

OPTIMIZING THE COUPLING BETWEEN TWO ISOMETRIC PROJECTIONS OF MATRICES*

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Abstract. In this paper, we analyze the coupling between the isometric projections of two square matrices. These two matrices of dimensions $m \times m$ and $n \times n$ are restricted to a lower k -dimensional subspace under isometry constraints. We maximize the coupling between these isometric projections expressed as the trace of the product of the projected matrices. First we connect this problem to notions such as the generalized numerical range, the field of values, and the similarity matrix. We show that these concepts are particular cases of our problem for special choices of m , n , and k . The formulation used here applies to both real and complex matrices. We characterize the objective function, its critical points, and its optimal value for Hermitian and normal matrices, and, finally, give upper and lower bounds for the general case. An iterative algorithm based on the singular value decomposition is proposed to solve the optimization problem.

Key words. trace maximization, generalized numerical range, isometry, singular value decomposition

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1. Introduction. The problem of projection of matrices in lower-dimensional subspaces is of great interest for a large field of applications. The projection of matrices provides an easier visualization and comprehension of the initial problem and is often used to reduce the complexity of some computational problems. Moreover the coupling between these projections can reveal some particularities inherent to the data which can be analyzed and interpreted.

We consider the coupling or similarity between two “projected” matrices A and B , respectively, of dimensions $m \times m$ and $n \times n$, expressed as the real part of the trace of the product of the isometric projections U^*AU and V^*BV :

$$(1.1) \quad \Re \operatorname{tr}(U^*AU V^*BV)$$

under the constraint that $U^*U = V^*V = I_k$, where I_k denotes the identity matrix of dimension k , with $k \leq \min(m, n)$. In this paper, we will consider both real and complex matrices. The notation will be different for the real and complex cases, i.e., T and $*$, respectively for the transpose and complex conjugate transpose, the real inner product and real-valued inner product, respectively, for the real and complex case (see the notations in section 2.1). In particular, for real matrices, the coupling we consider is the following:

$$(1.2) \quad \operatorname{tr}(U^T A U V^T B^T V).$$

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Most results are developed for the complex case. When results are different for the real and complex problems, we explicitly mention this; otherwise, we consider only the complex problem.

This is a generic problem which can be linked to various applications treated in the literature and which has been studied extensively in a variety of contexts for particular dimensions of the projection and of the matrices. A first field of application for real matrices lies in the analysis of graphs. The notion of the graph similarity matrix, which is a matrix that expresses how similar the nodes of two graphs are, has recently been introduced in [2]. For undirected graphs, the similarity matrix is the product of the isometries U and V^T maximizing (1.2) where A and B are real symmetric adjacency matrices and which is obtained with k equal to one. The graph similarity matrix is, e.g., useful for the development of efficient search engines or the automatic extraction of synonyms in a dictionary. Another important task in graph analysis is that of graph matching, which is a fundamental problem in pattern recognition and in shape and image analysis (see, e.g., [6] for an overview of graph matching techniques). A common class of methods in graph matching is the spectral methods in which spectral properties of characteristic matrices are used to compare the graphs. The spectral method developed in [4] combines a projection technique and a clustering algorithm to match the graphs in a lower-dimensional subspace. It can be shown that the step of projection used by the authors is equivalent to maximizing (1.2) for symmetric matrices A and B . A second field of application where relevant matrices are complex concerns experiments in quantum mechanics and in particular the task of maximizing the signal intensity in coherent ensemble spectroscopy (see, e.g., [7], [9], [16]). Indeed, the spectroscopic experiments require optimal unitary transformations of a given initial operator onto a target operator maximizing the overlap between these two operators. From a mathematical point of view, maximizing this overlap is equivalent to maximizing an expression similar to (1.1) where all of the matrices are square. The optimal value constitutes a transfer bound called the generalized numerical radius of A .

In the linear algebra literature, problem (1.1) has also been studied for particular cases and dimensions, and it hence constitutes an extension of a variety of known problems. For the case where all of the matrices are square, this problem corresponds to the generalized numerical range. See, e.g., [13] or [14] for a survey on the properties of the generalized numerical range. For the scalar case, which corresponds to a one-dimensional projection, the expression (1.1) is equivalent to the product of the field of values of two matrices (see, e.g., [12]). In this paper we consider matrices A and B of different dimensions and an arbitrary dimension k . We treat also the complex and real cases.

There exist many numerical algorithms to maximize (1.1) for particular dimensions of the matrices (e.g., [1], [3], [7], [9]). We develop here a simple recursive algorithm valid for the general case, i.e., for complex or real problems and for all dimensions of the matrices. Characterizations of the fixed points of the algorithm are presented.

The paper is organized as follows. In section 2, we introduce some notations. In section 3, we define the problem considered in the paper which consists of maximizing an expression similar to (1.1). We recall some important results from the literature that we can link to our problem. The first one concerns square matrices and appears in the field of the generalized numerical range and in the context of semidefinite programming relaxations. The second case is about one-dimensional projections and is linked to the field of values of matrices. We extend also some of these results. The

main new results are in section 4, where we characterize the critical points of the problem. Then we focus on the case of Hermitian and normal matrices, and we give lower and upper bounds for the optimal value. In section 5, we propose a simple algorithm to solve the optimization problem. Some numerical experiments are also presented. The last section 6 summarizes the results and describes some directions for future research.

2. Notations. In this section, we introduce some notations used in the paper. The first part treats the complex and real-valued inner product of matrices. The second part summarizes some definitions and results about gradients of functions with matrix arguments. Finally, the definitions of an isometry and of an isometric projection are given.

2.1. Inner product. Let $\mathbb{R}^{m \times n}$ and $\mathbb{C}^{m \times n}$ denote the set of all $m \times n$ real and complex matrices, respectively, and let X^T , \bar{X} , and X^* represent, respectively, the transpose, the complex conjugate, and the complex conjugate transpose of X . The inner product between matrices is defined as follows. For $X, Y \in \mathbb{R}^{m \times n}$, the *real inner product* is denoted by

$$(2.1) \quad \langle X, Y \rangle = \sum_{i=1}^m \sum_{j=1}^n X_{ij} Y_{ij}$$

and can be linked to the trace function of a matrix:

$$\langle X, Y \rangle = \text{tr}(XY^T) = \text{tr}(X^T Y).$$

For complex matrices $X, Y \in \mathbb{C}^{m \times n}$, another inner product often useful in optimization is the *real-valued inner product* defined by:

$$(2.2) \quad \langle X, Y \rangle_H = \langle \Re(X), \Re(Y) \rangle + \langle \Im(X), \Im(Y) \rangle,$$

where $\Re(X)$ and $\Im(X)$ represent the real and the imaginary part of X , respectively. This inner product can be linked again to the trace

$$\langle X, Y \rangle_H = \Re \text{tr}(X^* Y)$$

and satisfies the following properties:

$$(2.3) \quad \langle X, Y \rangle_H = \langle Y^*, X^* \rangle_H = \overline{\langle X^*, Y^* \rangle_H}.$$

For complex vectors $x, y \in \mathbb{C}^n$, the real-valued inner product is defined similarly by:

$$(2.4) \quad \langle x, y \rangle_H = \sum_{i=1}^n \Re(\bar{x}_i y_i) = \langle \Re(x), \Re(y) \rangle + \langle \Im(x), \Im(y) \rangle.$$

2.2. Gradients. Let $f: \mathbb{C}^{m \times n} \rightarrow \mathbb{R}$ be a differentiable real-valued function with matrix argument X . Then the first-order approximation of f at a point X can be expressed as

$$(2.5) \quad f(X + \Delta) = f(X) + \langle \nabla f(X), \Delta \rangle_H + o(\|\Delta\|),$$

where the gradient $\nabla f(X)$ is the $m \times n$ matrix whose (i, j) entry is $\frac{\partial f(X)}{\partial X_{i,j}}$. As particular examples, we provide some gradients of inner-product functions with respect to a matrix X :

$$(2.6) \quad \nabla \langle A, X^* X \rangle_H = X(A + A^*),$$

$$(2.7) \quad \nabla \langle X^* A X, B \rangle_H = A X B^* + A^* X B.$$

2.3. Isometry and isometric projection. Let $A \in \mathbb{C}^{m \times m}$ and $U \in \mathbb{C}^{m \times k}$, $k \leq m$, be given. If $U^*U = I_k$, with I_k the identity matrix of dimension k , then U is called an *isometry* and U^*AU is called an *isometric projection* of A .

3. Main known results and some extensions of these results. For $A \in \mathbb{C}^{m \times m}$ and $B \in \mathbb{C}^{n \times n}$, we consider the following problem:

$$(3.1) \quad \max_{\substack{U^*U=I_k \\ V^*V=I_k}} \langle U^*AU, V^*BV \rangle_H,$$

where $U \in \mathbb{C}^{m \times k}$ and $V \in \mathbb{C}^{n \times k}$, with $k \leq \min(m, n)$. If the matrices A and B are real, one could restrict U and V to be real also which is then a different problem expressed by:

$$(3.2) \quad \max_{\substack{U^T U=I_k \\ V^T V=I_k}} \langle U^T AU, V^T BV \rangle.$$

It will be clear, depending on the context, which case we consider. Since the algebraic structure of the constraints and the objective function is the same, most results for both problems will be essentially the same. Let us remark that, for $k = \min(m, n)$, (3.1) is equivalent to

$$(3.3) \quad \max_{Q^*Q=I_n} \langle Q^*AQ, B \rangle_H,$$

where $Q = UV^*$ is an isometry of dimension $m \times n$. The general problem is then reduced to an optimization problem over only one variable Q .

This problem has largely been studied for particular dimensions of m, n , and k . Section 3.1 contains results for $k = m = n$, while section 3.2 summarizes some properties for $k = 1$.

3.1. Square matrices U and V . In the case where m, n , and k are equal, U and V are square matrices, and the problem is reduced to (3.3). This problem has been studied in a variety of contexts. In the rest of the section, we summarize some important results for the generalized numerical range (or C -numerical range) and for semidefinite programming relaxations providing bounds on the problem. To link the notations used in the literature for this problem with (3.3), we point out that

$$\langle Q^*AQ, B \rangle_H = \Re(\text{tr}(AQB^*Q^*)) = \Re(\text{tr}(B^*Q^*AQ)).$$

3.1.1. C -numerical range. The problem (3.3) is equivalent to maximizing the real part of the C -numerical range of A (or generalized numerical range) introduced by [8] and defined by

$$(3.4) \quad W_C(A) := \{\text{tr}(C^*Q^*AQ) : Q \text{ is unitary}\}.$$

See, e.g., [13] for a survey on the properties of the C -numerical range. In the literature it is pointed out that the C -numerical range and in particular its geometry can be quite complicated. For all $A \in \mathbb{C}^{n \times n}$, $W_C(A)$ is convex if C is Hermitian or if C is normal with its eigenvalues colinear in the complex plane. Moreover, for general A and C , $W_C(A)$ is always star-shaped with respect to the star-center $(\text{tr } A)(\text{tr } C)/n$ [5] but not necessarily convex. For example, [19] gave an example in which C is normal but not Hermitian and where $W_C(A)$ is not convex. Upper bounds on the size of

$W_C(A)$ are given in [9]. In the general case there is no closed formula for computing the C -numerical range. One can only come up with an approximation. For example, [9] provides a gradient flow leading to a numerical algorithm to approach the set of critical points of $\Re(\text{tr}(C^*Q^*AQ))$. See also [3] and [7].

The C -numerical range has been studied by many authors in the past few decades and has many domains of applications, e.g., in quantum dynamics for the study of the efficiency of polarization or coherence transfer between quantized states under unitary transformations. This application is equivalent to computing the C -numerical radius of A for certain sparse nilpotent matrices C and A (e.g., [7], [9], [16]). Some authors have also used the numerical range to study problems on norms of operators (see, e.g., [15]).

3.1.2. Semidefinite programming relaxations.

Real matrices. In the case of real and symmetric matrices A and B , the problem (3.3) is reduced to a classical problem called the quadratically constrained quadratic program defined over orthogonal matrices:

$$(3.5) \quad \mu_P = \max_{Q^T Q = I} \text{tr}(AQBQ^T).$$

This problem can be solved exactly, and the optimal value is obtained by performing spectral decompositions of A and B (see, e.g., [1] or [18]). Let us suppose that the orthogonal diagonalizations of A, B are $A = UD_AU^T$ and $B = VD_BV^T$, respectively, where the eigenvalues in D_A and in D_B are ordered in a nondecreasing fashion. Then the optimal value of (3.5) is $\text{tr} D_A D_B$, and the optimal solution is obtained by using the orthogonal matrices that yield the diagonalizations, i.e., $Q_{opt} = UV^T$.

For real matrices and by a reasoning similar to the one developed in [20], we construct the following primal problem ν_P and its semidefinite programming relaxation ν_D :

$$(3.6) \quad \begin{aligned} \nu_P &= \max_{\substack{Q^T Q = I \\ Q Q^T = I}} \text{tr}(AQB^T Q^T), \\ \nu_D &= \min \text{tr} S + \text{tr} T \\ \text{such that (s.t.)} \quad &\frac{B \otimes A}{2} + \frac{B^T \otimes A^T}{2} - S \otimes I - I \otimes T \preceq 0, \\ &S = S^T, \\ &T = T^T, \end{aligned}$$

where S and T are the symmetric matrices of Lagrange multipliers used to relax the constraints $Q^T Q = I$ and $Q Q^T = I$ and \otimes denotes the Kronecker product. The redundant constraint $Q Q^T = I$ is added in order to close the duality gap for symmetric matrices A and B . Indeed, for symmetric A and B , it is proved that strong duality holds; $\nu_P = \nu_D$ [1]. A few examples show that there can be a nonzero duality gap in the case of arbitrary matrices which are not symmetric. Strong duality does not hold in this case, but this semidefinite relaxation provides an upper bound ν_D for the problem we consider $\nu_P \leq \nu_D$. See section 5.3.2 for an example where a duality gap occurs.

Complex matrices. A complex matrix $A = A_R + jA_I$, with $j = \sqrt{-1}$, of dimension $n \times n$ can be represented by a real matrix \tilde{A} of dimension $2n \times 2n$ of the form:

$$(3.7) \quad \tilde{A} = \begin{pmatrix} A_R & A_I \\ -A_I & A_R \end{pmatrix}.$$

For a Hermitian matrix A , \tilde{A} is symmetric, while, for a unitary matrix Q , \tilde{Q} is orthogonal. If the matrices A , B , and $Q \in \mathbb{C}^{n \times n}$ are represented by the matrices \tilde{A} , \tilde{B} , and $\tilde{Q} \in \mathbb{C}^{2n \times 2n}$, respectively, we obtain the following link between the two trace functions:

$$(3.8) \quad 2\Re \operatorname{tr}(AQB^*Q^*) = \operatorname{tr}(\tilde{A}\tilde{Q}\tilde{B}^T\tilde{Q}^T).$$

One can easily prove this relation by developing the two terms of the equality. The problem (3.5) in terms of complex matrices is thus equivalent to maximizing

$$(3.9) \quad \max_{\tilde{Q}^T\tilde{Q}=I} \frac{1}{2} \operatorname{tr}(\tilde{A}\tilde{Q}\tilde{B}^T\tilde{Q}^T)$$

expressed in terms of real matrices. The dual method developed previously for real matrices can then be applied in the same way and provides an upper bound for the problem.

For Hermitian matrices A and B , strong duality holds because the representations \tilde{A} and \tilde{B} are symmetric, and then the gap between the primal and dual problems is zero. In this case, we know that the solution is simply the trace of the product of the diagonal matrices of the eigenvalues of \tilde{A} and \tilde{B} ordered in an adequate way $\operatorname{tr} D_{\tilde{A}}D_{\tilde{B}}$. By developing the expressions one can easily see that $\operatorname{tr} D_{\tilde{A}}D_{\tilde{B}} = 2 \operatorname{tr} D_A D_B$. The optimal value obtained for Hermitian matrices is then the product of the eigenvalues of the matrices. For general complex matrices A and B , the dual problem provides only an upper bound for the initial problem.

3.2. The one-dimensional case. When k equals one, the matrices U and V are reduced to vectors u and v , respectively, and the problem (3.1) becomes

$$(3.10) \quad \max_{\substack{u^*u=1 \\ v^*v=1}} \langle u^*Au, v^*Bv \rangle_H.$$

This problem is related to the notion of the field of values. The field of values of a matrix A (also known as the numerical range) is defined by [12]

$$F(A) := \{x^*Ax : x \in \mathbb{C}^n, x^*x = 1\}.$$

The problem is then reduced to obtaining the maximum of the products of the elements from the fields of values of A and of B .

The field of values is known to be a convex subset of the complex plane, while the product of two fields of values $F(A)F(B)$ is generally not a convex set. We provide a simple counterexample.

Example 1. Let

$$A = \begin{pmatrix} 1 & 0 \\ 0 & j \end{pmatrix}, \quad B = \begin{pmatrix} -1 & 0 \\ 0 & -j \end{pmatrix}.$$

Then $F(A)$ is the line segment joining 1 and j , and $F(B)$ is the line segment joining -1 and $-j$. Thus $F(A)F(B)$ is not a convex set since $1, -1 \in F(A)F(B)$ and $0 \notin F(A)F(B)$.

In the real and Hermitian cases, we obtain the exact optimal value of the function.

3.2.1. Hermitian case. For a Hermitian matrix A , the field of values is the interval

$$[\lambda_{\min}(A), \lambda_{\max}(A)],$$

with $\lambda_{\min}(A)$ and $\lambda_{\max}(A)$ the smallest and largest eigenvalues of A , respectively. The solution of (3.10) is then the product of the adequate extremal (smallest and largest) eigenvalues of the Hermitian matrices A and B depending on their signs. The solutions u and v providing the optimum are the eigenvectors of A and B corresponding to the eigenvalues providing the solution, respectively.

3.2.2. Real case. For a real matrix A , the field of values could be complex in general. The *real* field of values associated with a real square matrix A is defined by [12]

$$F_R(A) := \{x^T A x : x \in \mathbb{R}^n, x^T x = 1\}.$$

If we notice that $F_R(A) = F_R(A_H)$, with $A_H = \frac{A+A^T}{2}$ the symmetric part of A , then it is sufficient to consider only the symmetric part of the matrix in order to study the real field of values. $F_R(A)$ is the real interval joining the smallest and the largest eigenvalues of A_H and is thus always convex. The solution of (3.10), for A , B , u , and v real, is then the product of the adequate extremal eigenvalues of A_H and B_H depending on their signs.

In the particular case of real symmetric matrices, this scalar case can be linked to the concept of the similarity matrix S introduced in [2]. This matrix expresses how similar vertices of two graphs are and is defined as a particular fixed point of the iteration

$$(3.11) \quad S_{k+1} = \frac{AS_k B^T + A^T S_k B}{\|AS_k B^T + A^T S_k B\|_F},$$

with the Frobenius norm $\|\cdot\|_F = \sqrt{\langle \cdot, \cdot \rangle}$ and where A and B , representing the adjacency matrices of the graphs, have nonnegative elements. In the case where the adjacency matrix of one graph is normal, the similarity matrix has rank one and can then be decomposed into the product of two vectors u and v , $S = uv^T$, and it satisfies the equation $\rho S = ASB^T + A^T SB$ [2]. In the case of undirected graphs which are characterized by symmetric adjacency matrices, u and v are the Perron vectors of A and B . The solutions u and v of (3.10) are then those giving the similarity matrix S . In general S is not of rank one, but we will see in section 5.1 an algorithm to solve the corresponding optimization problem. The similarity matrix can be linked to our problem and is obtained as the limit of the normalized iterates $Au_i v_i^T B^T + A^T u_i v_i^T B$.

4. The general case. In this section we provide some results obtained for the general problem

$$(4.1) \quad \max_{\substack{U^* U = I_k \\ V^* V = I_k}} \langle U^* A U, V^* B V \rangle_H,$$

where $A \in \mathbb{C}^{m \times m}$, $B \in \mathbb{C}^{n \times n}$, $U \in \mathbb{C}^{m \times k}$, and $V \in \mathbb{C}^{n \times k}$, with $k \leq \min(m, n)$.

We derive first the expressions for the critical points of the optimization problem. Then we consider some particular cases, i.e., when one matrix is Hermitian and when the two matrices are normal. An upper and a lower bound to the general problem are also obtained by decomposing the problem into the sum of two Hermitian problems. Let us mention that the techniques used in the rest of the section are quite similar to the ones used in [9].

4.1. Critical points. We consider the following problem:

$$(4.2) \quad \max_{\substack{U^*U=I_k \\ V^*V=I_k}} F(U, V),$$

where the objective function

$$(4.3) \quad F(U, V) = \langle U^*AU, V^*BV \rangle_H = \frac{1}{2} [\langle U^*AU, V^*BV \rangle_H + \langle U^*A^*U, V^*B^*V \rangle_H]$$

according to the trace properties (2.3). The problem is equivalent to maximizing the coupling between two constrained matrices A and B . This is an optimization problem of a continuous function $F(U, V)$ on a compact domain. In particular, the constraint set constitutes a smooth manifold as a product of two compact Stiefel manifolds (see, e.g., [10]). There always exists a solution U and V optimizing the function such that the first-order conditions are satisfied.

The first-order optimality conditions for (4.2) can be derived from the Lagrangian $L(U, V, X, Y)$

$$(4.4) \quad L(U, V, X, Y) = \frac{1}{2} [\langle U^*AU, V^*BV \rangle_H + \langle U^*A^*U, V^*B^*V \rangle_H + \langle X, I - U^*U \rangle_H + \langle Y, I - V^*V \rangle_H],$$

where X and Y are Hermitian matrices of Lagrange multipliers for the isometry constraints. Partial gradients of L with respect to (U, V) according to (2.6) and (2.7) lead to the following first-order optimality conditions:

$$\begin{aligned} \nabla_U L &= AU(V^*B^*V) + A^*U(V^*BV) - UX = 0, \\ \nabla_V L &= BV(U^*A^*U) + B^*V(U^*AU) - VY = 0 \end{aligned}$$

or, equivalently,

$$\begin{aligned} UX &= AU(V^*B^*V) + A^*U(V^*BV), \\ VY &= BV(U^*A^*U) + B^*V(U^*AU), \end{aligned}$$

and of course the constraints $U^*U = V^*V = I$. It easily follows from this that $X = Y$. If we decompose $X = Y$ by an eigendecomposition $\hat{U}\Lambda\hat{U}^*$, where $\hat{U} \in \mathbb{C}^{k \times k}$ is an unitary matrix, then we can replace U by $U\hat{U}$ and V by $V\hat{U}$ which amounts to changing the bases in which we describe the spaces $Im(U)$ and $Im(V)$, the images of U and V . In this particular coordinate system the above first-order conditions would have a real diagonal matrix Λ with ordered diagonal elements $\lambda_i \geq \lambda_{i+1}$, $i = 1, \dots, k - 1$:

$$(4.5) \quad \begin{aligned} U\Lambda &= AU(V^*B^*V) + A^*U(V^*BV), \\ V\Lambda &= BV(U^*A^*U) + B^*V(U^*AU). \end{aligned}$$

4.2. Case where one matrix is Hermitian. If A is Hermitian or $A = A^*$, the maximum of (4.1) is achieved for matrices U and V corresponding, respectively, to the dominant eigenvectors of A and $(B + B^*)$. Moreover $U\Lambda V^*$ is exactly of rank k . In other words, in this case the problem is decoupled regarding the matrices A and B , and the solutions U and V satisfy

$$(4.6) \quad \begin{aligned} AU &= UA_{sub}, \\ (B + B^*)V &= VB_{sub}, \end{aligned}$$

where A_{sub} and B_{sub} are diagonal matrices of dimension k whose elements are the dominant eigenvalues of A and $(B+B^*)$, respectively. The following theorem provides a characterization of the maximum of (4.1).

THEOREM 4.1. *If $A = A^*$,*

$$(4.7) \quad \max_{\substack{U^*U=I_k \\ V^*V=I_k}} \langle U^*AU, V^*BV \rangle_H = \frac{1}{2} \max_{\pi_1, \pi_2} \left(\sum_{i=1}^k \alpha_{\pi_1(i)} \beta_{\pi_2(i)} \right),$$

where $\alpha_1, \dots, \alpha_m$ and β_1, \dots, β_n are the real eigenvalues of A and $(B+B^*)$ and $\pi_1(\cdot)$ and $\pi_2(\cdot)$ permutations of $1, \dots, m$ and $1, \dots, n$, respectively.

Proof. The solution (U, V) satisfies the equations for the critical points

$$(4.8) \quad \begin{aligned} \Lambda &= U^*AUV^*(B+B^*)V, \\ \Lambda &= V^*(B+B^*)VU^*AU, \end{aligned}$$

which point out that the two matrices U^*AU and $V^*(B+B^*)V$ commute and are thus simultaneously diagonalizable under the same unitary transformation W such that

$$(4.9) \quad \begin{aligned} W^*U^*AUW &= D_A, \\ W^*V^*(B+B^*)VW &= D_B. \end{aligned}$$

The expressions in (4.8) become

$$(4.10) \quad \begin{aligned} W^*\Lambda W &= \hat{\Lambda} = D_A D_B, \\ W^*\Lambda W &= \hat{\Lambda} = D_B D_A, \end{aligned}$$

where $\hat{\Lambda}$ is diagonal as a product of two diagonal matrices D_A and D_B . In this coordinate system, the critical point condition (4.5) can be expressed as

$$\begin{aligned} u_i \lambda_i &= A u_i \beta_i, \\ v_i \lambda_i &= (B+B^*) v_i \alpha_i, \end{aligned}$$

where α_i and β_i are the eigenvalues of A and $(B+B^*)$, respectively. If $\lambda_i \neq 0$, it is obvious that u_i and v_i are eigenvectors of A and $(B+B^*)$, respectively. The matrices U and V providing the optimum are thus composed of the dominant eigenvectors. If $\lambda_i = 0$, the above formulas do not imply that both u_i and v_i are eigenvectors, since only one of α_i and β_i needs to be zero, but it is easy to see that one can choose both u_i and v_i to be eigenvectors without altering the objective function.

It follows from (4.8) and (4.10) that the value of F for a critical point is equal to the trace of

$$(4.11) \quad \frac{1}{2} W^*U^*AUV^*(B+B^*)VW.$$

The maximal value for all of the critical points is therefore obtained by

$$(4.12) \quad \frac{1}{2} \max_{\pi_1, \pi_2} \left(\sum_{i=1}^k \alpha_{\pi_1(i)} \beta_{\pi_2(i)} \right),$$

where $\alpha_1, \dots, \alpha_m$ and β_1, \dots, β_n are the real eigenvalues of A and $(B+B^*)$ and $\pi_1(\cdot)$ and $\pi_2(\cdot)$ permutations of $1, \dots, m$ and $1, \dots, n$, respectively. \square

Let us remark that, in the square case ($k = m = n$), Theorem 4.1 is a well-known fact (see, e.g., [1]). In practice, problem (4.12) can be solved by the following theorem (see Figure 4.1 for the notations).

LEMMA 4.2. *Let $\{\alpha_i, i = 1, \dots, m\}$ and $\{\beta_i, i = 1, \dots, n\}$ be the eigenvalues of A and $(B + B^*)$, respectively, ordered in a decreasing fashion. Let m_+ and m_- be the number of nonnegative (positive or zero) and negative eigenvalues of A and n_+ and n_- the number of nonnegative and negative eigenvalues of $(B + B^*)$, and let $k_+ = \min(m_+, n_+)$, $k_- = \min(m_-, n_-)$, and $l = k - (k_+ + k_-)$.*

If $k \leq k_+ + k_-$, the couples of eigenvalues yielding (4.12) are obtained as follows. Take the k_+ products formed with $\{(\alpha_i, \beta_i), i = 1, \dots, k_+\}$ and the k_- products formed with $\{(\alpha_{m-i+1}, \beta_{n-i+1}), i = 1, \dots, k_-\}$ whose values are all nonnegative. Order the values of these products in a decreasing fashion, and keep the pairs of eigenvalues producing the k largest products.

If $k > k_+ + k_-$, take the $k_+ + k_-$ pairs as explained above whose products all have a nonnegative value. The l remaining pairs will give products of negative values which have to be as small as possible in absolute value. These pairs are the following:

$$(4.13) \quad \begin{cases} (\alpha_{m_+ - i + 1}, \beta_{n_+ + l - i + 1}), i = 1, \dots, l & \text{if } k_- = m_-, \\ (\alpha_{m_+ + l - i + 1}, \beta_{n_+ - i + 1}), i = 1, \dots, l & \text{if } k_- = n_-. \end{cases}$$

Proof. Let us put the points $\{\alpha_i, i = 1, \dots, m\}$ and $\{\beta_i, i = 1, \dots, n\}$ on two parallel axes and connect the elements of the selected couples by a line (see Figure 4.1). The optimal couples satisfy two properties.

1. The elements have to be coupled such that no crossing between the pairs appears. In other words, only parallel couplings are allowed. Indeed, if we consider the couples (α_p, β_q) and (α_r, β_s) , with $p > r$, $q > s$, i.e., $\alpha_p \leq \alpha_r$ and $\beta_q \leq \beta_s$, we have

$$\alpha_p \beta_q + \alpha_r \beta_s - \alpha_p \beta_s - \alpha_r \beta_q = (\alpha_p - \alpha_r)(\beta_q - \beta_s) \geq 0.$$

The combination of the two couples (α_p, β_q) and (α_r, β_s) produces therefore a larger value than the value obtained for (α_p, β_s) and (α_r, β_q) .

2. The pairs formed by elements of the same sign have to be chosen first, since their product is nonnegative and therefore larger than a product of two elements of different sign.

Following these two properties, one can easily see that, for $k \leq k_+ + k_-$, the couples of eigenvalues producing (4.12) are the couples formed by the extremal eigenvalues of A and $(B + B^*)$. Indeed these products are all nonnegative and maximize the function.

For $k > k_+ + k_-$, we take into account as well negative products that have to be as small as possible in absolute value for all of the combinations of eigenvalues. Two cases may occur: $k_- = m_-$ or $k_- = n_-$. We consider $k_- = m_-$ (see Figure 4.1), and the reasoning for $k_- = n_-$ is similar. In this case, the first $k_+ + k_-$ pairs are the pairs formed by elements of the same sign according to the second property. The l remaining couples are formed as expressed by (4.13), which takes into account the first property of no crossing between the elements. This expression also takes into account that only the elements closest to zero are kept. Indeed, permuting any element from this set with an element farther from zero will give a product, of negative value, greater in absolute value. For example, if we take $\alpha_{m_+ - 3}$ instead of $\alpha_{m_+ - 2}$ in Figure 4.1, we obtain the couple $\alpha_{m_+ - 3} \beta_{n_+ + 1}$, which is smaller than $\alpha_{m_+ - 2} \beta_{n_+ + 1}$. By reasoning similarly for all of the elements, one proves that only the elements closest to zero yield (4.12). \square

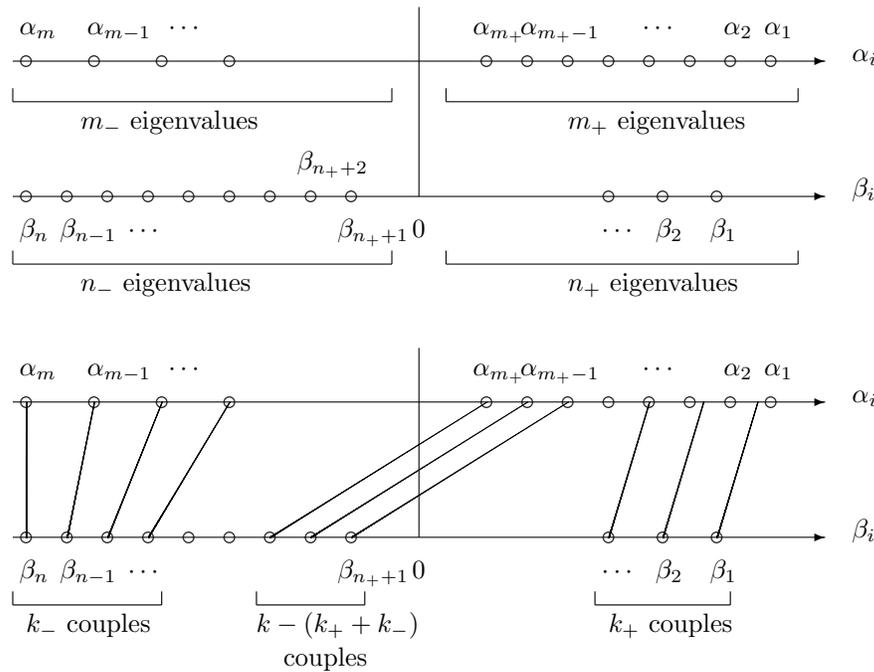


FIG. 4.1. Representation of the eigenvalues α_i of A and β_i of B with their numbering (on the top) and of the k adequate couples for finding the maximal combination (4.12) (on the bottom).

4.3. Sum of two Hermitian problems. The square matrices A and B can always be decomposed into

$$A = A_H + jA_S, \quad B = B_H + jB_S,$$

where the matrices $A_H = \frac{A+A^*}{2}$ and $A_S = \frac{A-A^*}{2j}$ are Hermitian matrices. The objective function can also then be decomposed into a sum of two Hermitian problems

$$(4.14) \quad \frac{1}{2} \langle U^* A_H U, V^* B_H V \rangle_H + \frac{1}{2} \langle U^* A_S U, V^* B_S V \rangle_H.$$

This expression of the objective function provides an upper bound for the optimal value. This bound is expressed in the following corollary.

COROLLARY 4.3. *By Theorem 4.1, an upper bound for (4.2) where $F(U, V)$ is expressed by (4.14) is*

$$(4.15) \quad \frac{1}{2} \max_{\pi_1, \pi_2} \left(\sum_{i=1}^k \alpha_{\pi_1(i)}^H \beta_{\pi_2(i)}^H \right) + \frac{1}{2} \max_{\pi_1, \pi_2} \left(\sum_{i=1}^k \alpha_{\pi_1(i)}^S \beta_{\pi_2(i)}^S \right),$$

with α_i^H and β_i^H the eigenvalues of A_H and B_H , respectively, and α_j^S and β_j^S the eigenvalues of A_S and B_S , respectively. $\pi_1(\cdot)$ and $\pi_2(\cdot)$ are permutations of $1, \dots, m$ and $1, \dots, n$, respectively.

Let us point out that the permutations π_1 and π_2 in these two terms at the respective maxima can be different. A lower bound can also be found by choosing the matrices U and V optimizing one of the two Hermitian problems and by calculating the value of (4.14) for this pair of matrices (U, V) . For example, if we take U_1, V_1 optimum

for $\frac{1}{2}\langle U^*A_HU, V^*B_HV \rangle_H$, the optimal solution is lower and upper bounded by

$$\begin{aligned}
 & \frac{1}{2} \max_{\pi_1, \pi_2} \left(\sum_{i=1}^k \alpha_{\pi_1(i)}^H \beta_{\pi_2(i)}^H \right) + \frac{1}{2} \langle U_1^* A_S U_1, V_1^* B_S V_1 \rangle_H \\
 (4.16) \quad & \leq \max_{\substack{U^*U=I_k \\ V^*V=I_k}} \frac{1}{2} \langle U^* A_H U, V^* B_H V \rangle_H + \frac{1}{2} \langle U^* A_S U, V^* B_S V \rangle_H \\
 & \leq \frac{1}{2} \max_{\pi_1, \pi_2} \left(\sum_{i=1}^k \alpha_{\pi_1(i)}^H \beta_{\pi_2(i)}^H \right) + \frac{1}{2} \max_{\pi_1, \pi_2} \left(\sum_{i=1}^k \alpha_{\pi_1(i)}^S \beta_{\pi_2(i)}^S \right).
 \end{aligned}$$

4.4. Case of two normal matrices. In the case of normal matrices A and B (i.e., $AA^* = A^*A$ and $BB^* = B^*B$), the optimal value for the objective function can be found for $k = 1$ and $k = m = n$. For general $k \leq \min(m, n)$, only an upper bound for the optimal value of the problem can be obtained. The following developments are based on the fact that all normal matrices are diagonalizable under unitary transformation. We can thus make the matrices A and B diagonal matrices D_A and D_B by unitary transformations, with $D_A = D_{A_R} + jD_{A_I}$ and $D_B = D_{B_R} + jD_{B_I}$, where the subscripts R and I denote, respectively, the real and imaginary parts of the matrices. In the rest of the section, $\alpha_i, i = 1, \dots, m$, and $\beta_i, i = 1 \dots, n$, are the eigenvalues of A and B , respectively.

4.4.1. One-dimensional case.

THEOREM 4.4. For $k = 1$ and for A and B normal matrices,

$$(4.17) \quad \max_{\substack{u^*u=1 \\ v^*v=1}} \langle u^* D_A u, v^* D_B v \rangle_H = \max_{i,j} \Re(\alpha_i \beta_j).$$

Proof. For $k = 1$, and by using the diagonalization of the normal matrices A and B , the maximization (4.1) can be expressed as follows:

$$(4.18) \quad \max_{\substack{u^*u=1 \\ v^*v=1}} \langle u^* D_A u, v^* D_B v \rangle_H.$$

This problem is equivalent to

$$\begin{aligned}
 (4.19) \quad & \max \Re \left(\sum_{i=1}^n \mu_i \alpha_i \right) \left(\sum_{i=1}^m \nu_i \beta_i \right) \\
 & \text{s.t.} \quad \sum \mu_i = 1, \\
 & \quad \sum \nu_i = 1, \\
 & \quad \mu_i \geq 0, \nu_i \geq 0,
 \end{aligned}$$

where $\mu_i = |u_i|^2$ and $\nu_i = |v_i|^2$ are nonnegative real numbers. This amounts to optimizing the real part of the products of convex combinations of the eigenvalues of A and B . This problem is a bilinear form with respect to μ_i and ν_i . If we fix μ_i , the problem is linear in ν_i and amounts to a linear programming problem. The feasible set forms a polyhedron, and the optimal solution is situated on a vertex of this polyhedron (or on a face of the polyhedron). We then apply the same reasoning for μ_i to obtain the optimal solution. The problem is then equivalent to finding the indices i and j maximizing

$$(4.20) \quad \max_{i,j} \Re(\alpha_i \beta_j) = \max_{i,j} (\alpha_{i_R} \beta_{j_R} + \alpha_{i_I} \beta_{j_I}),$$

where the subscripts R and I denote, respectively, the real and imaginary parts. □

This problem can be solved in $O(mn)$ operations by merely trying out all products.

4.4.2. Square matrices.

THEOREM 4.5. *For $k = m = n$ and for A and B normal matrices,*

$$(4.21) \quad \max_{Q^*Q=I} \langle Q^*AQ, B \rangle_H = \max_{\pi_2} \sum_{i=1}^n (\alpha_{i_R} \beta_{\pi_2(i)_R} + \alpha_{i_I} \beta_{\pi_2(i)_I}),$$

where $\pi_2(\cdot)$ is a permutation of $1, 2, \dots, n$.

Proof. By using again the diagonalization of the matrices, the maximization can be expressed as follows:

$$(4.22) \quad \max_{Q^*Q=I} (\langle Q^*D_{A_R}Q, D_{B_R} \rangle_H + \langle Q^*D_{A_I}Q, D_{B_I} \rangle_H).$$

If we develop the first term in the function and we define $d_{A_R} = \text{diag}(D_{A_R})$, $d_{B_R} = \text{diag}(D_{B_R})$, α_{i_R} and β_{i_R} the elements i of d_{A_R} and d_{B_R} , and q_i the row i of Q , we obtain

$$\langle Q^*D_{A_R}Q, D_{B_R} \rangle_H = \sum_{i=1}^n \langle |q_i|^2, d_{A_R} \rangle \beta_{i_R}.$$

The last expression is equivalent to

$$\langle \hat{Q}d_{A_R}, d_{B_R} \rangle_H,$$

where $\hat{Q}_{ij} = |Q_{ij}|^2$. \hat{Q} is an orthostochastic¹ matrix and hence a type of doubly stochastic matrix, i.e., $\hat{Q}_{ij} \geq 0$ for all i, j and $\hat{Q}e = \hat{Q}^T e = e$, with e the vector whose entries are all equal to 1. The fact that the row and column sums are all +1 follows from the fact that the rows and columns of Q are all Euclidean unit vectors. From Birkhoff's theorem (see [11]), \hat{Q} is a convex combination of permutation matrices, i.e., $\hat{Q} = \sum_{i=1}^{n!} c_i P_i$, with $\sum_{i=1}^{n!} c_i = 1$ and $c_i > 0$. The above quantity $\langle \hat{Q}d_{A_R}, d_{B_R} \rangle$ is real, and then the problem (4.22) is bounded by the maximum of

$$(4.23) \quad \langle \hat{Q}d_{A_R}, d_{B_R} \rangle + \langle \hat{Q}d_{A_I}, d_{B_I} \rangle$$

for all \hat{Q} doubly stochastic matrices. We are optimizing over the set of doubly stochastic matrices, but the solution is a permutation matrix and hence corresponds to a permutation matrix Q as well. The maximal value of (4.23) is the solution of a corresponding linear programming problem. This value is simply

$$(4.24) \quad \max_{\pi_2} \sum_{i=1}^n (\alpha_{i_R} \beta_{\pi_2(i)_R} + \alpha_{i_I} \beta_{\pi_2(i)_I}),$$

where $\pi_2(\cdot)$ is a permutation of $1, 2, \dots, n$. \square

In the case of Hermitian matrix A or B , the problem simplifies further and is equivalent to optimizing

$$\langle \hat{Q}d_{A_R}, d_{B_R} \rangle$$

because the eigenvalues of a Hermitian matrix are real. We retrieve then the original problem developed in section 4.2.

¹A square matrix X of the form $X = U \circ \bar{U}$ (i.e., X is the Hadamard product of U with itself, $X_{ij} = U_{ij}^2$) for some unitary U is said to be orthostochastic.

TABLE 4.1

Summary of the results and bounds obtained for particular matrices and dimensions.

Dimensions	Matrices	Optimum/Upper bound
$k = m = n$	A Hermitian, B arbitrary	Optimum: maximal combination of the eigenvalues of A and $(B + B^*)$ (4.7): $\frac{1}{2} \max_{\pi_1, \pi_2} (\sum_{i=1}^k \alpha_{\pi_1(i)} \beta_{\pi_2(i)})$
	A, B normal	Optimum: maximal combination of the eigenvalues of A and B (4.24): $\max_{\pi_2} \sum_{i=1}^n (\alpha_{i_R} \beta_{\pi_2(i)_R} + \alpha_{i_I} \beta_{\pi_2(i)_I})$
	A, B arbitrary	Bound: solution of the semidefinite programming relaxation ν_D (3.6) or (4.15).
$k = 1$	A, B real	Optimum: product of the adequate extremal eigenvalues of the symmetric parts of A and B (section 3.2.2)
	A, B Hermitian	Optimum: product of the adequate eigenvalues of A and B (section 3.2.1)
	A, B normal	Optimum: maximal combination of the real and imaginary parts of an eigenvalue of A and an eigenvalue of B (4.20): $\max_{i,j} (\alpha_{R_i} \beta_{R_j} + \alpha_{I_i} \beta_{I_j})$
	A, B arbitrary	Bound: maximal sum of the products of the adequate extremal eigenvalues of the Hermitian and skew-Hermitian parts of A and B (4.15)
$k \leq \min(m, n)$	A Hermitian, B arbitrary	Optimum: maximal sum of the products of k eigenvalues of A and $(B + B^*)$ (4.7): $\frac{1}{2} \max_{\pi_1, \pi_2} (\sum_{i=1}^k \alpha_{\pi_1(i)} \beta_{\pi_2(i)})$
	A, B normal	Bound: maximal sum of the combinations of the real and imaginary parts of k eigenvalues of A and B (4.25): $\max_{\pi_1, \pi_2} \sum_{i=1}^k (\alpha_{\pi_1(i)_R} \beta_{\pi_2(i)_R}) + \max_{\pi_1, \pi_2} \sum_{i=1}^k (\alpha_{\pi_1(i)_I} \beta_{\pi_2(i)_I})$
	A, B arbitrary	Bound: maximal sum of the combinations of the eigenvalues of k Hermitian and skew-Hermitian parts of A and B (4.15): $\frac{1}{2} \max_{\pi_1, \pi_2} (\sum_{i=1}^k \alpha_{\pi_1(i)}^H \beta_{\pi_2(i)}^H) + \frac{1}{2} \max_{\pi_1, \pi_2} (\sum_{i=1}^k \alpha_{\pi_1(i)}^S \beta_{\pi_2(i)}^S)$

4.4.3. General case. In the general case of normal matrices $A \in \mathbb{C}^{m \times m}$ and $B \in \mathbb{C}^{n \times n}$, for $1 \leq k \leq \min(m, n)$ an upper bound for the general problem (4.1) can be found. We optimize the function

$$\max_{\substack{U^* U = I_k \\ V^* V = I_k}} (\langle U^* D_{A_R} U, V^* D_{B_R} V \rangle_H + \langle U^* D_{A_I} U, V^* D_{B_I} V \rangle_H).$$

An upper bound to this problem is then

$$(4.25) \quad \max_{\pi_1, \pi_2} \sum_{i=1}^k (\alpha_{\pi_1(i)_R} \beta_{\pi_2(i)_R}) + \max_{\pi_1, \pi_2} \sum_{i=1}^k (\alpha_{\pi_1(i)_I} \beta_{\pi_2(i)_I}),$$

where α_{i_R} and β_{i_R} are the elements of $\text{diag}(D_{A_R})$ and $\text{diag}(D_{B_R})$, respectively, and α_{i_I} and β_{i_I} the elements of $\text{diag}(D_{A_I})$ and $\text{diag}(D_{B_I})$, respectively. This problem is combinatorial and differs from (4.24).

4.5. Summary of optimal values and bounds. Table 4.1 summarizes the results and the bounds for the problem (4.1) developed in the previous sections. These results and bounds depend on the kind of matrices and their sizes.

5. Numerical computation. In this section we present first an iterative algorithm to find a critical point of (4.1). We then show the equivalence between the fixed

points of the iteration and the critical points of (4.1). At the end of the section, we present some numerical experiments of the algorithm applied to nilpotent matrices.

5.1. Algorithm. The proposed algorithm to solve (4.1) is based on the following relations:

$$\begin{aligned} F(U, V) &= \langle U^*AU, V^*BV \rangle_H \\ &= \frac{1}{2} \langle UV^*, AUV^*B^* + A^*UV^*B \rangle_H \\ &= \frac{1}{2} (\langle UV^*, AUV^*B^* + A^*UV^*B + sUV^* \rangle_H - sk) \end{aligned}$$

resulting from the properties (2.3) and where s is a constant scalar. Let us now define the linear map $M_s(X) = AXB^* + A^*XB + sX$, and then the problem of maximizing $F(U, V)$ is equivalent to the following constrained maximization problem:

$$(5.1) \quad \max_X G(X) = \langle X, M_s(X) \rangle_H \quad \text{s.t.} \quad X = UV^*, U^*U = V^*V = I_k.$$

An algorithm for this problem is given in this section, but it relies on a few intermediate results. In order to show the uniqueness of the iterates of our algorithm, we will need the following two lemmas.

LEMMA 5.1. *Let the singular value decomposition of the matrix $M \in \mathbb{C}^{m \times n}$ be partitioned as*

$$M = [P_1 \mid P_2] \left[\begin{array}{c|c} \Sigma_1 & 0 \\ \hline 0 & \Sigma_2 \end{array} \right] [Q_1 \mid Q_2]^*,$$

with $P_1 \in \mathbb{C}^{m \times k}$, $P_2 \in \mathbb{C}^{m \times (m-k)}$, $Q_1 \in \mathbb{C}^{n \times k}$, $Q_2 \in \mathbb{C}^{n \times (n-k)}$, $\Sigma_1 \in \mathbb{R}^{k \times k}$, and $\Sigma_2 \in \mathbb{R}^{(m-k) \times (n-k)}$ and where $k \leq \min(m, n)$. Then the product $P_1Q_1^*$ is unique if $\sigma_{\min}(\Sigma_1) > \sigma_{\max}(\Sigma_2)$ for $k < \min(m, n)$ and if $\sigma_{\min}(\Sigma_1) > 0$ for $k = \min(m, n)$.

Proof. This is a well-known result, discussed, e.g., in [12, Theorems 3.1.1 and 3.1.1']. \square

Notice that the pairs of matrices (P_1, Q_1) are not unique but are all given by (P_1R, Q_1R) , where R is a unitary matrix commuting with Σ_1 . But the degree of freedom R disappears in the product $P_1Q_1^*$.

LEMMA 5.2. *Let $a_i, b_i \in \mathbb{R}$, $i = 1, \dots, m$, and let $b_1 \geq b_2 \geq \dots \geq b_m \geq 0$. If $\sum_{i=1}^m a_i \leq k$, $k \leq m$, and $0 \leq a_i \leq 1$, $i = 1, \dots, m$, then*

$$\sum_{i=1}^m a_i b_i \leq \sum_{i=1}^k b_i.$$

The upper bound is achieved if $a_i = 1$, $i \leq k$, and $a_i = 0$, $i > k$. Moreover, this is the unique solution achieving the upper bound if $b_k > b_{k+1}$ ($k < m$) or $b_k > 0$ ($k = m$).

Proof. The inequality results from Proposition B.7 for majorized sequences in [17] by remarking that $\sum_{i=1}^m a_i b_i = b^T a$ and $\sum_{i=1}^k b_i = b^T v$, with

$$v = (\underbrace{1, \dots, 1}_k, \underbrace{0, \dots, 0}_{m-k}).$$

The upper bound is achieved if $\sum_{i=1}^k (1 - a_i)b_i = \sum_{i=k+1}^m a_i b_i$. The terms are all nonnegative because $b_i \geq 0$ and $0 \leq a_i \leq 1$ for $i = 1, \dots, m$. The condition $\sum_{i=1}^m a_i \leq k$ implies that

$$\sum_{i=1}^k a_i \leq k - \epsilon, \quad \sum_{i=k+1}^m a_i \leq \epsilon,$$

with $0 \leq \epsilon$. Therefore

$$\sum_{i=1}^k (1 - a_i) b_i \geq b_k \sum_{i=1}^k (1 - a_i) \geq b_k \epsilon$$

and

$$\sum_{i=k+1}^m a_i b_i \leq b_{k+1} \epsilon.$$

If $b_k > b_{k+1}$ (or $b_k > 0$ if $k = m$), the equality $\sum_{i=1}^k (1 - a_i) b_i = \sum_{i=k+1}^m a_i b_i$ is thus achieved if and only if $\epsilon = 0$, i.e., all of the terms equal 0. This happens if $a = v$, which is the unique solution. \square

We now propose an algorithm to solve (5.1) by using an iteration

$$X_{i+1} = \arg \max_X \langle X, M_s(X_i) \rangle_H$$

which is analyzed in the following theorem.

THEOREM 5.3. *Let $M_s(X_i) \in \mathbb{C}^{m \times n}$ be given by*

$$M_s(X_i) = AX_i B^* + A^* X_i B + sX_i, \quad X_i = U_i V_i^*, U_i^* U_i = I_k = V_i^* V_i,$$

with $A \in \mathbb{C}^{m \times m}$, $B \in \mathbb{C}^{n \times n}$, $U_i \in \mathbb{C}^{m \times k}$, and $V_i \in \mathbb{C}^{n \times k}$, where $k \leq \min(m, n)$, and s a constant which is strictly larger than $s_{min} := 4\|A\|_2\|B\|_2$. Assume that $M_s(X_i)$ has an ordered singular value decomposition

$$(5.2) \quad M_s(X_i) = \begin{bmatrix} P_1 & | & P_2 \end{bmatrix} \begin{bmatrix} \Sigma_1 & | & 0 \\ 0 & | & \Sigma_2 \end{bmatrix} \begin{bmatrix} Q_1 & | & Q_2 \end{bmatrix}^* = P \Sigma Q^*,$$

with $P_1 \in \mathbb{C}^{m \times k}$, $P_2 \in \mathbb{C}^{m \times (m-k)}$, $Q_1 \in \mathbb{C}^{n \times k}$, $Q_2 \in \mathbb{C}^{n \times (n-k)}$, $\Sigma_1 \in \mathbb{R}^{k \times k}$, and $\Sigma_2 \in \mathbb{R}^{(m-k) \times (n-k)}$. Let also $U \in \mathbb{C}^{m \times k}$, $V \in \mathbb{C}^{n \times k}$ be isometries. Then

$$(5.3) \quad \max_{\substack{X=UV^* \\ U^*U=I_k=V^*V}} \langle X, M_s(X_i) \rangle_H = \sum_{i=1}^k \sigma_i(M_s)$$

where $\{\sigma_i(M_s)\}$ is the set of singular values of $M_s(X_i)$ ordered in a decreasing way. Moreover the maximizing solution X is unique and equals $P_1 Q_1^*$.

Proof. We first show that $\sigma_k(M_s) > s_{min}/2$ and $\sigma_{k+1}(M_s) \leq s_{min}/2$ and hence that there is a gap between $\sigma_k(M_s)$ and $\sigma_{k+1}(M_s)$. This is proved as follows. The k leading singular values of sX_i are given by s and the others by 0, and the largest singular value $\sigma_1(M_0)$ of $M_0(X_i) = AX_i B^* + A^* X_i B$ is upper bounded by $s_{min}/2$ because

$$\begin{aligned} \sigma_1(M_0) &= \|AX_i B^* + A^* X_i B\|_2 \\ &\leq \|AX_i B^*\|_2 + \|A^* X_i B\|_2 \\ &\leq \|A\|_2\|B\|_2 + \|A\|_2\|B\|_2 = 2\|A\|_2\|B\|_2 = s_{min}/2. \end{aligned}$$

We now apply the perturbation result (Theorem 3.3.16 in [12]) to $M_S(X_i) = M_0(X_i) + sX_i$ and obtain

$$\sigma_{k+1}(M_s) \leq \sigma_{k+1}(sX_i) + \sigma_1(M_0) \leq s_{min}/2$$

and

$$\sigma_k(M_s) \geq \sigma_k(sX_i) - \sigma_1(M_0) > s_{min}/2.$$

We have

$$\langle X, M_s(X_i) \rangle_H = \langle X, P\Sigma Q^* \rangle_H = \langle P^*XQ, \Sigma \rangle_H,$$

and the following two problems are equivalent:

$$\max_{\substack{X=UV^* \\ U^*U=I_k=V^*V}} \langle X, M_s(X_i) \rangle_H = \max_{\substack{\tilde{X}=\tilde{U}\tilde{V}^* \\ \tilde{U}^*\tilde{U}=I_k=\tilde{V}^*\tilde{V}}} \langle \tilde{X}, \Sigma \rangle_H,$$

where $\tilde{U} = P^*U$ and $\tilde{V} = Q^*V$. Without loss of generality, we assume that $n \leq m$ (otherwise the proof is very similar). Then

$$(5.4) \quad \langle \tilde{X}, \Sigma \rangle_H = \sum_{i=1}^n \Re(\tilde{X}_{ii})\sigma_i(M_s) \leq \sum_{i=1}^n |\tilde{X}_{ii}\sigma_i(M_s)| \leq \sum_{i=1}^n \sigma_i(\tilde{X}^*\Sigma) \leq \sum_{i=1}^k \sigma_i(M_s)$$

according to Formula 3.3.10b and Lemma 3.3.1 in [12]. Moreover, since \tilde{U} and \tilde{V} are isometries, we have

$$0 \leq |\tilde{X}_{ii}| \leq 1, \quad i = 1, \dots, n,$$

and, by a reasoning similar to (5.4) with a matrix $M_s(X_i)$ for which $\sigma_i(M_s) = 1, i = 1, \dots, n,$

$$\sum_{i=1}^n |\tilde{X}_{ii}| \leq k.$$

According to Lemma 5.2, $\sum_{i=1}^n |\tilde{X}_{ii}|\sigma_i(M_s) = \sum_{i=1}^k \sigma_i(M_s)$ in (5.4) when $|\tilde{X}_{ii}| = 1$ for $i = 1, \dots, k$ and $|\tilde{X}_{ii}| = 0$ for $i > k$. The upper bound in (5.4) is achieved if all inequalities are equalities. This implies that $\Re(\tilde{X}_{ii}) = |\tilde{X}_{ii}| = 1, i = 1, \dots, k,$ and $\Re(\tilde{X}_{ii}) = |\tilde{X}_{ii}| = 0, i > k,$ i.e., if and only if $\tilde{X}_{ii} = 1, i = 1, \dots, k,$ and $\tilde{X}_{ii} = 0, i > k.$ Since $\tilde{X} = \tilde{U}\tilde{V}^*$ and \tilde{U} and \tilde{V} are isometries, it happens only when $\tilde{X} = \tilde{U}\tilde{V}^* = P^*UV^*Q = \begin{pmatrix} I_k & 0 \\ 0 & 0 \end{pmatrix},$ i.e., when $X = UV^* = P_1Q_1^*$. The conditions of Lemma 5.1 are satisfied, and the solution X is therefore unique. \square

The proposed iterative algorithm to solve (4.1) is then the following one. Choose initial isometries $U_0, V_0,$ and, for $i \geq 0$ until convergence, compute

$$(5.5) \quad X_{i+1} = f_s(X_i) = \arg \max_{\substack{X=UV^* \\ U^*U=I_k=V^*V}} \langle X, M_s(X_i) \rangle_H,$$

where we assume that $\sigma_k(M_s) > \sigma_{k+1}(M_s),$ which is always satisfied by choosing adequately $s.$ Theorem 5.3 gives the maximizing solution and shows that it is unique. In practice, we apply the following procedure in which we switch again to the formulation in terms of U and $V:$ Choose initial isometries U_0 and V_0 and a value for $s,$ and, for $i = 0, 1, \dots$ until convergence, compute the SVD:

$$\left[\begin{array}{c|c} U_{i+1} & U_{\perp} \end{array} \right] \left[\begin{array}{c|c} \Sigma_1 & 0 \\ \hline 0 & \Sigma_2 \end{array} \right] \left[\begin{array}{c|c} V_{i+1} & V_{\perp} \end{array} \right]^* = AU_iV_i^*B^* + A^*U_iV_i^*B + sU_iV_i^*.$$

When the product $U_i V_i^*$ converges (i.e., when $\|U_i V_i^* - U_{i+1} V_{i+1}^*\| \rightarrow 0$), there exists a diagonal matrix $\Lambda = \Sigma_1 - sI_k$ such that

$$(5.6) \quad U\Lambda V^* = AUV^*B^* + A^*UV^*B - U_\perp \Sigma_2 V_\perp^*,$$

where U_\perp and V_\perp are matrices such that every column of U_\perp (resp., V_\perp) is orthogonal to every column of U (resp., V). Σ_2 is a diagonal matrix with elements which are all smaller than the elements of Σ_1 . The scalar s must be larger than $s_{min} = 4\|A\|_2\|B\|_2$. The convergence is not proved, but in all experiments the process always converged linearly to a solution.

Remark 1. An indication that the method has typically linear convergence can be seen from the case $k = 1$ and one of the matrices Hermitian (say, $A = A^*$) (with $|\alpha_1| \geq |\alpha_i|, i = 1, \dots, m, |\beta_1| \geq |\beta_i|, i = 1, \dots, n$, and $\alpha_1\beta_1 > 0$ to simplify the reasoning; indeed the parameter s could then be zero). In this particular case, the iteration becomes

$$(5.7) \quad u_{i+1}\sigma_{i+1}v_{i+1}^* = Au_i v_i^*(B + B^*)$$

because the right-hand side is exactly of rank one. This algorithm corresponds to the combination of two power methods for A and $B + B^*$. Linear convergence is thus guaranteed. The reasoning could be extended for arbitrary $k \leq \min(m, n)$ and for $s = 0$ in the iteration.

5.2. Relation to the optimization problem. In this part we show that solving the iteration (5.5) is equivalent to solving the optimization problem (4.1), whose critical points are expressed by (4.5).

THEOREM 5.4. *Let $s \geq s_{min}$ in $M_s(UV^*)$. Then every fixed point of $f_s(UV^*)$ yields a pair (U, V) that is a critical point of $F(U, V)$. Conversely, every critical point (U, V) of $F(U, V)$ yields a fixed point UV^* of $f_s(UV^*)$.*

Proof. Let UV^* be a fixed point of $f_s(UV^*)$. Then according to Theorem 5.3

$$U\Sigma_1 V^* + U_\perp \Sigma_2 V_\perp^* = AUV^*B^* + A^*UV^*B + sUV^*.$$

Multiply this matrix by V and its Hermitian conjugate by U to get

$$\begin{aligned} U(\Sigma_1 - sI_k) &= AUV^*B^*V + A^*UV^*BV, \\ V(\Sigma_1 - sI_k) &= BVU^*A^*U + B^*VU^*AU. \end{aligned}$$

This is nothing but the condition for a critical point (U, V) of $F(U, V)$ (see (4.5)).

Conversely, let (U, V) be a critical point of $F(U, V)$, and then

$$\begin{aligned} U\Lambda &= AU(V^*B^*V) + A^*U(V^*BV), \\ V\Lambda &= BV(U^*A^*U) + B^*V(U^*AU), \end{aligned}$$

where we have chosen the diagonal ordered form for Λ (see (4.5)). Then, if we define $\Sigma_1 = \Lambda + sI$, with $s > 4\|A\|_2\|B\|_2$,

$$U\Sigma_1 = M_s(UV^*)V, \quad \Sigma_1 V^* = U^*M_s(UV^*).$$

These equations express that the diagonal elements of Σ_1 are singular values of $M_s(UV^*)$ and that the columns of U and V are corresponding right and left singular vectors. Hence there exists an SVD

$$M_s(UV^*) = [U \mid U_\perp] \left[\begin{array}{c|c} \Sigma_1 & 0 \\ \hline 0 & \Sigma_2 \end{array} \right] [V \mid V_\perp]^*,$$

TABLE 5.1
Conjectured values for (5.10) given in [9].

n	1	2	3	4	5	6
f_n^{max}	2	4	$4(1 + \sqrt{3})$	$8(1 + \sqrt{3})$	$16(1 + \sqrt{3}) + 4\sqrt{5}$	$32(1 + \sqrt{3}) + 8\sqrt{5}$

where $\Sigma_2, U_\perp, V_\perp$ contain the remaining singular values and vectors of $M_s(UV^*)$ (where we can choose to order the diagonal elements of Σ_2 as well). Moreover $\sigma_{min}(\Sigma_1) > 2\|A\|_2\|B\|_2 \geq \sigma_{max}(\Sigma_2)$ (see proof of Theorem 5.3). This is the condition for a fixed point UV^* of $f_s(UV^*)$, according to Theorem 5.3. \square

Remark that, for arbitrary matrices A and B , local minima and local maxima can exist, and then the algorithm may not always converge to the global optimum of the function.

5.3. Numerical experiments. As an illustration of the algorithm, we consider the problem of maximizing (4.1) in the case of special nilpotent matrices A_n and B_n . For any $n \in \mathbb{N}$, the nilpotent ($2^{n+1} \times 2^{n+1}$) matrices are recursively defined by

$$(5.8) \quad A_n = \begin{pmatrix} N_n & 0 \\ 0 & N_n \end{pmatrix}, \quad B_n = \begin{pmatrix} 0 & 0 \\ I_{2^n} & 0 \end{pmatrix},$$

with I_m the $m \times m$ identity matrix and N_n given inductively by

$$(5.9) \quad N_n = \begin{pmatrix} N_{n-1} & 0 \\ I_{2^{n-1}} & N_{n-1} \end{pmatrix}, \quad N_0 = 0.$$

The matrices U and V are chosen of the same dimension $2^{n+1} \times 2^{n+1}$. The problem (3.1) is equivalent to maximizing the C -numerical range of A_n

$$(5.10) \quad \max_{Q^*Q=I} \langle Q^* A_n Q, B_n \rangle_H.$$

In [9], the authors provide conjectured maximal values of the function, depending on n . These values are represented in Table 5.1 and have been proved to be correct for $n = 1, 2$.

5.3.1. Numerical values by application of the algorithm. We apply the algorithm given in section 5.1 for nilpotent matrices A_n and B_n defined above (for $n = 1, \dots, 6$). Initial unitary matrices U_0 and V_0 are randomly generated. The results are presented in Figure 5.1. Each plot combines the trajectories for three different initial values. The function

$$(5.11) \quad \text{residual} = f_n^{max} - \max_{\substack{U^*U=I \\ V^*V=I}} \langle U^* A_n U, V^* B_n V \rangle_H$$

is plotted on a logarithmic scale against the number of iterations. The values of f_n^{max} are taken from the above conjecture. The termination criteria we used for the different plots are represented in Table 5.2. We observe a convergence to a maximum defined by the values of the conjecture given in [9].

5.3.2. Duality gap. In this part we show that a duality gap can occur for the problem (3.6) in the case of nonsymmetric matrices. Consider (3.6) for nilpotent matrices A_3 and B_3 . In the assumption that the conjecture in [9] is true, $\nu_P = 4(1 + \sqrt{3}) = 10.92$. The value obtained for the dual problem is $\nu_D = 11$. That proves that a nonduality gap can occur, i.e., $\nu_P \leq \nu_D$.

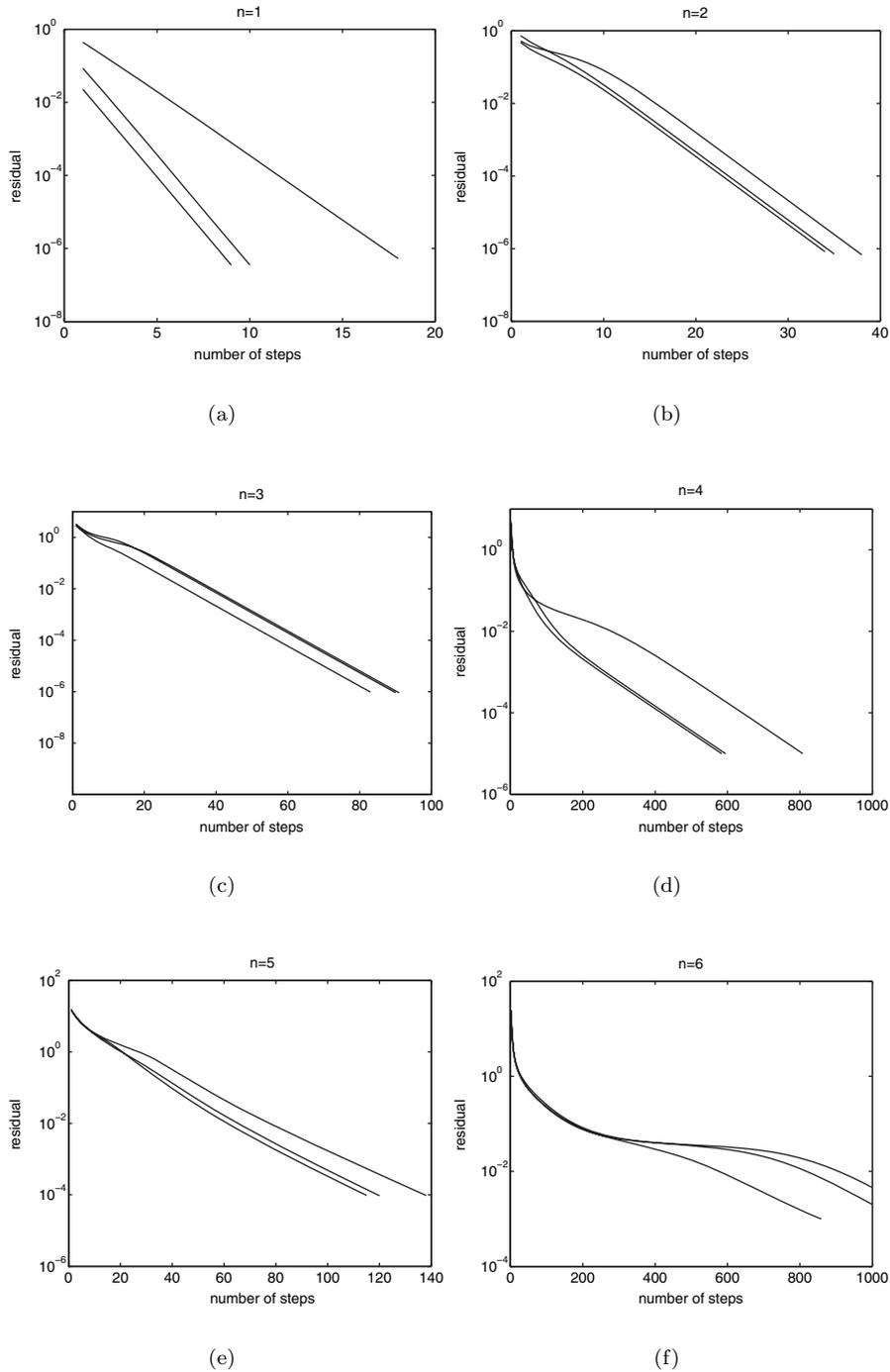


FIG. 5.1. Minimization of the residual (5.11) by application of the SVD algorithm.

TABLE 5.2
Termination criteria for the plots.

n	Residual	or	Number of steps
1	$< 10^{-6}$		> 1000
2	$< 10^{-6}$		> 1000
3	$< 10^{-6}$		> 1000
4	$< 10^{-5}$		> 1000
5	$< 10^{-4}$		> 1000
6	$< 10^{-3}$		> 1000

6. Conclusion. In this paper, we analyze the coupling between two restricted matrices under isometry constraints. Our problem provides a method to project simultaneously the matrices in a subspace of arbitrary dimension k and can be applied to both real and complex matrices. We indicate that it is an extension of various problems found in the literature. Many applications can arise from this formulation.

We present some mathematical properties of the problem and we characterize the maximal coupling for particular matrices such as Hermitian or normal matrices. In general only an upper bound can be found theoretically.

We develop an iterative algorithm in order to reach the optimum, and we characterize the fixed points. This algorithm is very simple to implement and is based on the singular value decomposition. Because this problem is not convex, the analysis of convergence and stability of the fixed points is difficult to realize.

Investigations of mathematical properties and applications of the similarity between restricted matrices can be pursued in several directions. A deeper analysis of the convergence of the algorithm is worthwhile to consider. We outline in the rest of the section a nonexhaustive list of some possible improvements and future research directions.

The first possible improvement concerns the convergence of the algorithm. Experimentally we observe a linear convergence to the optimum, but this convergence has not yet been proved and remains an important point to develop in the future. Second, because the problem is not convex, the analysis of the stability of the fixed points and the study of their basins of attraction are not easy to obtain. This last point is thus a delicate but interesting task to explore. From a more applied point of view, another topic of interest is to investigate how the mathematical concepts proposed here can be used, possibly in modified form, for applications in various areas. Some research for the use of the algorithm in the graph matching problem has been initiated but still needs further investigation. We can conclude that the problem envisaged in this paper gives rise to the study of interesting mathematical properties but also to various applications in different areas.

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