrivial intersection.*

The first estimate, for the cosine, does give a better constant, compare to one, but our constant is sharper, e.g.,

$$\cos\left(\theta_{\min}\{\mathcal{F},\, (\mathcal{G}+\widetilde{\mathcal{G}})\ominus G\}\right) \le \cos\left(\theta_{\min}\{\mathcal{F},\, \mathcal{G}+\widetilde{\mathcal{G}}\}\right).$$

Our more complex identities used to derive perturbation bounds provide an extra projector in the error term, which allows us to obtain better constants.

We can now establish an estimate of absolute sensitivity of cosine and sine of principle angles with respect to *perturbations of subspaces.*

THEOREM 5.3. *Let* $\sigma_1, \sigma_2, \ldots, \sigma_q$*, and* $\widetilde{\sigma}_1, \widetilde{\sigma}_2, \ldots, \widetilde{\sigma}_q$*, be cosine of principle angles between subspaces* $\mathcal{F}$, $\mathcal{G}$*, and* $\widetilde{\mathcal{F}}$, $\widetilde{\mathcal{G}}$*, correspondingly, computed in the A-based scalar product. Then*

$$|\sigma_k - \widetilde{\sigma}_k| \le c_1 \mathrm{gap}_A(\mathcal{F},\widetilde{\mathcal{F}}) + c_2 \mathrm{gap}_A(\mathcal{G},\widetilde{\mathcal{G}}),\ k=1,\ldots,q, \tag{5.8}$$

where

$$c_1 = \max\left\{\cos\left(\theta_{\min}\{(\mathcal{G}+\widetilde{\mathcal{G}})\ominus\mathcal{G},\, \mathcal{F}\}\right);\, \cos\left(\theta_{\min}\{(\mathcal{G}+\widetilde{\mathcal{G}})\ominus\widetilde{\mathcal{G}},\, \mathcal{F}\}\right)\right\},$$

$$c_2 = \max\left\{\cos\left(\theta_{\min}\{(\mathcal{F}+\widetilde{\mathcal{F}})\ominus\mathcal{F},\, \widetilde{\mathcal{G}}\}\right);\, \cos\left(\theta_{\min}\{(\mathcal{F}+\widetilde{\mathcal{F}})\ominus\widetilde{\mathcal{F}},\, \widetilde{\mathcal{G}}\}\right)\right\},$$

where $\theta_{\min}$ *is the smallest angle between corresponding subspaces in the A-based scalar product.*

Proof. First, by Lemma 5.1, for $k=1,\ldots,q$:

$$|\sigma_k - \widehat{\sigma}_k| \le \max\left\{\cos\left(\theta_{\min}\{(\mathcal{G}+\widetilde{\mathcal{G}})\ominus\mathcal{G},\, \mathcal{F}\}\right);\, \cos\left(\theta_{\min}\{(\mathcal{G}+\widetilde{\mathcal{G}})\ominus\widetilde{\mathcal{G}},\, \mathcal{F}\}\right)\right\}\mathrm{gap}_A(\mathcal{G},\widetilde{\mathcal{G}}).$$

Second, we apply a similar statement to cosine of principle angles between subspaces $\mathcal{F}$, $\widetilde{\mathcal{G}}$ and $\widetilde{\mathcal{F}}$, $\widetilde{\mathcal{G}}$, correspondingly, computed in the A-based scalar product:

$$|\widetilde{\sigma}_k - \widehat{\sigma}_k| \le \max\left\{\cos\left(\theta_{\min}\{(\mathcal{F}+\widetilde{\mathcal{F}})\ominus\mathcal{F},\, \widetilde{\mathcal{G}}\}\right);\, \cos\left(\theta_{\min}\{(\mathcal{F}+\widetilde{\mathcal{F}})\ominus\widetilde{\mathcal{F}},\, \widetilde{\mathcal{G}}\}\right)\right\}\mathrm{gap}_A(\mathcal{F},\widetilde{\mathcal{F}}).$$

The statement of the theorem now follows from the triangle inequality. ☐

THEOREM 5.4. *Let* $\mu_1, \mu_2, \ldots, \mu_q$*, and* $\widetilde{\mu}_1, \widetilde{\mu}_2, \ldots, \widetilde{\mu}_q$ *be sine of principle angles between subspaces* $\mathcal{F}$, $\mathcal{G}$*, and* $\widetilde{\mathcal{F}}$, $\widetilde{\mathcal{G}}$*, correspondingly, computed in the A-based scalar product. Then*

$$|\mu_k - \widetilde{\mu}_k| \le c_3 \mathrm{gap}_A(\mathcal{F},\widetilde{\mathcal{F}}) + c_4 \mathrm{gap}_A(\mathcal{G},\widetilde{\mathcal{G}}),\ k=1,\ldots,q, \tag{5.9}$$

where

$$c_3 = \max\left\{\sin\left(\theta_{\max}\{(\mathcal{G}+\widetilde{\mathcal{G}})\ominus\mathcal{G},\, \mathcal{F}\}\right);\, \sin\left(\theta_{\max}\{(\mathcal{G}+\widetilde{\mathcal{G}})\ominus\widetilde{\mathcal{G}},\, \mathcal{F}\}\right)\right\},$$

$$c_4 = \max\left\{\sin\left(\theta_{\max}\{(\mathcal{F}+\widetilde{\mathcal{F}})\ominus\mathcal{F},\, \widetilde{\mathcal{G}}\}\right);\, \sin\left(\theta_{\max}\{(\mathcal{F}+\widetilde{\mathcal{F}})\ominus\widetilde{\mathcal{F}},\, \widetilde{\mathcal{G}}\}\right)\right\},$$

where $\theta_{\max}$ *is the largest angle between corresponding subspaces in the A-based scalar product.*

Proof. First, by Lemma 5.2, $k=1,\ldots,q$:

$$|\mu_k - \widehat{\mu}_k| \le \max\left\{\sin\left(\theta_{\max}\{(\mathcal{G}+\widetilde{\mathcal{G}})\ominus\mathcal{G},\, \mathcal{F}\}\right);\, \sin\left(\theta_{\max}\{(\mathcal{G}+\widetilde{\mathcal{G}})\ominus\widetilde{\mathcal{G}},\, \mathcal{F}\}\right)\right\}\mathrm{gap}_A(\mathcal{G},\widetilde{\mathcal{G}}).$$

Second, we apply a similar statement to sine of principle angles between subspaces $\mathcal{F}$, $\widetilde{\mathcal{G}}$ and $\widetilde{\mathcal{F}}$, $\widetilde{\mathcal{G}}$, correspondingly, computed in the A-based scalar product:

$$|\widetilde{\mu}_k - \widehat{\mu}_k| \leq \max\left\{\sin\left(\theta_{\max}\{(\mathcal{F}+\widetilde{\mathcal{F}})\ominus\mathcal{F},\, \widetilde{\mathcal{G}}\}\right);\, \sin\left(\theta_{\max}\{(\mathcal{F}+\widetilde{\mathcal{F}})\ominus\widetilde{\mathcal{F}},\, \widetilde{\mathcal{G}}\}\right)\right\}\operatorname{gap}_A(\mathcal{F},\widetilde{\mathcal{F}}).$$

The statement of the theorem now follows from the triangle inequality. □

Finally, we want a perturbation analysis in terms of matrices F and G that generate subspaces $\mathcal{F}$ and $\mathcal{G}$. For that, we have to estimate the sensitivity of a column space of a matrix, for example, matrix G.

LEMMA 5.5. *Let*

$$\kappa_A(G) = \frac{s_{\max}(A^{1/2}G)}{s_{\min}(A^{1/2}G)}$$

denote the corresponding A-based condition number of G, where $s_{\max}$ and $s_{\min}$ are, respectively, largest and smallest singular values of matrix $A^{1/2}G$. Let $\mathcal{G}$ and $\widetilde{\mathcal{G}}$ be column spaces of matrices G and $\widetilde{G}$, respectively. Then

$$\operatorname{gap}_A(\mathcal{G},\widetilde{\mathcal{G}}) \leq \kappa_A(G)\frac{\|A^{1/2}(G-\widetilde{G})\|}{\|A^{1/2}G\|}. \tag{5.10}$$

Proof. Here, we essentially just adopt the corresponding proof of [22] for the A-based scalar product using the same approach as in Theorem 4.2.

Let us consider the polar decompositions

$$A^{1/2}G = A^{1/2}Q_GT_G \text{ and } A^{1/2}\widetilde{G} = A^{1/2}Q_{\widetilde{G}}T_{\widetilde{G}},$$

where matrices $A^{1/2}Q_G$ and $A^{1/2}Q_{\widetilde{G}}$ have orthonormal columns and matrices T_G and $T_{\widetilde{G}}$ are q-by-q symmetric positive definite, e.g., $T_G = (Q_GQ_G^T)^{1/2}$. Singular values of T_G and $T_{\widetilde{G}}$ are, therefore, the same as singular values of $A^{1/2}G$ and $A^{1/2}\widetilde{G}$, correspondingly. Then,

$$(I-P_{\widetilde{G}})(G-\widetilde{G}) = (I-P_{\widetilde{G}})Q_GT_G.$$

Therefore,

$$A^{1/2}(I-P_{\widetilde{G}})Q_G = \left(A^{1/2}(I-P_{\widetilde{G}})A^{-1/2}\right)A^{1/2}(G-\widetilde{G})T_G^{-1},$$

and

$$\operatorname{gap}_A(\mathcal{G},\widetilde{\mathcal{G}}) \leq \|A^{1/2}(G-\widetilde{G})\|\|T_G^{-1}\| = \frac{\|A^{1/2}(G-\widetilde{G})\|}{s_{\min}(A^{1/2}G)},$$

as $\|A^{1/2}(I-P_{\widetilde{G}})A^{-1/2}\| = \|I-P_{\widetilde{G}}\|_A \leq 1$. The statement of the lemma follows. □

REMARK 5.4. *Some matrices allow improvement of their condition numbers by column scaling, which trivially does not change the column range. Our simple Lemma 5.5 does not capture this property. A more sophisticated variant can be easily obtained using technique developed in [11, 10].*

Our cosine theorem follows next. It generalizes results of [20, 10, 11] to A-based scalar product, and somewhat improves the constant.

THEOREM 5.6. *Under assumptions of Theorem 5.3,*

$$|\sigma_k - \widetilde{\sigma}_k| \leq c_1\kappa_A(F)\frac{\|A^{1/2}(F-\widetilde{F})\|}{\|A^{1/2}F\|} + c_2\kappa_A(G)\frac{\|A^{1/2}(G-\widetilde{G})\|}{\|A^{1/2}G\|},\ k=1,\ldots,q. \tag{5.11}$$

The theorem above does not provide an accurate estimate for small angles. To fill the gap, we suggest the following perturbation theorem in terms of sine of principal angles, cf. [20, 10] for $A = I$.

THEOREM 5.7. *Under assumptions of Theorem 5.4,*

$$|\mu - \widetilde{\mu}_k| \leq c_3 \kappa_A(F) \frac{\|A^{1/2}(F - \widetilde{F})\|}{\|A^{1/2}F\|} + c_4 \kappa_A(G) \frac{\|A^{1/2}(G - \widetilde{G})\|}{\|A^{1/2}G\|}, \; k = 1, \ldots, q. \tag{5.12}$$

We consider an algorithm of computing principal angles in the next section.

6. Algorithm Implementation. In this section, we provide a detailed description of our MATLAB code SUBSPACEA.m and discuss the algorithm implementation.

ALGORITHM 6.1 : **SUBSPACEA.m.**

Input: *real matrices F and G with the same number of rows, and a symmetric positive definite matrix A for the scalar product, or a device to compute: Ax for a given vector x.*

1. *Compute A-orthogonal bases $Q_F = \mathrm{ortha}(F)$, $Q_G = \mathrm{ortha}(G)$ of column-spaces of F and G.*
2. *Compute SVD for cosine $[Y, \mathrm{diag}\,(\sigma_1, \ldots, \sigma_q), Z] = \mathrm{svd}(Q_F^T A\, Q_G)$.*
3. *Compute matrices of left $U_{\cos} = Q_F Y$ and right $V_{\cos} = Q_G Z$ principal vectors.*
4. *Compute the matrix* $S = \begin{cases} Q_G - Q_F(Q_F^T A\, Q_G), & \text{if } \mathrm{rank}(Q_F) \geq \mathrm{rank}(Q_G), \\ Q_F - Q_G(Q_G^T A\, Q_F), & \text{otherwise.} \end{cases}$
5. *Compute SVD for sine: $[Y, \mathrm{diag}\,(\nu_1, \ldots, \nu_q), Z] = \mathrm{svd}(S^T A S)$.*
6. *Compute matrices $U_{\sin}$ and $V_{\sin}$ of left and right principal vectors:*
   $V_{\sin} = Q_G Z$, $U_{\sin} = Q_F(Q_F^T A V_{\sin})$, *if* $\mathrm{rank}(Q_F) \geq \mathrm{rank}(Q_G)$;
   $U_{\sin} = Q_F Z$, $V_{\sin} = Q_G(Q_G^T A U_{\sin})$, *otherwise.*
7. *Compute the principle angles, for $k = 1, \ldots, q$:*
   $\theta_k = \begin{cases} \arccos(\sigma_k), & \text{if } \sigma_k^2 \geq 1/2, \\ \arcsin(\sqrt{\nu_{q-k+1}}), & \text{if } \nu_{q-k+1} \leq 1/2. \end{cases}$
8. *Form matrices U and V by picking up corresponding columns of $U_{\sin}$, $V_{\sin}$ and $U_{\cos}$, $V_{\cos}$, according to the choice for θ_k above.*

Output: *Principal angles $\theta_1, \ldots, \theta_q$ between column-spaces of matrices F and G in the A-based scalar product, and corresponding matrices of left, U, and right, V, principal vectors.*

REMARK 6.1. *On Step 1 of the algorithm, the A-orthogonalization can be performed using the QR method, or the SVD, where the latter is apparently more robust for almost linearly dependent columns and ill-conditioned matrices A. In the actual code, we use our SVD-based function ORTHA.m.*

REMARK 6.2. *A check* $\mathrm{rank}(Q_F) \geq \mathrm{rank}(Q_G)$ *on Steps 4 and 6 of the algorithm removes the need for our assumption* $p = \mathrm{rank}(Q_F) \geq \mathrm{rank}(Q_G) = q$.

REMARK 6.3. *We replace here*

$$(I - Q_F Q_F^T A) Q_G = Q_G - Q_F(Q_F^T A G_Q)$$

to avoid having any matrices of the size n-by-n in the algorithm, thus, making it efficient for large-scale problems.

REMARK 6.4. *We compute singular values of $S^T A S$ instead of eigenvalues to increase robustness of the algorithm for small angles. SVD provides better relative accuracy in the presence of round-off errors, which we observe in numerical tests.*

REMARK 6.5. *Our actual code is written for a more general complex case.*

7. Numerical Examples. Our first example is taken from [2] with $p = 13$ and $m = 26$. Matrices F and G were called A and B in [2]. F was orthogonal, while G was an m-by-p Vandermonde matrix with $\mathrm{cond}(G) \approx 10^4$. Matrix G was generated in double precision and then rounded to single precision.

According to our theory above and a perturbation analysis of [2, 20, 10, 11], in this example an absolute change in principle angles is bounded by a perturbation in matrix G times its condition

k	$\sin(\theta_k)$	$\cos(\theta_k)$
1	0.00000000000	1.00000000000
2	0.05942261363	0.99823291519
3	0.06089682091	0.99814406635
4	0.13875176720	0.99032719194
5	0.14184708183	0.98988858230
6	0.21569434797	0.97646093022
7	0.27005046021	0.96284617096
8	0.33704307148	0.94148922881
9	0.39753678833	0.91758623677
10	0.49280942462	0.87013727135
11	0.64562133627	0.76365770483
12	0.99815068733	0.06078820101
13	0.99987854229	0.01558527040

TABLE 7.1: **Computed sine and cosine of principle angles of the example of [2].**

number. Thus, we should expect sine and cosine of principle angles computed in [2] to be accurate with approximately four decimal digits.

In our code, all computations are performed in double precision, therefore, answers in Table 7.1 should be accurate up to twelve decimal digits.

We observe, as expected, that our results are consistent with those of [2] within four digits.

In our next series of tests, we define

$$d = [10^{10}\ 10^{8}\ 2\ 1\ 0.5\ 10^{-10}\ 10^{-20}]$$

and first take

$$F_1 = [I\ 0]^T,\ G_1 = [I\ \mathrm{diag}\,(d)]^T, \tag{7.1}$$

where I and 0 are 7-by-7 identity and zero matrices. We notice that condition numbers of F_1 and G_1 are, respectively, one and 10^{10}, and that G_1 can be scaled column-wise to decrease the condition number almost to one.

The exact values of sine and cosine of principle angles are given by

$$\frac{d_k}{\sqrt{1+d_k^2}},\ \frac{1}{\sqrt{1+d_k^2}},\quad k = 1,\ldots,7, \tag{7.2}$$

correspondingly, see Table 7.2.

We also put in Table 7.2 absolute and relative errors for sine and cosine of principal angles between column-spaces of F_1 and G_1 from (7.1), computed using our code.

We observe that computed results are sharp for the sine. For the cosine, we see an absolute error at the level of double precision, $\epsilon \approx 10^{-16}$, which confirms results of [11, 10] on column scaling of ill-conditioned matrices. Namely, our ill-conditioned matrix G_1 can be made well-conditioned by column scaling, thus, perturbations in the angles should be small. The relative error for the cosine, however, is not apparently bounded by the perturbation even in this simplest test.

For the second test, we multiply both matrices by a random 14-by-14 orthogonal matrix U on the left:

$$F_2 = U * F_1,\ G_2 = U * G_1. \tag{7.3}$$

This transformation does not change angles and condition numbers. It removes, however, a possibility to improve condition number 10^{10} of G_2 by column scaling, so we could expect a loss of accuracy by factor 10^{10}. In a few “atypical” tests, not shown here, we indeed detect an absolute error in sin and

k	exact sin	exact cos	abs sin	rel sin	abs cos	rel cos
1	9.999999999999998e-21	1.000000000000000	0	0	0	0
2	1.000000000000000e-10	1.000000000000000	0	0	0	0
3	4.472135954999580e-01	8.944271909999159e-01	0	0	0	0
4	7.071067811865475e-01	7.071067811865475e-01	0	0	1e-16	1e-16
5	8.944271909999159e-01	4.472135954999580e-01	0	0	1e-16	2e-16
6	1.000000000000000	1.000000000000000e-08	0	0	4e-19	4e-11
7	1.000000000000000	1.000000000000000e-10	0	0	6e-17	7e-07

TABLE 7.2: *Exact values of sine and cosine, and absolute and relative errors for sine and cosine of angles between* F_1 *and* G_1.

k	sin	cos	abs sin	rel sin	abs cos	rel cos
1	3.160689533451956e-16	1.000000000000000	3e-16	3e+04	0	0
2	1.000000725940658e-10	1.000000000000000	7e-17	7e-07	0	0
3	4.472135954999580e-01	8.944271909999159e-01	0	0	0	0
4	7.071067811865474e-01	7.071067811865477e-01	-1e-16	-1e-16	2e-016	3e-16
5	8.944271909999159e-01	4.472135954999580e-01	0	0	1e-16	2e-16
6	1.000000000000000	9.999999556366398e-09	0	0	-4e-16	-4e-08
7	1.000000000000000	1.000000695043548e-10	0	0	7e-17	7e-07

TABLE 7.3: *Sine and cosine of angles between* F_2 *and* G_2*, and corresponding absolute and relative errors.*

cosine at the level up to 10^{-8}. In most cases, however, we do not observe this, see Table 7.3, which shows "typical" computed values sin and cosine of principal angles between column-spaces of F_2 and G_2 from (7.3) and corresponding absolute and relative errors.

The main difference between results in Table 7.2 and Table 7.3 is that the computed values are no longer sharp for the sine, moreover, the relative error for the sine is not apparently bounded by the perturbation, which is consistent with observation of [10] that relative errors of sine and cosine of principal angles are not, in general, bounded.

Finally, we multiply both matrices by random nonsingular 7-by-7 matrices on the right:

$$F_3 = F_2 * P_F, \; G_3 = G_2 * P_G. \tag{7.4}$$

This transformation does not change angles and gives a general case. We only accept random matrices with condition number no more then a hundred, to make sure that condition numbers of matrices F_3 and G_3 are not much larger than those of F_1 and G_1. "Typical" computed results are shown in Table 7.4. We observe absolute errors in sine and cosine at the level up to 10^{-6}, which is consistent with a perturbation analysis of [2, 11] in double precision, as $\text{cond}(G_3) \approx 10^{10}$ and F_3 is well-conditioned. Surprisingly, the absolute error of cosine of small angles is much better. We do not have a perfect explanation of such a good behavior, but our theory suggests that perturbations resulting from round-off errors in ill-conditioned part of G in this case are apparently approximately orthogonal to subspace F, thus, decreasing the effect of ill-conditioning.

Our last numerical results demonstrate robustness of our code for ill-conditioned scalar products.

We take G to be first ten columns of the identity matrix of the size twenty, and F to be the last ten columns of the Vandermonde matrix of the size twenty with elements $v_{i,j} = i^{20-j}$, $i, j = 1, \ldots, 20$. Matrix F is ill-conditioned, $\text{cond}F \approx 10^{13}$. We compute principal angles and vectors between F and G in an A-based scalar product for the following family of matrices

$$A = A_l = 10^{-l} I + H, \, l = 1, \ldots, 16,$$

where I is identity and H is the Hilbert matrix of the order twenty, whose elements are given by $h_{i,j} = 1/(i + j - 1)$, $i, j = 1, \ldots, 20$. Our subspaces $\mathcal{F}$ and $\mathcal{G}$ do not change with l, only the scalar product that describes the geometry of the space, changes. When $l = 1$, we observe three angels with cosine less then 10^{-3} and three angles with sine less then 10^{-3}. When l increases we are getting closer

k	sin	cos	abs sin	rel sin	abs cos	rel cos
1	4.940183241923373e-8	9.999999999999988e-01	4e-8	4e+12	-1e-15	-1e-15
2	1.278801813590290e-6	9.999999999991824e-01	1e-6	1e+04	-8e-13	-8e-13
3	4.472138673096326e-1	8.944270550950270e-01	2e-7	6e-07	-1e-07	-1e-07
4	7.071073700303603e-1	7.071061923422445e-01	5e-7	8e-07	-5e-07	-8e-07
5	8.944269164662731e-1	4.472141445668220e-01	-2e-7	-3e-07	5e-07	1e-06
6	1.000000000000000	1.000000222090166e-08	0	0	2e-15	2e-07
7	1.000000000000000	9.999984745974988e-11	0	0	-1e-16	-1e-06

TABLE 7.4: *Sine and cosine of angles between F_3 and G_3, and corresponding absolute and relative errors.*

to the Hilbert matrix, which emphasizes first rows in matrices F and G, effectively ignoring last rows. By construction of F, its large elements, which make subspace $\mathcal{F}$ to be further away from subspace $\mathcal{G}$, are all in last rows. Thus, we should expect large principal angles between $\mathcal{F}$ and $\mathcal{G}$ to decrease monotonically when l grows. We observe this in our numerical tests, see Figure 7.1, which plots in logarithmic scale sine of all ten principal angles as functions of l.

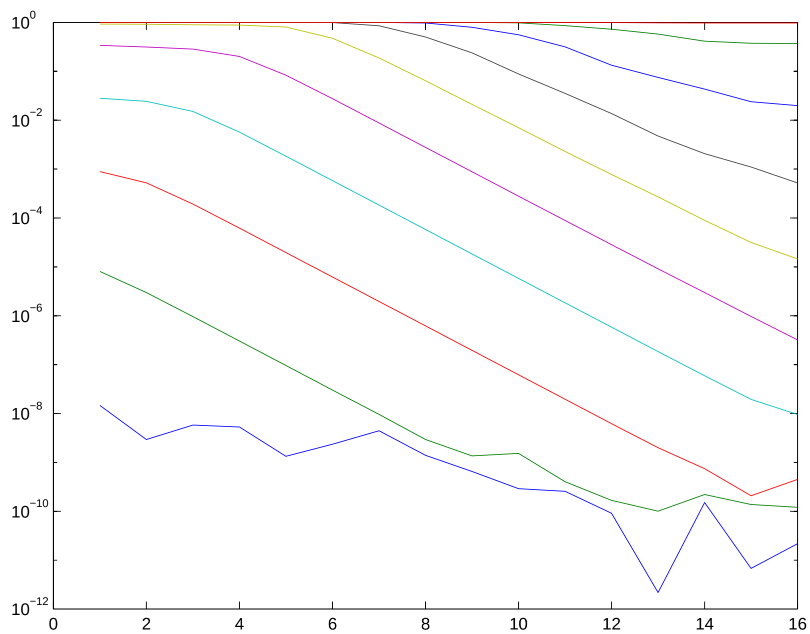

FIG. 7.1: **Sine of principal angles as functions of l.**

Of course, such change in geometry that makes sine of an angle to decrease 10^4 times, means that matrix A_l, describing the scalar product, gets more and more ill-conditioned, as it gets closer to Hilbert matrix H, namely, $\text{cond}(A) \approx 10^l$ in our case. It is known that ill-conditioned problems usually lead to a significant increase of the resulting error, as ill-conditioning amplifies round-off errors. To investigate this effect for our code, we introduce the error as the following sum

$$\text{error} = \|V^T AV - I\| + \|U^T AU - I\| + \|\Sigma - U^T AU\|,$$

where the first two terms control orthogonality of principal vectors and the last term measures the accuracy of cosine of principal angles. We observe in our experiments that different terms in the sum are close to each other, and none dominates. The accuracy of sine of principal angles is not important in this example. As U and V are constructed directly from columns of F and G, they span the same subspaces with high accuracy independently of condition number of A, as we observe in the tests.

We plot the error on the y-axis of Figure 7.2 for Pentium III 500 running two different operating systems: MS Windows NT 4.0 SP6 (red stars) and RedHat LINUX 6.1 (blue diamonds), where the x-axis presents condition number of A, both axes are in logarithmic scale. The MATLAB Version 5.3.1.29215a (R11.1) is the same on both operating systems.

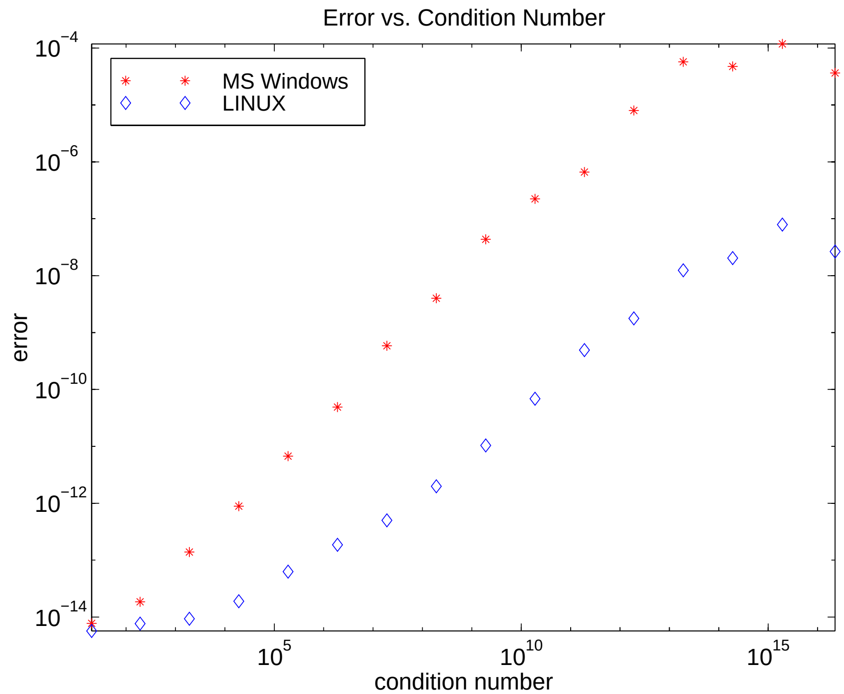

FIG. 7.2: **Error increase for MS Windows and LINUX as functions of condition number.**

We see, as expected, that the error grows, apparently linearly, with the condition number. We also observe, now with quite a surprise, that the error on LINUX is much smaller than the error on MS Windows!

As the same MATLAB's version and the same code SUBSPACEA.m is ran on the same hardware, this fact deserves an explanation. As a result of a discussion with Nabeel and Lawrence Kirby at the News Group *sci.math.num-analysis*, it has been found that MATLAB was apparently compiled on LINUX to take advantage of extended 80 bit precision of FPU registers of PIII, while Windows and specifically Microsoft compilers apparently set the FPU to 64 bit operations. To demonstrate this, Nabeel suggested the following elegant example: compute scalar product

$$(1\ 10^{-19}\ \ -1)^T\ (1\ 1\ 1).$$

On MS Windows, the result is zero, as it should be with double precision, while on LINUX the result is 1.084210^{-19}.

Figure 7.2 shows that our algorithm can turn this seemingly tiny difference into significant error improvement for an ill-conditioned problem and provide numerical results of much better quality.

Finally, our code SUBSPACEA.m has been used for a year in the code LOBPCG.m, see [15], to control accuracy of invariant subspaces of large symmetric generalized eigenvalue problems, and, thus, has been tested for a variety of practical problems.

8. Availability of the Software. Our code SUBSPACEA.m and the function ORTHA.m it uses have been submitted to MathWorks. They are publicly available at
http://www.mathworks.com/support/ftp/linalgv5.shtml
as well as our fix for SUBSPACE.m.

9. Conclusion. Let us formulate here the main points of the present paper:

- A bug in the cosine-based algorithm of computing principle angles between subspaces, which prevents one from computing small angles accurately in computer arithmetic, is illustrated.
- An algorithm is presented that computes all principle angles accurately in computer arithmetic and is proved to be equivalent to the standard algorithm in exact arithmetic.
- A generalization of the algorithm to an arbitrary scalar product given by a symmetric positive definite matrix is suggested and justified theoretically.
- Perturbation estimates for absolute errors in cosine and sine of principal angles, with improved constants and for an arbitrary scalar product, are derived.
- A description of the code is given as well as results of numerical tests. The code is very robust and provides accurate angles for large-scale and ill-conditioned cases.

Acknowledgments. The authors thank CU-Denver graduate students: Sean Jenson, who helped to test our code SUBSPACEA.m; and Chan-Chai Aniwathananon and Saulo Oliveira, who participated in testing the code ORTHA.m.

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