

SYMPLECTIC EIGENVALUE PROBLEM VIA TRACE MINIMIZATION AND RIEMANNIAN OPTIMIZATION*

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Abstract. We address the problem of computing the smallest symplectic eigenvalues and the corresponding eigenvectors of symmetric positive-definite matrices in the sense of Williamson’s theorem. It is formulated as minimizing a trace cost function over the symplectic Stiefel manifold. We first investigate various theoretical aspects of this optimization problem such as characterizing the sets of critical points, saddle points, and global minimizers as well as proving that non-global local minimizers do not exist. Based on our recent results on constructing Riemannian structures on the symplectic Stiefel manifold and the associated optimization algorithms, we then propose solving the symplectic eigenvalue problem in the framework of Riemannian optimization. Moreover, a connection of the sought solution with the eigenvalues of a special class of Hamiltonian matrices is discussed. Numerical examples are presented.

Key words. Symplectic eigenvalue problem, Williamson’s diagonal form, trace minimization, Riemannian optimization, symplectic Stiefel manifold, positive-definite Hamiltonian matrices

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1. Introduction. Given a positive integer n , let us consider the matrix

$$J_{2n} = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix} \in \mathbb{R}^{2n \times 2n},$$

where I_n denotes the $n \times n$ identity matrix. A matrix $X \in \mathbb{R}^{2n \times 2k}$ with $k \leq n$ is said to be *symplectic* if it holds $X^T J_{2n} X = J_{2k}$. Although the term “symplectic” previously seemed to apply to square matrices only, it has recently been used for rectangular ones as well [48, 29]. Note that J_{2n} is orthogonal, skew-symmetric, symplectic, and sometimes referred to as the Poisson matrix [48]. Symplectic matrices appear in a variety of applications including quantum mechanics [20], Hamiltonian dynamics [34, 53], systems and control theory [28, 32, 42] and optimization problems [26, 18]. The set of all symplectic matrices is denoted by $\text{Sp}(2k, 2n)$. When $k = n$, we write $\text{Sp}(2n)$ instead of $\text{Sp}(2k, 2n)$. These matrix sets have a rich geometry structure: $\text{Sp}(2k, 2n)$ is a Riemannian manifold [29], also known as the symplectic Stiefel manifold, whereas $\text{Sp}(2n)$ forms additionally a noncompact Lie group [27, Lemma 1.15].

There are fundamental differences between symplectic and orthonormal matrices: notably, $\text{Sp}(2k, 2n)$ is unbounded [29]. However, their definitions look alike (replacing J by I in the definition of symplectic matrices yields that of orthonormal ones) and several properties of orthonormal matrices have their counterparts for symplectic matrices, e.g., they have full rank and they form a submanifold. Of interest here is the diagonalization of symmetric positive-definite (spd) matrices. The fact that every spd matrix can be reduced by an orthogonal congruence to a diagonal matrix with

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positive diagonal elements is well-known and can be found in any standard linear algebra textbook. This problem is also called the eigenvalue decomposition as the diagonal entries of the diagonalized matrix are the eigenvalues of the given one. Its symplectic counterpart is known as Williamson's theorem [58] which states that for any spd matrix $M \in \mathbb{R}^{2n \times 2n}$, there exists $S \in \text{Sp}(2n)$ such that

$$(1.1) \quad S^T M S = \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix},$$

where $D = \text{diag}(d_1, \dots, d_n)$ with positive diagonal elements. This decomposition is referred to as Williamson's diagonal form or Williamson's normal form of M . The values d_i are called the *symplectic eigenvalues* of M , and the columns of S form a *symplectic eigenbasis* in \mathbb{R}^{2n} . Constructive proofs of Williamson's theorem can be found in [52, 47, 37]. Symplectic eigenvalues have wide applications in quantum mechanics and optics; they are important quantities to characterize quantum systems and their subsystems with Gaussian states [33, 47, 40]. Especially, in the Gaussian marginal problem, knowledge on symplectic eigenvalues helps to determine local entropies which are compatible with a given joint state [22].

The computation of standard eigenvalues is a well-established subfield in numerical linear algebra, see, e.g., [41, 56, 49] and many other textbooks related to matrix analysis and computations. Particularly, numerical methods based on optimization were extensively studied where either a matrix trace or Rayleigh quotient is minimized with some constraints. The generalized eigenvalue problems (EVPs) were investigated in [51, 39, 50, 44] using trace minimization. This approach was also applied to a special class of Hamiltonian matrices in the context of (generalized) linear response EVP [8, 9, 10]. The authors of [21, 2, 1, 11] approached the Rayleigh quotient or trace minimization problem by using Riemannian optimization on an appropriately chosen matrix manifold [4] such as the Stiefel manifold and the Grassmann manifold. However, only very few works devoted to computing symplectic eigenvalues can be found in the literature. In addition to some constructive proofs, e.g., [52, 47], which lead to numerical methods suitable for small to medium-sized problems only, the approaches in [6, 37] are based on the one-to-one correspondence between spd matrices and a special class of Hamiltonian ones, the so-called positive-definite Hamiltonian (pdH) matrices. Specifically, it was proposed in [37] to compute the symplectic eigenvalues of M by transforming the pdH matrix $J_{2n}M$ into a normal form by using elementary symplectic transformations as described in [36]. Furthermore, the symplectic Lanczos method for computing several extreme eigenvalues of pdH matrices developed in [5, 6] was also based on a similar relation. Perturbation bounds for Williamson's diagonal form were presented in [35].

To the best of our knowledge, there is no algorithmic work that relates the computation of symplectic eigenvalues to the optimization framework similar to that for the standard EVP. In [33, 17], a connection between the sum of the k smallest symplectic eigenvalues of an spd matrix and the minimal trace of a matrix function defined on the set of symplectic matrices was established. Note that computation was not the focus and no algorithms were discussed in these works. Moreover, no practical procedure can be directly implied from the relation.

In this paper, building on results of [33, 17] and on various additional properties of the trace minimization problem, we construct an algorithm to compute the smallest symplectic eigenvalues via solving an optimization problem with symplectic constraints by exploiting the Riemannian structure of $\text{Sp}(2k, 2n)$ investigated recently in [29]. Our goal is not merely to find a way to minimize the trace cost function, but

also to investigate the intrinsic connection between the symplectic EVP and the trace minimization problem. To this end, our contributions are mainly reflected in the following aspects. (i) We characterize the set of eigenbasis matrices in Williamson’s diagonal form of an spd matrix (Theorem 3.6) as well as the sets of critical points (Theorem 4.3 and Corollary 4.4), saddle points (Proposition 4.12) and the minimizers (Theorem 4.6 and Corollary 4.7) of the associated trace minimization problem and prove the non-existence of non-global local minimizers (Proposition 4.11). Some of these findings turn out to be important extensions of the existing results for the standard EVP. (ii) Based on a recent development on symplectic optimization derived in [29], we propose an algorithm (Algorithm 5.2) to solve the symplectic EVP via Riemannian optimization. (iii) As an application, we consider computing the standard eigenvalues and the corresponding eigenvectors of the associated pdH matrix. Numerical examples are reported to verify the effectiveness of the proposed algorithm.

To avoid ambiguity, we would like to mention that the term “symplectic eigenvalue problem” or “symplectic eigenproblem” was also used in some works, e.g., [19, 13, 24], in a different meaning. There, symplectic matrices are used as a tool to compute standard eigenvalues of structured matrices such as Hamiltonian, skew-Hamiltonian, and symplectic matrices. The motivation behind this is that symplectic similarity transformations preserve these special structures. The resulting structure-preserving methods are, therefore, referred to as symplectic methods. Here, we focus instead on the computation of the symplectic eigenvalues of spd matrices, where symplectic matrices are involved due to Williamson’s diagonal form (1.1), and a special Hamiltonian EVP is considered as an application only.

The rest of the paper is organized as follows. In section 2, we introduce the notation and review some basic facts for structured matrices. In section 3, we define the symplectic EVP, revisit Williamson’s theorem on diagonalization of spd matrices, and characterize the set of symplectically diagonalizing matrices. We also establish a relation between the standard and symplectic eigenvalues for spd and skew-Hamiltonian matrices. In section 4, we go deeply into the symplectic trace minimization problem and study the connection between the symplectic EVP and trace minimization. In section 5, we present a Riemannian optimization algorithm for computing the smallest symplectic eigenvalues as well as the corresponding eigenvectors. Additionally, we discuss the computation of standard eigenvalues of pdH matrices. Some numerical results are given in section 6. Finally, the conclusion is provided in section 7.

2. Notation and preliminaries. In this section, after stating some conventions for notation, we introduce several structured matrices used in this paper and collect their useful properties.

In the Euclidean space \mathbb{R}^{2n} , e_i denotes the i -th canonical basis vector for $i = 1, \dots, 2n$. The Euclidean inner product of two matrices $X, Y \in \mathbb{R}^{n \times m}$ is denoted by $\langle X, Y \rangle := \text{tr}(X^T Y)$, where $\text{tr}(\cdot)$ is the trace operator and X^T stands for the transpose of X . Given $A \in \mathbb{R}^{m \times m}$, $\text{sym}(A) := \frac{1}{2}(A + A^T)$ denotes the symmetric part of A . We let $\text{diag}(a_1, \dots, a_m) \in \mathbb{R}^{m \times m}$ denote the diagonal matrix with the components a_1, \dots, a_m on the diagonal. This notation is also used for block diagonal matrices, where each a_i is a submatrix block. We use $\text{span}(A)$ to express the subspace spanned by the columns of A . Furthermore, $\mathcal{S}_{\text{sym}}(n)$, $\mathcal{SPD}(n)$, and $\mathcal{S}_{\text{skew}}(n)$ denote the sets of all symmetric, symmetric positive-definite, and skew-symmetric $n \times n$ matrices, respectively. For a twice continuously differentiable function $f : \mathbb{R}^{n \times m} \rightarrow \mathbb{R}$, we denote by $\nabla f(X)$ and $\nabla^2 f(X)$, respectively, the Euclidean gradient and the Hessian of f at X . Moreover, $Dh(X)$ stands for the Fréchet derivative at X of a mapping h

between Banach spaces, if it exists.

A matrix $H \in \mathbb{R}^{2n \times 2n}$ is called *Hamiltonian* if $(J_{2n}^T H)^T = J_{2n}^T H$. It is well-known, e.g., [45], that the eigenvalues of such a matrix appear in pairs $(\lambda, -\lambda)$, if $\lambda \in \mathbb{R} \cup i\mathbb{R}$, or in quadruples $(\lambda, -\lambda, \bar{\lambda}, -\bar{\lambda})$, if $\lambda \in \mathbb{C} \setminus \{\mathbb{R} \cup i\mathbb{R}\}$. Here, $i = \sqrt{-1}$ denotes the imaginary unit. Further, a Hamiltonian matrix $H \in \mathbb{R}^{2n \times 2n}$ is called *positive-definite Hamiltonian* (pdH) if its symmetric generator $J_{2n}^T H$ is positive definite. The eigenvalues of the pdH matrix are purely imaginary [7].

A matrix $N \in \mathbb{R}^{2n \times 2n}$ is called *skew-Hamiltonian* if $(J_{2n}^T N)^T = -J_{2n}^T N$. Each eigenvalue of N has even algebraic multiplicity. Skew-Hamiltonian matrices play an important role in the computation of eigenvalues and invariant subspaces of Hamiltonian matrices, see [16] for a survey.

A matrix $K \in \mathbb{R}^{2n \times 2n}$ is called *orthosymplectic*, if it is both orthogonal and symplectic, i.e., $K^T K = I_{2n}$ and $K^T J_{2n} K = J_{2n}$. We denote the set of $2n \times 2n$ orthosymplectic matrices by $\text{OrSp}(2n)$. It is well-known that similarity transformations of Hamiltonian, skew-Hamiltonian and symplectic matrices with (ortho)symplectic matrices preserve the corresponding matrix structure. This property is often used in structure-preserving algorithms for solving structured EVPs, e.g., [45, 24, 16].

Next, we present some useful facts on symplectic and orthosymplectic matrices which will be exploited later.

PROPOSITION 2.1. *i) Let $S \in \text{Sp}(2n)$. Then $S^{-1}, S^T \in \text{Sp}(2n)$.*

ii) The set of orthosymplectic matrices $\text{OrSp}(2n)$ is a group characterized by

$$\text{OrSp}(2n) = \left\{ K = \begin{bmatrix} K_1 & K_2 \\ -K_2 & K_1 \end{bmatrix} : K_1^T K_2 = K_2^T K_1, K_1^T K_1 + K_2^T K_2 = I \right\}.$$

iii) For $S, T \in \text{Sp}(2k, 2n)$, $\text{span}(S) = \text{span}(T)$ if and only if there exists a matrix $K \in \text{Sp}(2k)$ such that $T = SK$.

Proof. i) These facts have been proved in various sources, e.g., [33, Section 2] or [34, Proposition 2 in Chapter 1].

ii) The representation for elements of $\text{OrSp}(2n)$ has been proved in [20, Section 2.1.2] or [30, Section 7.8.1]. This set is a group because it is the intersection of two groups with the same operation and identity element.

iii) If $k = n$, the proof is straightforward since $\text{Sp}(2n)$ is a group. Otherwise, the sufficiency immediately follows from the relation $T = SK$. To prove the necessity, we assume that $S, T \in \text{Sp}(2k, 2n)$ with $\text{span}(S) = \text{span}(T)$. Then there exists a nonsingular matrix $K \in \mathbb{R}^{2k \times 2k}$ such that $T = SK$. The simplicity of K is verified by $K^T J_{2k} K = K^T S^T J_{2n} S K = T^T J_{2n} T = J_{2k}$. \square

3. Williamson's theorem revisited. In this section, we discuss Williamson's theorem and related issues in detail. This includes a definition of symplectic eigenvectors, a characterization of symplectically diagonalizing matrices, and the methods for computing Williamson's diagonal form for general spd matrices and for spd and skew-Hamiltonian matrices.

3.1. Williamson's diagonal form and symplectic eigenvectors. First, we review some facts related to Williamson's theorem. Let a matrix $M \in \text{SPD}(2n)$ be transformed into Williamson's diagonal form (1.1) with a symplectic transformation matrix $S = [s_1, \dots, s_n, s_{n+1}, \dots, s_{2n}]$ and a diagonal matrix $D = \text{diag}(d_1, \dots, d_n)$ with the symplectic eigenvalues on the diagonal in the non-decreasing order, i.e., $0 < d_1 \leq \dots \leq d_n$. In this case, we will say that S *symplectically diagonalizes* M or that S is a *symplectically diagonalizing* matrix, when M is clear from the context.

Note that the set of symplectic eigenvalues, also called the *symplectic spectrum* of M , is known to be unique [20, Theorem 8.11], while the symplectically diagonalizing matrix S is not unique. It has been shown in [20, Proposition 8.12] that if S and T symplectically diagonalize M , then $S^{-1}T \in \text{OrSp}(2n)$.

The *multiplicity* of the symplectic eigenvalue d_j , $j = 1, \dots, n$, is the number of times it is repeated in D . Note that this definition differs from that for standard eigenvalues, where the appearance of the eigenvalue in $\text{diag}(D, D)$ is counted. The reasons for this discrepancy will get cleared after introducing symplectic eigenvectors, see, e.g., [17, 38] and the references therein.

A pair of vectors (u, v) in \mathbb{R}^{2n} is called (*symplectically*) *normalized* if $\langle u, J_{2n}v \rangle = 1$. Two pairs of vectors (u_1, v_1) and (u_2, v_2) are said to be *symplectically orthogonal* if

$$\langle u_i, J_{2n}v_j \rangle = \langle u_i, J_{2n}u_j \rangle = \langle v_i, J_{2n}v_j \rangle = 0 \quad \text{for } i \neq j, i, j = 1, 2.$$

A matrix $X = [u_1, \dots, u_k, v_1, \dots, v_k] \in \mathbb{R}^{2n \times 2k}$ is said to be *normalized* if each pair (u_i, v_i) , $i = 1, \dots, k$, is normalized. It is called *symplectically orthogonal* if the pairs of vectors (u_i, v_i) are mutually symplectically orthogonal. Note that the symplecticity of X is equivalent to the fact that X is normalized and symplectically orthogonal. For $k = n$, a normalized and symplectically orthogonal vector set forms a *symplectic basis* in \mathbb{R}^{2n} .

The two columns of a matrix $X \in \mathbb{R}^{2n \times 2}$ are called a *symplectic eigenvector pair* of $M \in \text{SPD}(2n)$ associated with a symplectic eigenvalue λ if it holds

$$(3.1) \quad MX = J_{2n}X \begin{bmatrix} 0 & -\lambda \\ \lambda & 0 \end{bmatrix}.$$

If X is additionally symplectic, we call its columns a *normalized symplectic eigenvector pair*. Since each symplectic eigenvalue always needs a pair of symplectic eigenvectors to define, this explains the above definition of the multiplicity.

More general, the columns of $X \in \mathbb{R}^{2n \times 2k}$ are called a *symplectic eigenvector set* of $M \in \text{SPD}(2n)$ associated with the symplectic eigenvalues $\lambda_1, \dots, \lambda_k$, if it holds

$$(3.2) \quad MX = J_{2n}X \begin{bmatrix} 0 & -\Lambda \\ \Lambda & 0 \end{bmatrix}$$

with $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_k)$. If X is, in addition, symplectic, we say that its columns form a *normalized symplectic eigenvector set*.

REMARK 3.1. *If $X \in \text{Sp}(2k, 2n)$ satisfies (3.2), then due to the uniqueness of the symplectic eigenvalues (conventionally arranged in non-decreasing order), there always exists a strictly increasingly ordered index set $\mathcal{I}_k = \{i_1, \dots, i_k\} \subset \{1, \dots, n\}$ such that $\Lambda = \text{diag}(d_{i_1}, \dots, d_{i_k})$. Therefore, in this paper, we will use $X_{\mathcal{I}_k}$ to denote any normalized symplectic eigenvector set associated with the symplectic eigenvalues d_{i_1}, \dots, d_{i_k} . If $\mathcal{I}_k = \{1, \dots, k\}$, we will write $X_{1:k}$.*

Multiplying both sides of Williamson's diagonal form (1.1) from the left with $S^{-T} = J_{2n}S J_{2n}^T$, we obtain

$$(3.3) \quad MS = J_{2n}S J_{2n}^T \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} = J_{2n}S \begin{bmatrix} 0 & -D \\ D & 0 \end{bmatrix}.$$

This implies that for any ordered index set $\mathcal{I}_k = \{i_1, \dots, i_k\} \subset \{1, \dots, n\}$, the columns of the symplectic submatrix $[s_{i_1}, \dots, s_{i_k}, s_{n+i_1}, \dots, s_{n+i_k}]$ of S form a normalized symplectic eigenvector set of M associated with d_{i_1}, \dots, d_{i_k} . Note that $[cs_i, cs_{n+i}]$ with $c \notin \{-1, 0, 1\}$ is a symplectic eigenvector pair associated with d_i but not normalized.

Taking into account (3.3), Williamson's theorem can alternatively be restated as follows: For any $M \in \mathcal{SPD}(2n)$, there exists a normalized symplectic eigenvector set of M that constitutes a symplectic basis in \mathbb{R}^{2n} .

Next, we collect some useful facts on symplectic eigenvectors.

PROPOSITION 3.2. [38, Corollaries 2.4 and 5.3] *Let $M \in \mathcal{SPD}(2n)$.*

- i) Any two symplectic eigenvector pairs corresponding to two distinct symplectic eigenvalues of M are symplectically orthogonal.*
- ii) Let λ be a symplectic eigenvalue of M of multiplicity m and let the columns of $X \in \mathbb{R}^{2n \times 2m}$ be a normalized symplectic eigenvector set associated with λ . Then the columns of a matrix $Y \in \mathbb{R}^{2n \times 2m}$ form also a normalized symplectic eigenvector set associated with λ if and only if there exists $K \in \text{OrSp}(2m)$ such that $Y = XK$.*

We conclude this subsection by mentioning a connection between the symplectic eigenvalues and eigenvectors of the spd matrix M and the standard eigenvalues and eigenvectors of the pdH matrix $J_{2n}M$. This result is not new and has already been established in a slightly different form in [20, Theorem 8.11] and [38, Lemma 2.2].

PROPOSITION 3.3. *Let $M \in \mathcal{SPD}(2n)$ and let $S = [s_1, \dots, s_{2n}]$ be a symplectically diagonalizing matrix of M . Then $d_j, j = 1, \dots, n$, are the symplectic eigenvalues of M if and only if $\pm id_j, j = 1, \dots, n$, are the standard eigenvalues of the pdH matrix $H = J_{2n}M$. Moreover, for any $j = 1, \dots, n$, $s_j \pm is_{n+j}$ is an eigenvector of H corresponding to the eigenvalue $\pm id_j$.*

Proof. The result immediately follows from the relation (3.3). \square

This proposition shows that the eigenvalues of a pdH matrix H are purely imaginary and that they can be determined by computing the symplectic eigenvalues of the corresponding spd matrix $M = J_{2n}^T H$.

3.2. Characterization of the set of symplectically diagonalizing matrices. As we mentioned before, the diagonalizing matrix in Williamson's diagonal form (1.1) is not unique. In this subsection, we aim to characterize the set of all symplectically diagonalizing matrices.

First, note that if $M \in \mathcal{SPD}(2n)$ has only one symplectic eigenvalue of multiplicity n , then by Proposition 3.2(ii) such a set is given by $S\text{OrSp}(2n)$, where S is any symplectically diagonalizing matrix of M . For general case, we present two special classes of symplectically diagonalizing matrices.

PROPOSITION 3.4. *Let $M \in \mathcal{SPD}(2n)$ and let $S \in \text{Sp}(2n)$ symplectically diagonalize M . Then the following statements hold.*

- i) Let $R_{(j,\theta)} \in \mathbb{R}^{2n \times 2n}$ be the Givens rotation matrix of angle θ in the plane spanned by e_j and e_{n+j} . Then $SR_{(j,\theta)}$ symplectically diagonalizes M for any $j = 1, \dots, n$ and $\theta \in [0, 2\pi)$.*
- ii) Let $Q = \text{diag}(Q_1, \dots, Q_q, Q_1, \dots, Q_q)$, where $Q_j \in \mathbb{R}^{m_j \times m_j}$, $j = 1, \dots, q$, are orthogonal, m_1, \dots, m_q are multiplicities of the symplectic eigenvalues and $m_1 + \dots + m_q = n$. Then SQ symplectically diagonalizes M .*

Proof. As the product of two symplectic matrices is again symplectic, we have to show that $R_{(j,\theta)}$ and Q are symplectic, and that they congruently preserve $\text{diag}(D, D)$, i.e., $R_{(j,\theta)}^T \text{diag}(D, D) R_{(j,\theta)} = \text{diag}(D, D)$ and $Q^T \text{diag}(D, D) Q = \text{diag}(D, D)$. This can be verified by direct calculations. \square

In the case $n = 1$, it follows from [20, Proposition 8.12] that the set of all symplectically diagonalizing matrices is $S\mathbb{SO}(2)$, where $\mathbb{SO}(2)$ is the orthogonal group of

rotations in \mathbb{R}^2 . In other words, the first class of matrices in Proposition 3.4 completely characterizes the set of all symplectically diagonalizing matrices when $n = 1$.

For the general case $n > 1$, it turns out that Proposition 3.2 plays an important role in establishing the required result. Using the first statement in this proposition, we can show that the symplectic eigenvectors associated with distinct symplectic eigenvalues are linearly independent, see, e.g., [20, Theorem 1.15]. Let

$$A^{(i)} = \begin{bmatrix} A_1^{(i)} & A_2^{(i)} \\ A_3^{(i)} & A_4^{(i)} \end{bmatrix} \in \mathbb{R}^{2k_i \times 2k_i}, \quad i = 1, \dots, q,$$

be matrices that have been decomposed into four square blocks. We will denote by

$$\text{dab}(A^{(1)}, \dots, A^{(q)}) = \begin{bmatrix} A_1 & A_2 \\ A_3 & A_4 \end{bmatrix}$$

the $2(k_1 + \dots + k_q) \times 2(k_1 + \dots + k_q)$ matrix generated by diagonally assembling the blocks $A_\ell^{(i)}$ such that $A_\ell = \text{diag}(A_\ell^{(1)}, \dots, A_\ell^{(q)})$, $\ell = 1, \dots, 4$. Hence the notation ‘‘dab’’. If each matrix $A^{(i)}$ belongs to a set of matrices $\Phi^{(i)}$, then $\text{dab}(\Phi^{(1)} \times \dots \times \Phi^{(q)})$ denotes the set of all matrices $\text{dab}(A^{(1)}, \dots, A^{(q)})$ with $A^{(i)} \in \Phi^{(i)}$, $i = 1, \dots, q$. It is straightforward to verify the following lemma.

LEMMA 3.5. *For any set of integers k_1, \dots, k_q , it holds that*

$$\text{dab}(\text{OrSp}(2k_1) \times \dots \times \text{OrSp}(2k_q)) \subset \text{OrSp}(2(k_1 + \dots + k_q)).$$

One can check that the matrices $R_{(j,\theta)}$ and Q in Proposition 3.4 are elements of the set $\text{dab}(\text{OrSp}(2k_1) \times \dots \times \text{OrSp}(2k_q))$ with appropriately chosen k_1, \dots, k_q . Indeed, for any $j = 1, \dots, n$, $R_{(j,\theta)} \in \text{dab}(\text{OrSp}(2(j-1)) \times \text{OrSp}(2) \times \text{OrSp}(2(n-j)))$. Similarly, the matrix Q belongs to the set $\text{dab}(\text{OrSp}(2m_1) \times \dots \times \text{OrSp}(2m_q))$.

We are now ready to state the main result in this subsection. Theorem 3.6 below is an important improvement of the classical result [20, Proposition 8.12] in the sense that it characterizes exactly the set of symplectically diagonalizing matrices of $M \in \text{SPD}(2n)$. Moreover, its sufficiency part covers the matrix classes in Proposition 3.4 as special cases. Finally, it is also a nontrivial generalization of Proposition 3.2(ii).

THEOREM 3.6. *Let $M \in \text{SPD}(2n)$ have $q \leq n$ distinct symplectic eigenvalues d_1, \dots, d_q with multiplicities m_1, \dots, m_q , respectively, and let $S \in \text{Sp}(2n)$ be a symplectically diagonalizing matrix of M . Then $T \in \text{Sp}(2n)$ symplectically diagonalizes M if and only if there exists $K \in \text{dab}(\text{OrSp}(2m_1) \times \dots \times \text{OrSp}(2m_q))$ such that $T = SK$.*

Proof. First, we show the sufficiency. Lemma 3.5 implies that $K \in \text{OrSp}(2n)$. Then we obtain

$$T^T M T = K^T S^T M S K = K^T \text{diag}(D, D) K = K^T K \text{diag}(D, D) = \text{diag}(D, D),$$

where the third equality follows from the fact that $K \in \text{dab}(\text{OrSp}(2m_1) \times \dots \times \text{OrSp}(2m_q))$. This means that T symplectically diagonalizes M .

Conversely, let T symplectically diagonalize M . Let us pick any symplectic eigenvalue d_i of multiplicity m_i , $i = 1, \dots, q$, and let $\mathcal{I}_{m_i} = \{j_i + 1, \dots, j_i + m_i\}$ with $j_i = m_1 + \dots + m_{i-1}$. Then the columns of $S_{\mathcal{I}_{m_i}}, T_{\mathcal{I}_{m_i}} \in \mathbb{R}^{2n \times 2m_i}$ form the normalized symplectic eigenvector sets associated with d_i . Therefore, by Proposition 3.2(ii) there exists $K^{(i)} \in \text{OrSp}(2m_i)$ such that $T_{\mathcal{I}_{m_i}} = S_{\mathcal{I}_{m_i}} K^{(i)}$. Ordering the columns of $T_{\mathcal{I}_{m_i}}$ and $S_{\mathcal{I}_{m_i}}$ for $i = 1, \dots, q$ as in T and S , respectively, we obtain $T = SK$ with $K = \text{dab}(K^{(1)}, \dots, K^{(q)}) \in \text{dab}(\text{OrSp}(2m_1) \times \dots \times \text{OrSp}(2m_q))$. \square

3.3. Computation of Williamson's diagonal form. Here, we present an algorithm based on [47] for computing a symplectically diagonalizing matrix S of M in (1.1). This procedure can also be viewed as a constructive proof of Williamson's theorem. Since M is spd, its real symmetric square root $M^{1/2}$ exists. It is easy to check that $\tilde{M} = M^{1/2}J_{2n}M^{1/2}$ is skew-symmetric and nonsingular. This matrix can be transformed into the real Schur form

$$(3.4) \quad Q^T \tilde{M} Q = \text{diag} \left(\begin{bmatrix} 0 & d_1 \\ -d_1 & 0 \end{bmatrix}, \dots, \begin{bmatrix} 0 & d_n \\ -d_n & 0 \end{bmatrix} \right),$$

where Q is orthogonal, and $0 < d_1 \leq \dots \leq d_n$, see [30, Theorem 7.4.1]. Further, let

$$(3.5) \quad P = [e_1, e_3, \dots, e_{2n-1}, e_2, e_4, \dots, e_{2n}]$$

denote the perfect shuffle permutation matrix. Obviously, QP is orthogonal and it holds

$$P^T Q^T \tilde{M} Q P = \begin{bmatrix} 0 & D \\ -D & 0 \end{bmatrix},$$

where $D = \text{diag}(d_1, \dots, d_n)$. Finally, we set

$$(3.6) \quad S = J_{2n} M^{1/2} Q P \begin{bmatrix} 0 & -D^{-1/2} \\ D^{-1/2} & 0 \end{bmatrix}.$$

It can be verified that S is symplectic and $S^T M S = \text{diag}(D, D)$. For ease of reference, we summarize these steps in Algorithm 3.1.

Algorithm 3.1 Williamson's diagonal form

Input: $M \in \mathcal{SPD}(2n)$.

Output: $S \in \text{Sp}(2n)$, $D = \text{diag}(d_1, \dots, d_n)$ such that $S^T M S = \text{diag}(D, D)$.

- 1: Compute the symmetric square root $M^{1/2}$ of M .
 - 2: Compute the real Schur form (3.4) of $\tilde{M} = M^{1/2}J_{2n}M^{1/2}$.
 - 3: Set $D = \text{diag}(d_1, \dots, d_n)$ and compute the symplectic matrix S as in (3.6) with P given in (3.5).
-

Note that $M^{1/2}$ can be computed using the spectral decomposition of M , see [31, Section 6.2]. For the computation of the real Schur form (3.4), we can employ the skew-symmetric QR algorithm [54]. In this case, Algorithm 3.1 requires about $125n^3$ flops.

3.4. Williamson's diagonal form for skew-Hamiltonian matrices. To close this section, we present an alternative algorithm for computing Williamson's diagonal form of spd matrices which are additionally assumed to be skew-Hamiltonian. This algorithm and Proposition 3.7 below will be of crucial importance and employed as a step, which is faster than Algorithm 3.1 designed for general spd matrices, in our optimization method for computing the symplectic eigenvalues and eigenvectors of general spd matrices presented in Section 5.

PROPOSITION 3.7. *Let $N \in \mathbb{R}^{2n \times 2n}$ be spd and skew-Hamiltonian. If S symplectically diagonalizes N , then $S \in \text{OrSp}(2n)$.*

Proof. It has been constructively shown in [16] that any skew-Hamiltonian matrix N can be transformed into a real skew-Hamiltonian-Schur form

$$(3.7) \quad K^T N K = \begin{bmatrix} \Omega_{11} & \Omega_{12} \\ 0 & \Omega_{11}^T \end{bmatrix},$$

where $K \in \text{OrSp}(2n)$ and $\Omega_{11} \in \mathbb{R}^{n \times n}$ is quasi-triangular with diagonal blocks of order one and two corresponding, respectively, to real and complex standard eigenvalues of N . Since N is spd, we obtain that Ω_{11} is diagonal and $\Omega_{12} = 0$. Thus, K symplectically diagonalizes N .

Let S be any symplectically diagonalizing matrix of N and let $K \in \text{OrSp}(2n)$ be the diagonalizing matrix as in (3.7). Then by [20, Proposition 8.12], we have $K^{-1}S \in \text{OrSp}(2n)$. This implies that $S \in \text{OrSp}(2n)$. \square

It immediately follows from Proposition 3.7 that the standard eigenvalues of an spd and skew-Hamiltonian matrix N coincide with the symplectic eigenvalues. Moreover, we obtain that the symplectically diagonalizing matrix of N constructed by Algorithm 3.1 is orthosymplectic.

An alternative method for computing Williamson's diagonal form of N , based on the construction of the skew-Hamiltonian-Schur form (3.7) as presented in [16, Algorithm 10], is now summarized in Algorithm 3.2. Note that this algorithm is strongly backward stable and costs about $23n^3$ flops.

Algorithm 3.2 Williamson's diagonal form for spd and skew-Hamiltonian matrices

Input: $N \in \mathbb{R}^{2n \times 2n}$ is spd and skew-Hamiltonian.

Output: $K \in \text{OrSp}(2n)$, $D = \text{diag}(d_1, \dots, d_n)$ such that $K^T N K = \text{diag}(D, D)$.

- 1: Compute the symmetric Paige/Van Loan form $N = U \text{diag}(\Omega_1, \Omega_1) U^T$ with $U \in \text{OrSp}(2n)$ and tridiagonal $\Omega_1 \in \mathcal{SPD}(n)$ as described in [45].
 - 2: Compute the symmetric Schur form $\Omega_1 = Q_1 D Q_1^T$, where Q_1 is orthogonal and $D = \text{diag}(d_1, \dots, d_n)$.
 - 3: Compute the orthosymplectic matrix $K = U \text{diag}(Q_1, Q_1)$.
-

4. Symplectic trace minimization problem. In this section, we establish the connection between the symplectic EVP and the symplectic trace minimization problem. The following result is one of the main sources that inspire our work.

THEOREM 4.1. [33, 17] *Let a matrix $M \in \mathcal{SPD}(2n)$ have symplectic eigenvalues $d_1 \leq \dots \leq d_n$. Then for any integer $1 \leq k \leq n$, it holds*

$$(4.1) \quad 2 \sum_{j=1}^k d_j = \min_{X \in \mathbb{R}^{2n \times 2k}} f(X) := \text{tr}(X^T M X) \quad \text{s.t.} \quad h(X) := X^T J_{2n} X - J_{2k} = 0.$$

Due to the constraint condition, the problem (4.1) can be viewed as the minimization problem restricted to the symplectic Stiefel manifold $\text{Sp}(2k, 2n)$. The following lemma establishes the homogeneity of the cost function f on $\text{OrSp}(2k)$.

LEMMA 4.2. *Let $M \in \mathcal{SPD}(2n)$. For $X \in \text{Sp}(2k, 2n)$ and $K \in \text{OrSp}(2k)$, the cost function f in (4.1) satisfies $f(XK) = f(X)$.*

Proof. For $X \in \text{Sp}(2k, 2n)$ and $K \in \text{OrSp}(2k)$, we obtain that $XK \in \text{Sp}(2k, 2n)$ and

$$f(XK) = \text{tr}(K^T X^T M X K) = \text{tr}(K^{-1} X^T M X K) = \text{tr}(X^T M X) = f(X).$$

Here, we used the fact that similar matrices have the same trace. \square

4.1. Critical points. First, we investigate the critical points of the optimization problem (4.1). For this purpose, we will invoke the associated Lagrangian function

$$\mathcal{L}(X, L) = \text{tr}(X^T M X) - \text{tr}(L(X^T J_{2n} X - J_{2k})),$$

where $L \in \mathbb{R}^{2k \times 2k}$ is the Lagrangian multiplier. Since the constraint function h maps $\mathbb{R}^{2n \times 2k}$ into $\mathcal{S}_{\text{skew}}(2k)$, the Lagrangian multiplier L can also be taken skew-symmetric. The gradient of \mathcal{L} with respect to the first argument at (X, L) takes the form

$$(4.2) \quad \nabla_X \mathcal{L}(X, L) = 2MX - 2J_{2n}XL.$$

Furthermore, the action of the Hessian of \mathcal{L} with respect to the first argument on $(W, W) \in \mathbb{R}^{2n \times 2k} \times \mathbb{R}^{2n \times 2k}$ reads

$$(4.3) \quad \nabla_{XX}^2 \mathcal{L}(X, L)[W, W] = 2 \operatorname{tr}(W^T(MW - J_{2n}WL)).$$

Next, let us recall the first- and the second-order necessary optimality conditions [46] for the constrained optimization problem (4.1). A point $X_* \in \mathbb{R}^{2n \times 2k}$ is called a *critical point* of the problem (4.1) if $h(X_*) = 0$ and there exists a Lagrangian multiplier $L_* \in \mathcal{S}_{\text{skew}}(2k)$ such that $\nabla_X \mathcal{L}(X_*, L_*) = 0$. These conditions are known as the Karush-Kuhn-Tucker conditions. The first condition implies that $X_* \in \operatorname{Sp}(2k, 2n)$. Using (4.2), the stationarity condition can equivalently be written as

$$(4.4) \quad MX_* = J_{2n}X_*L_*.$$

Comparing (3.2) with (4.4), we obtain that any normalized symplectic eigenvector set X of M is a critical point with the Lagrangian multiplier

$$L_* = \begin{bmatrix} 0 & -\Lambda \\ \Lambda & 0 \end{bmatrix}.$$

In this case, multiplying (4.4) with X_*^T on the left and taking the trace of the resulting equality lead to

$$(4.5) \quad f(X_*) = 2\operatorname{tr}(\Lambda) = 2(\lambda_1 + \cdots + \lambda_k).$$

The critical point $X_* \in \mathbb{R}^{2n \times 2k}$ with the associated Lagrangian multiplier L_* is said to satisfy the second-order necessary optimality condition if

$$\nabla_{XX}^2 \mathcal{L}(X_*, L_*)[W, W] = 2 \operatorname{tr}(W^T(MW - J_{2n}WL_*)) \geq 0$$

for all $W \in \operatorname{null}(\operatorname{Dh}(X_*)) := \{Y \in \mathbb{R}^{2n \times 2k} : \operatorname{Dh}(X_*)[Y] = Y^T J_{2n} X_* + X_*^T J_{2n} Y = 0\}$.

Based on Proposition 3.7, we can characterize the critical points of the optimization problem (4.1) as follows.

THEOREM 4.3. *Let $M \in \mathcal{SPD}(2n)$.*

- i) *If $X_* \in \operatorname{Sp}(2k, 2n)$ is a critical point of (4.1), then for any $K \in \operatorname{OrSp}(2k)$, the matrix X_*K is also a critical point of (4.1).*
- ii) *A matrix $X_* \in \operatorname{Sp}(2k, 2n)$ is a critical point of (4.1) if and only if there exists $K \in \operatorname{OrSp}(2k)$ such that the columns of X_*K form a normalized symplectic eigenvector set of M .*

Proof. i) If $X_* \in \operatorname{Sp}(2k, 2n)$ is a critical point of (4.1) with the associated Lagrangian multiplier L_* , then (4.4) is fulfilled. Therefore, for any $K \in \operatorname{OrSp}(2k)$, we obtain that $X_*K \in \operatorname{Sp}(2k, 2n)$ and $MX_*K = J_{2n}X_*L_*K = J_{2n}X_*KK^TL_*K$. This means that X_*K is also a critical point of (4.1) with the Lagrangian multiplier K^TL_*K .

ii) Assume that the columns of $Z_* = X_*K$ with $K \in \operatorname{OrSp}(2k)$ form a normalized symplectic eigenvector set of M . Then $Z_* \in \operatorname{Sp}(2k, 2n)$ is a critical point of (4.1), and, hence, by i), $X_* = Z_*K^{-1} \in \operatorname{Sp}(2k, 2n)$ is also a critical point of (4.1).

Conversely, let $X_* \in \text{Sp}(2k, 2n)$ be a critical point of (4.1). Then X_* satisfies (4.4) which immediately implies that

$$(4.6) \quad X_*^T M X_* = J_{2k} L_*$$

with a skew-symmetric matrix L_* . We now show that $X_*^T M X_*$ is spd and skew-Hamiltonian. Since M is spd and X_* has full column rank, we obtain that $X_*^T M X_*$ is spd. Furthermore, using (4.6), we get

$$(J_{2k} X_*^T M X_*)^T = (J_{2k} J_{2k} L_*)^T = L_* = -J_{2k} J_{2k} L_* = -J_{2k} X_*^T M X_*$$

implying that $X_*^T M X_*$ is skew-Hamiltonian. Then by Propostion 3.7, there exists $K \in \text{OrSp}(2k)$ such that

$$(4.7) \quad K^T (X_*^T M X_*) K = \begin{bmatrix} \Lambda & 0 \\ 0 & \Lambda \end{bmatrix}$$

with $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_k)$. Using (4.4), (4.6), (4.7) and $J_{2k}^T K = K J_{2k}^T$, we deduce

$$\begin{aligned} M X_* K &= J_{2n} X_* L_* K = J_{2n} X_* J_{2k}^T K K^T J_{2k} L_* K \\ &= J_{2n} X_* K J_{2k}^T K^T X_*^T M X_* K = J_{2n} X_* K \begin{bmatrix} 0 & -\Lambda \\ \Lambda & 0 \end{bmatrix}. \end{aligned}$$

Thus, the columns of $X_* K$ form a normalized symplectic eigenvector set of M . \square

Theorem 4.3 allows us to characterize the set of all critical points of the problem (4.1), and particularly the set of all minimizers as we will see in the next subsection.

COROLLARY 4.4. *The set of all critical points of the minimization problem (4.1) is the union of all $X \in \text{OrSp}(2k)$, where the columns of $X \in \text{Sp}(2k, 2n)$ form any possible normalized symplectic eigenvector set of M .*

REMARK 4.5. *We can extend Theorem 3.6 to the case $S \in \text{Sp}(2k, 2n)$ with $k < n$ by the same proof. Now, the picture is clear. We have three different tools to track different objects: $\text{Sp}(2k)$ for tracking the symplectic matrices that span the same subspace (Proposition 2.1(iii)), the ‘‘dab’’ set for the symplectically diagonalizing matrices of M (Theorem 3.6), and $\text{OrSp}(2k)$ for the set of feasible points at which the value of the cost function f in (4.1) is the same (Lemma 4.2) and for the set of all critical points of (4.1) (Theorem 4.3).*

4.2. Local and global minimizers. We now investigate the local and global minimizers of the optimization problem (4.1).

THEOREM 4.6. *Let $M \in \text{SPD}(2n)$.*

- i) If $X_* \in \text{Sp}(2k, 2n)$ is a global minimizer of (4.1), then for any $K \in \text{OrSp}(2k)$, the matrix $X_* K$ is also a global minimizer of (4.1).*
- ii) A matrix $X_* \in \text{Sp}(2k, 2n)$ is a global minimizer of (4.1) if and only if there exists $K \in \text{OrSp}(2k)$ such that the columns of $X_* K$ form a normalized symplectic eigenvector set of M associated with the symplectic eigenvalues d_1, \dots, d_k .*

Proof. i) Let $X_* \in \text{Sp}(2k, 2n)$ is a global minimizer of (4.1) and let $K \in \text{OrSp}(2k)$. Then $X_* K \in \text{Sp}(2k, 2n)$. Furthermore, by Lemma 4.2 we obtain $f(X_* K) = f(X_*)$, and, hence, $X_* K$ is a global minimizer of (4.1).

ii) In view of Lemma 4.2 and (4.5), the sufficiency immediately follows from $f(X_*) = f(X_* K) = 2(d_1 + \dots + d_k)$ for any $K \in \text{OrSp}(2k)$. Conversely, if X_* is a minimizer, it must be a critical point. Due to Theorem 4.3, there exists $K \in \text{OrSp}(2k)$

such that X_*K is a normalized symplectic eigenvector set corresponding to a set of symplectic eigenvalues, say d_{i_1}, \dots, d_{i_k} . Taking again Lemma 4.2 and (4.5) into account, we deduce from this fact that

$$2(d_1 + \dots + d_k) = f(X_*) = f(X_*K) = 2(d_{i_1} + \dots + d_{i_k}).$$

Because all d_{i_j} , $j = 1, \dots, k$, are taken from the set of positive numbers, where d_i , $i = 1, \dots, k$, are the k smallest ones, we can conclude, after a reordering if necessary, that $d_{i_j} = d_j$ for $j = 1, \dots, k$. \square

In Appendix A, we present an alternative proof of the necessity in Theorem 4.6(ii) which does not rely on Theorem 4.3.

Similarly to Corollary 4.4, we can now characterize the set of global minimizers of the problem (4.1).

COROLLARY 4.7. *The set of all global minimizers of (4.1) is the union of all $X_{1:k}\text{OrSp}(2k)$, where the columns of $X_{1:k} \in \text{Sp}(2k, 2n)$ form a normalized symplectic eigenvector set of M associated with the symplectic eigenvalues d_1, \dots, d_k .*

REMARK 4.8. *If $d_k < d_{k+1}$, Corollary 4.7 can be considered as a symplectic version of the corresponding result for the standard EVP, see, e.g., [50, Theorem 2.1]. In this case, $X_{1:k}$ can be constructed by taking the 1-st, ..., k -th, $(n+1)$ -st, ..., $(n+k)$ -th columns of any symplectically diagonalizing matrix S of M . Otherwise, let j be the largest index such that $d_j < d_k$. Then, the last $k-j$ columns in the first and second halves of $X_{1:k}$ can be any of those whose column indices are ranging from $j+1$ to $j+m_k$ and their counterparts in the second half of S , where m_k denotes the multiplicity of d_k . In all related statements in the rest of this paper, by $X_{1:k}$, we include all such cases.*

Next, we collect some consequences from Theorem 4.6 for the case $k = n$.

COROLLARY 4.9. *Let $M \in \text{SPD}(2n)$.*

- i) Any critical point of the minimization problem (4.1) with $k = n$ is a global minimizer.*
- ii) The set of all global minimizers of (4.1) with $k = n$ is $S\text{OrSp}(2n)$, where $S \in \text{Sp}(2n)$ is a symplectically diagonalizing matrix of M .*

We now consider the non-existence of non-global local minimizers. In view of Corollary 4.9, we restrict ourselves to the case $k < n$. A similar result for the generalized EVP can be found in [39, 44]. First, we state an important technical lemma.

LEMMA 4.10. *Let $M \in \text{SPD}(2n)$ and let the columns of $X_{1:k}$ and $X_{n-k+1:n}$ form any normalized symplectic eigenvector sets associated, respectively, with the k smallest and k largest symplectic eigenvalues of M . Then for any critical point X_0 of the optimization problem (4.1), there exist a global minimizer $X_* \in X_{1:k}\text{OrSp}(2k)$ and an $X^* \in X_{n-k+1:n}\text{OrSp}(2k)$ such that $X_*, X^* \in \text{null}(\text{Dh}(X_0))$.*

Proof. See Appendix B. \square

PROPOSITION 4.11. *Every local minimizer of the optimization problem (4.1) is a global one.*

Proof. Assume that there is a non-global local minimizer X_0 of the problem (4.1). Since X_0 is a critical point, there is an associated Lagrangian multiplier L_0 . Moreover, by Corollary 4.4, X_0 can be represented as $X_0 = X_{\mathcal{I}_k}K_0$, where $K_0 \in \text{OrSp}(2k)$, and the columns of $X_{\mathcal{I}_k}$ form a normalized symplectic eigenvector set associated with a set of the symplectic eigenvalues $\{d_{i_j}, i_j \in \mathcal{I}_k\}$ in which at least one of them is greater

than d_k . By Lemma 4.10, there exists a global minimizer $X_* \in \text{null}(Dh(X_0))$. On the account of (4.3), we get then

$$\begin{aligned} \nabla_{XX}^2 \mathcal{L}(X_0, L_0)[X_*, X_*] &= 2 \text{tr}(X_*^T M X_* - X_*^T J_{2n} X_* L_0) = 2 \text{tr}(X_*^T M X_* - J_{2k} L_0) \\ &= 2 \text{tr}(X_*^T M X_* - X_0^T M X_0) = 4 \sum_{i=1}^k d_i - 4 \sum_{j=1}^k d_{i_j} < 0, \end{aligned}$$

which contradicts to the second-order necessary optimality condition for X_0 . This completes the proof. \square

Saddle points of the cost function f in the problem (4.1) can be disclosed in the following.

PROPOSITION 4.12. *Any normalized symplectic eigenvector set X of a matrix $M \in \mathcal{SPD}(2n)$ associated with a symplectic eigenvalue set $\{d_{i_j}, i_j \in \mathcal{I}_k\}$, in which there is at least one d_{i_j} such that $d_k < d_{i_j} < d_{n-k+1}$, is a saddle point of (4.1).*

Proof. Obviously, X is a critical point. Then it follows from the proof of Proposition 4.11 that X is not a minimizer. Taking into account the existence of X^* in Lemma 4.10 and following the same proof of Proposition 4.11, we can show that X is not a maximizer of the cost function f in (4.1) either. Hence, X is a saddle point. \square

REMARK 4.13. *Unfortunately, we were unable to prove that each element in the matrix set $X_{n-k+1:n} \text{OrSp}(2k)$ is a local maximizer. Nevertheless, we can show that f in (4.1) has no global maximizer. Indeed, let us consider a symplectic matrix*

$$X_a = \begin{bmatrix} aI_{n,k} & 0 \\ 0 & 1/aI_{n,k} \end{bmatrix}, \quad a \neq 0,$$

where $I_{n,k}$ denotes a $n \times k$ submatrix of I_n . For any symplectically diagonalizing matrix S of M , $SX_a \in \text{Sp}(2k, 2n)$. We then get that

$$f(SX_a) = \text{tr}(X_a^T S^T M S X_a) = 2(a^2 + \frac{1}{a^2}) \text{tr}(I_{n,k}^T D I_{n,k})$$

which tends to infinity when $a \rightarrow 0$.

We close this section by considering some consequences for the case $k = 1$.

COROLLARY 4.14. *Let $M \in \mathcal{SPD}(2n)$ be in Williamson's diagonal form (1.1).*

- i) The two columns of $X \in \text{Sp}(2, 2n)$ form a normalized symplectic eigenvector pair of M if and only if X is a critical point of the minimization problem (4.1) with $k = 1$.*
- ii) The two columns of $X_1 \in \text{Sp}(2, 2n)$ form a normalized symplectic eigenvector pair of M associated with the smallest eigenvalue d_1 if and only if X_1 is a global minimizer of (4.1) with $k = 1$.*
- iii) For any $j = 2, \dots, n-1$ such that $d_1 < d_j < d_n$, a normalized symplectic eigenvector pair $X_j \in \text{Sp}(2, 2n)$ of M associated with d_j is a saddle point of (4.1) with $k = 1$.*

Corollary 4.14 can be considered as a symplectic version of the corresponding results on the trace minimization problem for standard eigenvalues. Especially, part (i) is similar to [3, Proposition 4.6.1]; part (ii) is similar to [3, Proposition 4.6.2(i)] with the note that X_1 is not unique; part (iii) is the same as [3, Proposition 4.6.2(iii)].

5. Eigenvalue computation via Riemannian optimization. In this section, we present a numerical method for solving the optimization problem (4.1). It is principally a constrained optimization problem for which some existing methods can be used, see, e.g., [46]. Nevertheless, maintaining the constraint is challenging. Recently, it has been shown in [29] that the feasible set $\text{Sp}(2k, 2n)$ constitutes a Riemannian manifold. Moreover, two efficient methods were proposed there for optimization on this manifold. In this section, we briefly review the necessary ingredients for a Riemannian optimization algorithm for solving (4.1) and discuss the computation of the smallest symplectic eigenvalues and the corresponding symplectic eigenvectors by using the presented optimization algorithm.

5.1. Riemannian optimization on the symplectic Stiefel manifold. Given $X \in \text{Sp}(2k, 2n)$, the tangent space of $\text{Sp}(2k, 2n)$ at X , denoted by $\text{T}_X \text{Sp}(2k, 2n)$, can be represented as $\text{T}_X \text{Sp}(2k, 2n) = \{AJ_{2n}X : A \in \mathcal{S}_{\text{sym}}(2n)\}$, see [29, Proposition 3.3] for detail. In view of [29, Proposition 4.1], a Riemannian metric for $\text{Sp}(2k, 2n)$, called the canonical-like metric, is defined as

$$g_\rho(Z_1, Z_2) := \text{tr} \left(Z_1^T \left(\frac{1}{\rho} J_{2n} X X^T J_{2n}^T - (J_{2n} X J_{2k} X^T J_{2n}^T - J_{2n})^2 \right) Z_2 \right),$$

where $Z_1, Z_2 \in \text{T}_X \text{Sp}(2k, 2n)$ and $\rho > 0$. Consequently, the associated Riemannian gradient of the cost function f in (4.1) has the following expression.

PROPOSITION 5.1. *Given $M \in \mathcal{SPD}(2n)$, the Riemannian gradient of the function $f : \text{Sp}(2k, 2n) \rightarrow \mathbb{R} : X \mapsto \text{tr}(X^T M X)$ associated with the metric g_ρ is given by $\text{grad}_\rho f(X) = A_X J_{2n} X$ with the matrices $A_X = 4 \text{sym}(H_X M X (X J_{2k})^T)$ and $H_X = I + \frac{\rho}{2} X X^T - J_{2n} X (X^T X)^{-1} X^T J_{2n}^T$.*

Proof. The result directly follows from $\nabla f(X) = 2MX$ and [29, Proposition 4.5]. \square

In [29], two searching strategies relying on quasi-geodesics and symplectic Cayley transform were proposed for the optimization on $\text{Sp}(2k, 2n)$. It has also been shown there that the Cayley-based method performs better than that based on quasi-geodesics. Therefore, we choose the Cayley retraction as the update formula. Specifically, the searching curve along $-\text{grad}_\rho f(X) \in \text{T}_X \text{Sp}(2k, 2n)$ is defined as

$$(5.1) \quad \mathcal{R}_X(-t \text{grad}_\rho f(X)) := \left(I + \frac{t}{2} A_X J_{2n} \right)^{-1} \left(I - \frac{t}{2} A_X J_{2n} \right) X,$$

where A_X is as in Proposition 5.1. Note that since the number k of required symplectic eigenvalues is usually small, the update (5.1) can be further assembled in an efficient way suggested in [29, Proposition 5.4].

In Algorithm 5.1, we present the Riemannian gradient method with non-monotone line search for solving (4.1). Practically, we can stop the iteration when the gradient of the cost function is smaller than a given tolerance ϵ . It has been proven in [29, Theorem 5.6] that with standard assumptions, Algorithm 5.1 generates an infinite sequence of which any accumulation point is a critical point of (4.1).

5.2. Computing the symplectic eigenvalues and eigenvectors. First, we consider the computation of the smallest symplectic eigenvalue d_1 of M . This case was briefly addressed in [29] as an example. We review it here and discuss the computation of the corresponding normalized symplectic eigenvector pair. Let $X_* \in \text{Sp}(2, 2n)$ be a minimizer computed by Algorithm 5.1. Then we have $d_1 = f(X_*)/2$ and by Corollary 4.14(ii) the columns of X_* provide the sought normalized symplectic eigenvector pair.

Algorithm 5.1 Riemannian gradient method for solving the problem (4.1)

Input: $M \in \mathcal{SPD}(2n)$; $X^{(0)} \in \text{Sp}(2k, 2n)$; $\rho > 0$, $\beta, \delta \in (0, 1)$, $\alpha \in [0, 1]$, $q_0 = 1$,
 $c_0 = f(X^{(0)})$, $\gamma_0 > 0$, $0 < \gamma_{\min} < \gamma_{\max} = 1$;

Output: Sequence of iterates $\{X^{(m)}\}$.

1: **for** $m = 0, 1, 2, \dots$ **do**

2: Set $Z^{(m)} = -\text{grad}_\rho f(X^{(m)})$.

3: **if** $m > 0$ **then**

4: $\gamma_m = \begin{cases} \frac{\langle W^{(m-1)}, W^{(m-1)} \rangle}{|\langle W^{(m-1)}, Y^{(m-1)} \rangle|} & \text{for odd } m, \\ \frac{|\langle W^{(m-1)}, Y^{(m-1)} \rangle|}{\langle Y^{(m-1)}, Y^{(m-1)} \rangle} & \text{for even } m, \end{cases}$

where $W^{(m-1)} = X^{(m)} - X^{(m-1)}$ and $Y^{(m-1)} = Z^{(m)} - Z^{(m-1)}$.

5: **end if**

6: Calculate the trial step size $\gamma_k = \max(\gamma_{\min}, \min(\gamma_k, \gamma_{\max}))$.

7: Find the smallest integer ℓ such that the non-monotone condition

$$f\left(\mathcal{R}_{X^{(m)}}(t_m Z^{(m)})\right) \leq c_m + \beta t_m g_\rho\left(\text{grad}_\rho f(X^{(m)}), Z^{(m)}\right)$$

holds, where $t_m = \gamma_m \delta^\ell$.

8: Set $X^{(m+1)} = \mathcal{R}_{X^{(m)}}(t_m Z^{(m)})$.

9: Update $q_m = \alpha q_{m-1} + 1$ and $c_m = \frac{\alpha q_{m-1}}{q_m} c_{m-1} + \frac{1}{q_m} f(X^{(m)})$.

10: **end for**

We now consider the general case $1 \leq k \leq n$. Assume that X_* is a minimizer of (4.1). According to Theorem 4.6(ii), there exists $K \in \text{OrSp}(2k)$ such that the columns of $X_* K$ form a normalized symplectic eigenvector set of M associated with the symplectic eigenvalues d_1, \dots, d_k . The sought matrix K can be computed by symplectically diagonalizing a $2k \times 2k$ matrix $X_*^T M X_*$. As $X_*^T M X_*$ is spd and skew-Hamiltonian, we can resort to Algorithm 3.2 for the sake of efficiency. We summarize the computation of the k smallest symplectic eigenvalues of M and the corresponding eigenvector set in Algorithm 5.2.

Algorithm 5.2 Symplectic EVP via Riemannian optimization

Input: $M \in \mathcal{SPD}(2n)$, $1 \leq k \leq n$.

Output: k smallest symplectic eigenvalues d_1, \dots, d_k and the corresponding normalized symplectic eigenvector set $X_{1:k} \in \text{Sp}(2k, 2n)$.

1: Solve the optimization problem (4.1) for $X_* \in \text{Sp}(2k, 2n)$ by using Algorithm 5.1.

2: Compute Williamson's diagonal form $X_*^T M X_* = K \text{diag}(D_{1:k}, D_{1:k}) K^T$ with $K \in \text{OrSp}(2k)$ and $D_{1:k} = \text{diag}(d_1, \dots, d_k)$ by using Algorithm 3.2.

3: Compute $X_{1:k} = X_* K$.

Algorithm 5.2 is comparable with typical methods for large standard EVPs in the sense that we first simplify and/or reduce the size of the problem and then solve the small and/or simpler (symplectic) EVP. This approach may be not efficient if all symplectic eigenvalues are required. In that case, Algorithm 3.1, for instance, could be used.

REMARK 5.2. *Unlike the standard eigenvalue trace minimization problem on the Stiefel manifold, as shown in Remark 4.13, the cost function f in (4.1) is unbounded*

from above. This comes from the fact that the Stiefel manifold is bounded while the symplectic Stiefel manifold is not. Therefore, we cannot find largest symplectic eigenvalues in a similar manner, i.e., by maximizing the cost function. Despite this fact, the largest symplectic eigenvalues of an spd matrix M can be computed by applying Algorithm 5.2 to the inverse of M . As in the standard case, this follows from the fact that the largest eigenvalues of M are the reciprocals of the corresponding smallest ones of its inverse [20, Theorem 8.14]. This task can be done as long as the linear equation $Mx = y$ can be solved efficiently.

5.3. Computing the eigenvalues of positive-definite Hamiltonian matrices. As an application of Algorithm 5.2, we consider the computation of standard eigenvalues and their corresponding eigenvectors of pdH matrices. Due to numerous applications, the EVPs for general Hamiltonian matrices have attracted a lot of attention and many different algorithms were developed for such problems, e.g., [45, 12, 55, 16, 15], just to name a few. It is noteworthy that some of these methods rely on the Hamiltonian-Schur form. Unfortunately, this form does not always exist, e.g., for real Hamiltonian matrices having purely imaginary eigenvalues, which is exactly the case for pdH matrices, see Proposition 3.3. In [5, 6], a symplectic Lanczos method was developed for computing a few extreme eigenvalues of a pdH matrix H , which exploits the symmetry and positive definiteness of its generator $M = J_{2n}^T H$.

Here, we present a different numerical approach for computing the eigenvalues of pdH matrices which relies on Riemannian optimization. To the best of our knowledge, this is the first geometric method for the special Hamiltonian EVP. Based on Proposition 3.3, we propose to compute the smallest (in modulus) eigenvalues of a pdH matrix H by applying Algorithm 5.2 to the spd matrix $M = J_{2n}^T H$.

6. Numerical examples. In this section, we present some results of numerical experiments demonstrating the proposed Riemannian trace minimization method, henceforth called Riemannian. The parameters in Algorithm 5.1 are set to default values as given in [29]. Although accumulation points of the iterates generated by this algorithm can be proven to be critical points of the cost function in (4.1) only [29], we never experience stagnation at a saddle point. This fact was observed in various works and arguably explained, see [43] and references therein. For reference and comparison, we also report the corresponding results for the restarted symplectic Lanczos algorithm [6] (sympLanczos) and the MATLAB function `eigs` applied to the associated Hamiltonian matrix. All computations were done on a workstation with two Intel(R) Xeon(R) Processors Silver 4110 (at 2.10GHz×8, 12M Cache) and 384GB of RAM running MATLAB R2018a under Ubuntu 18.10. The code that produced the results is available from <https://github.com/opt-gaobin/speig>.

The accuracy of computed symplectic eigenvalues and eigenvector sets of M are measured by using the normalized residual

$$\frac{\left\| M\tilde{X}_{1:k} - J_{2n}\tilde{X}_{1:k} \begin{bmatrix} 0 & -\tilde{D}_{1:k} \\ \tilde{D}_{1:k} & 0 \end{bmatrix} \right\|_F}{\|M\tilde{X}_{1:k}\|_F},$$

where $\tilde{X}_{1:k}$ is the computed symplectic eigenvector set associated with the symplectic eigenvalues on the diagonal of $\tilde{D}_{1:k} = \text{diag}(\tilde{d}_1, \dots, \tilde{d}_k)$. Here, $\|\cdot\|_F$ denotes the Frobenius matrix norm. For standard eigenvalues of $H = J_{2n}M$, the normalized residual is given by $\|H\tilde{V} - \tilde{V}\tilde{\Lambda}\|_F / \|H\tilde{V}\|_F$, where the columns of $\tilde{V} \in \mathbb{C}^{2n \times 2k}$ are the computed eigenvectors of H associated with the eigenvalues on the diagonal of

$$\tilde{\Lambda} = \text{diag}(\tilde{\lambda}_1, \dots, \tilde{\lambda}_{2k}).$$

6.1. A matrix with known symplectic eigenvalues. We consider the spd matrix $M = Q \text{diag}(D, D) Q^T$ with $D = \text{diag}(1, \dots, n)$ and $Q = KL(n/5, 1.2, -\sqrt{n/5})$, where $L(n/5, 1.2, -\sqrt{n/5}) \in \text{Sp}(2n)$ is the symplectic Gauss transformation defined in [23], and $K = \begin{bmatrix} \Re(U) & \Im(U) \\ -\Im(U) & \Re(U) \end{bmatrix} \in \text{OrSp}(2n)$ with unitary $U \in \mathbb{C}^{n \times n}$ produced by orthogonalizing a randomly generated complex matrix. Then, the k smallest symplectic eigenvalues of M are $1, \dots, k$. To exhibit the accuracy of computed symplectic eigenvalues $\tilde{d}_1, \dots, \tilde{d}_k$, we calculate the 1-norm error defined as $\sum_{i=1}^k |\tilde{d}_i - i|$. In our tests, we choose $k = 5$ and consider different values of n in the range between 100 and 2000. The mentioned errors and the corresponding residuals for the three methods are shown in Figure 6.1. The sought eigenvalues for $n = 2000$ are given in Table 6.1.

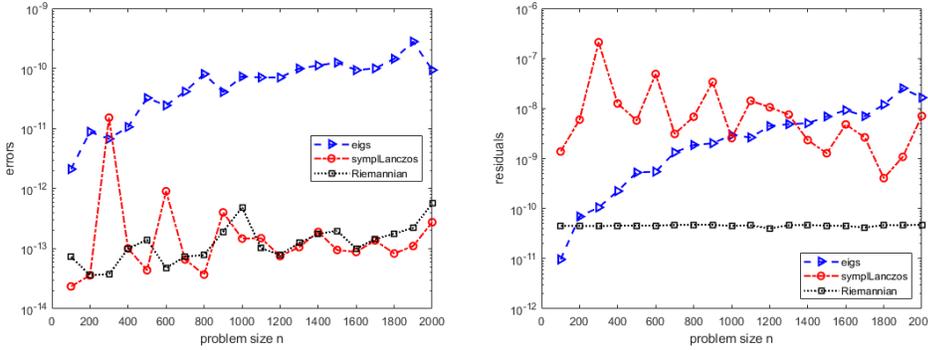


FIG. 6.1. A matrix with known symplectic eigenvalues: the 1-norm errors of the computed symplectic eigenvalues (left) and the corresponding normalized residuals (right)

TABLE 6.1
5 smallest symplectic eigenvalues of a 4000×4000 spd matrix M computed by different methods

$i \times \text{eigs}(H)$	$\text{symplLanczos}(M)$	$\text{Riemannian}(M)$
$0.000000000003296i + 1.000000000009247$	1.000000000000058	1.000000000000008
$-0.000000000022122i + 1.999999999995145$	2.000000000000043	1.999999999999957
$0.000000000015139i + 3.000000000002913$	3.000000000000062	3.000000000000074
$0.000000000023914i + 3.999999999977669$	3.999999999999927	3.999999999999944
$-0.000000000011256i + 4.999999999993021$	4.999999999999960	4.9999999999999617

6.2. Weakly damped gyroscopic systems. In the stability analysis of gyroscopic systems, one needs to solve a special quadratic eigenvalue problem (QEP) $(\lambda^2 M + \lambda \mathcal{G} + \mathcal{K})x = 0$, where $M \in \mathcal{SPD}(n)$, $\mathcal{G} \in \mathcal{S}_{\text{skew}}(n)$ and $\mathcal{K} \in \mathcal{SPD}(n)$ are, respectively, the mass, damping and stiffness matrices of the underlying mechanical structure. One can linearize this QEP and turn it into the standard EVP for the Hamiltonian matrix

$$H = \begin{bmatrix} I & -\frac{1}{2}\mathcal{G} \\ 0 & I \end{bmatrix} \begin{bmatrix} 0 & -\mathcal{K} \\ \mathcal{M}^{-1} & 0 \end{bmatrix} \begin{bmatrix} I & -\frac{1}{2}\mathcal{G} \\ 0 & I \end{bmatrix} = \begin{bmatrix} -\frac{1}{2}\mathcal{G}\mathcal{M}^{-1} & \frac{1}{4}\mathcal{G}\mathcal{M}^{-1}\mathcal{G} - \mathcal{K} \\ \mathcal{M}^{-1} & -\frac{1}{2}\mathcal{M}^{-1}\mathcal{G} \end{bmatrix},$$

see [14] for details. This leads to the fact that $J_{2n}^T H$ is symmetric negative definite if \mathcal{G} is small enough. In our experiments, we use therefore the spd matrix $M = J_{2n} H$.

In the first test, we generate \mathcal{M} , \mathcal{G} and \mathcal{K} by an eigenfunction discretization of a wire saw model as described in [57, Section 2] with the wire speed $v = 0.0306$ and the dimension $n = 2000$ followed by a scaling down of \mathcal{G} by $1e-3$. The eigenvalues computed by the three methods and the corresponding normalized residuals are given in Table 6.2.

TABLE 6.2

5 smallest symplectic eigenvalues of a 4000×4000 spd matrix $M = J_{2n}H$ generated from the wire saw model computed by different methods

$i \times \mathbf{eigs}(H)$	$\text{symplLanczos}(M)$	$\text{Riemannian}(M)$
$0.0000000000000002i + 3.140121476801627$	3.140121476801632	3.140121476801794
$-0.0000000000000001i + 6.280242953603250$	6.280242953603265	6.280242953605164
$0.00000000000000013i + 9.420364430404952$	9.420364430404895	9.420364430404506
$0.00000000000000037i + 12.560485907206663$	12.560485907206548	12.560485907211794
$-0.00000000000000077i + 15.700607384008093$	15.700607384008212	15.700607384223552
Residual:	1.4e-12	1.3e-14

In the second test, we employ the data matrices \mathcal{M} and \mathcal{K} from a discretized model of a piston rod inside a combustion engine [25]. This model has size $n = 8053$. Because matrix \mathcal{G} in this model is not skew-symmetric, we replace it with a sparse randomly generated skew-symmetric matrix whose pattern is the same as that of \mathcal{M} . As the matrices in this model are large in magnitude, to improve the efficiency of our method, we scale the matrix H by a factor of $1e-5$. The obtained results given in Table 6.3 are for these scaled data.

TABLE 6.3

5 smallest symplectic eigenvalues of a 16106×16106 spd matrix $M = J_{2n}H$ generated from the piston rod model computed by different methods

$i \times \mathbf{eigs}(H)$	$\text{symplLanczos}(M)$	$\text{Riemannian}(M)$
$-0.0000000000000001i + 0.162084145743768$	0.162084145770035	0.162084145232661
$0.0000000000000001i + 0.325674702254120$	0.325674702270259	0.325674702005421
$0.0000000000000006i + 0.663619676318176$	0.663619676324319	0.663619676186475
$0.0000000000000001i + 1.350097974209022$	1.350097974210526	1.350097974141396
$-0.0000000000000004i + 2.173559065028063$	2.173559065366786	2.173559064987688
Residual:	4.4e-10	9.9e-12

Some observations and remarks can be stated from these numerical examples. The comparisons might be a bit biased since \mathbf{eigs} is not designed for structured matrices, whereas the symplectic Lanczos method and the Riemannian optimization method exploit the structure of the EVP. This explains why in all three test examples the eigenvalues computed by $\mathbf{eigs}(H)$ are not purely imaginary. Though, in the symplectic Lanczos method, the residuals, which also depend on the accuracy of the symplectic eigenvectors, are not as small as expected, the first example shows that this method produces good approximations to symplectic eigenvalues. Compared to that, our method yields satisfying results in the sense that both errors and residuals are small. It should however be noted that slow convergence, especially near minimizers, was sometimes experienced in our tests. This is well-known for first-order optimization methods and poses a need for development of second-order methods.

7. Conclusion. We have established various theoretical properties for the symplectic eigenvalue trace minimization problem. Many of them are symplectic extensions of known results for the standard problem. We have also proposed a Riemannian optimization-based numerical method that resorts to a recent development about op-

timization on the symplectic Stiefel manifold. This method can also be employed to compute standard eigenvalues of positive-definite Hamiltonian matrices. Numerical examples demonstrate that the proposed method is comparable to existing approaches in the sense of accuracy.

Acknowledgments. We would like to thank B. Fröhlich for providing us with the data for the piston rod model.

Appendix A. Alternative proof of the necessity in Theorem 4.6(ii).

Theorem 4.3 is so strong that it does not only characterize the set of the critical points of the minimization problem (4.1) but also helps to obtain the set of the global minimizers as clarified in Theorem 4.6(ii). In this extra section, we will present another proof of this theorem which does not resort to Theorem 4.3 and its consequences.

Let $X_* \in \text{Sp}(2k, 2n)$ be a minimizer of (4.1). Then it satisfies the KKT condition (4.4) or, equivalently, $X_*^T M X_* = J_{2k} L_*$. Since $X_*^T M X_*$ is spd, an application of Williamson's theorem implies the existence of $K \in \text{Sp}(2k)$ such that

$$(A.1) \quad K^T J_{2k} L_* K = K^T X_*^T M X_* K = \begin{bmatrix} \Lambda & 0 \\ 0 & \Lambda \end{bmatrix}$$

with $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_k)$.

Next, we show that $\lambda_j = d_j$, $j = 1, \dots, k$. To this end, let us add more columns to X_* to make $\tilde{X}_* \in \text{Sp}(2n)$ such that its 1-st, \dots , k -th, $(n+1)$ -th, \dots , $(n+k)$ -th columns are those of X_* , see [20, Theorem 1.15]. It was shown in [20, Proposition 8.14], that the symplectic spectrum is symplectic invariant. This yields that the symplectic eigenvalues of $\tilde{X}_*^T M \tilde{X}_*$ are still d_j , $j = 1, \dots, n$. Moreover, $X_*^T M X_*$ is the so-called s-principal $2k \times 2k$ submatrix of $\tilde{X}_*^T M \tilde{X}_*$, i.e., $X_*^T M X_*$ is obtained from $\tilde{X}_*^T M \tilde{X}_*$ by deleting its row and columns with the indices $k+1, \dots, n, n+k+1, \dots, 2n$. From the symplectic analog of Cauchy's interlacing theorem [40, 17], we deduce that $d_j \leq \lambda_j$ for $j = 1, \dots, k$. On the other hand, taking into account that X_* is a global minimizer of (4.1), we obtain

$$2 \sum_{j=1}^k \lambda_j = \text{tr}(K^T J_{2k} L_* K) = \min_{Y \in \text{Sp}(2k)} \text{tr}(Y^T X_*^T M X_* Y) \leq \text{tr}(X_*^T M X_*) = 2 \sum_{j=1}^k d_j,$$

and, hence, $\lambda_j = d_j$ for $j = 1, \dots, k$. Further, it follows from (4.4) and (A.1) that

$$M X_* K = J_{2n} X_* K K^{-1} L_* K = J_{2n} X_* K \begin{bmatrix} 0 & -\Lambda \\ \Lambda & 0 \end{bmatrix}.$$

This implies that the columns of $X_{1:k} := X_* K$ form a normalized symplectic eigenvector set associated with the symplectic eigenvalues d_1, \dots, d_k .

It remains to show that $K \in \text{OrSp}(2k)$. Define $F = K^{-1}$. Since $X_* = X_{1:k} F$ is a global minimizer of (4.1), it follows that

$$(A.2) \quad 2 \sum_{i=1}^k d_i = \text{tr}(X_*^T M X_*) = \text{tr}(F^T X_{1:k}^T M X_{1:k} F) = \text{tr}(F^T \text{diag}(\Lambda, \Lambda) F).$$

We now express F in the block form as $F = \begin{bmatrix} A & B \\ C & G \end{bmatrix}$. By Proposition 2.1(i), we have $F^T \in \text{Sp}(2k)$. This results in the following constraints for the submatrices

$$(A.3) \quad A G^T - C B^T = I, \quad A B^T = B A^T, \quad C G^T = G C^T.$$

Then the right-hand side of (A.2) can be more detailed as

$$\begin{aligned} 2 \sum_{i=1}^k d_i &= \text{tr}(F^T \text{diag}(\Lambda, \Lambda) F) = \text{tr}(A^T \Lambda A + C^T \Lambda C + B^T \Lambda B + G^T \Lambda G) \\ &= \sum_{i=1}^k d_i \sum_{j=1}^k (a_{ij}^2 + g_{ij}^2 + c_{ij}^2 + b_{ij}^2) \geq 2 \sum_{i=1}^k d_i \sum_{j=1}^k (a_{ij} g_{ij} - c_{ij} b_{ij}) = 2 \sum_{i=1}^k d_i, \end{aligned}$$

where “ \geq ” appears due to the facts that $(a_{ij} - g_{ij})^2 \geq 0$ and $(c_{ij} + b_{ij})^2 \geq 0$ for all $i, j = 1, \dots, k$, and the last equality follows from the first relation in (A.3). The equality case happens if and only if $a_{ij} = g_{ij}$ and $c_{ij} = -b_{ij}$ for $i, j = 1, \dots, k$. Thus, $A = G$ and $C = -B$. Then by Proposition 2.1(ii), we obtain that $F \in \text{OrSp}(2k)$ and, hence, $K = F^{-1} \in \text{OrSp}(2k)$. \square

The last part of this proof is based on the ideas in [17, Theorems 5, 6]. It is however more direct and does not invoke the notions of doubly stochastic and doubly superstochastic matrices.

Appendix B. Proof of Lemma 4.10. We show the existence of X_* only, as the proof for X^* is similar. By Corollaries 4.4 and 4.7, we can replace X_0 and X_* by $X_{\mathcal{I}_k} K_0$ and $X_{1:k} K_*$, respectively, with some $K_0, K_* \in \text{OrSp}(2k)$ and $\mathcal{I}_k \subset \{1, \dots, n\}$. Let us assume that this lemma holds for the critical point $X_{\mathcal{I}_k}$, i.e., there exists a global minimizer X_* of (4.1) satisfying

$$(B.1) \quad X_*^T J_{2n} X_{\mathcal{I}_k} + X_{\mathcal{I}_k}^T J_{2n} X_* = 0.$$

Then we have

$$\begin{aligned} (X_* K_0)^T J_{2n} X_0 + X_0^T J_{2n} (X_* K_0) &= K_0^T X_*^T J_{2n} X_{\mathcal{I}_k} K_0 + K_0^T X_{\mathcal{I}_k}^T J_{2n} X_* K_0 \\ &= K_0^T (X_*^T J_{2n} X_{\mathcal{I}_k} + X_{\mathcal{I}_k}^T J_{2n} X_*) K_0 = 0. \end{aligned}$$

This means that $X_* K_0$ is the sought global minimizer corresponding to $X_0 = X_{\mathcal{I}_k} K_0$.

We now prove the above assumption. Our goal is to construct $K_* \in \text{OrSp}(2k)$ such that $X_* = X_{1:k} K_*$ satisfies (B.1) and is the global minimizer of (4.1). Let $O = X_{1:k}^T J_{2n} X_{\mathcal{I}_k}$ for $\mathcal{I}_k = \{i_1, \dots, i_k\} \subset \{1, \dots, n\}$. We can see that O can be written in the block form as

$$O = \begin{bmatrix} 0 & O_1 \\ -O_1 & 0 \end{bmatrix} \in \mathbb{R}^{2k \times 2k},$$

where $O_1 = [x_1, \dots, x_k]^T J_{2n} [x_{n+i_1}, \dots, x_{n+i_k}] \in \mathbb{R}^{k \times k}$. Let c denote the number of common indices $\{1, \dots, k\} \cap \mathcal{I}_k$ with $0 \leq c \leq k$. Taking Proposition 2.1(ii) into account, we are searching for $K_* \in \text{OrSp}(2k)$ of the form

$$K_* = \begin{bmatrix} K_1 & K_2 \\ -K_2 & K_1 \end{bmatrix},$$

where K_1 and K_2 satisfy

$$(B.2) \quad K_1^T K_2 = K_2^T K_1, \quad K_1^T K_1 + K_2^T K_2 = I,$$

$$(B.3) \quad K_1^T O_1 = -O_1^T K_1, \quad K_2^T O_1 = O_1^T K_2.$$

The conditions (B.2) guarantee the orthosymplecticity of K_* , whereas the conditions (B.3) imply (B.1). By definition, O_1 contains exactly c 1's. Let us denote their positions by $(i_1, j_1), \dots, (i_c, j_c)$. We moreover choose other $k - c$ positions $(i_{c+1}, j_{c+1}), \dots, (i_k, j_k)$ in such a way that if we put 1 in O_1 at all these positions, then the resulting matrix becomes a permutation of the identity. Let us note that while the set $(i_1, j_1), \dots, (i_c, j_c)$ is fixed upon the given matrix O_1 , there are multiple choices for $(i_{c+1}, j_{c+1}), \dots, (i_k, j_k)$. We will construct K_* as follows:

$$(K_1)_{ij} = \begin{cases} \cos \phi_l, & \text{if } (i, j, l) \in \{(i_{c+1}, j_{c+1}, c+1), \dots, (i_k, j_k, k)\}, \\ 0, & \text{otherwise,} \end{cases}$$

$$(K_2)_{ij} = \begin{cases} 1, & \text{if } (i, j) \in \{(i_1, j_1), \dots, (i_c, j_c)\}, \\ \sin \phi_l, & \text{if } (i, j, l) \in \{(i_{c+1}, j_{c+1}, c+1), \dots, (i_k, j_k, k)\}, \\ 0, & \text{otherwise,} \end{cases}$$

with $\phi_l \in \mathbb{R}$. Note that we can use -1 instead of 1 in K_2 . One directly verifies that

$$(K_1^T K_2)_{ij} = (K_2^T K_1)_{ij} = \begin{cases} \cos \phi_l \sin \phi_l, & \text{if } (i, j, l) \in \{(c+1, c+1, c+1), \dots, (k, k, k)\}, \\ 0, & \text{otherwise,} \end{cases}$$

$$(K_1^T K_1)_{ij} = \begin{cases} \cos^2 \phi_l, & \text{if } (i, j, l) \in \{(c+1, c+1, c+1), \dots, (k, k, k)\}, \\ 0, & \text{otherwise,} \end{cases}$$

$$(K_2^T K_2)_{ij} = \begin{cases} 1, & \text{if } (i, j) \in \{(1, 1), \dots, (c, c)\}, \\ \sin^2 \phi_l, & \text{if } (i, j, l) \in \{(c+1, c+1, c+1), \dots, (k, k, k)\}, \\ 0, & \text{otherwise.} \end{cases}$$

and, hence, the relations in (B.2) are satisfied. Furthermore, we have

$$(K_1^T O_1)_{ij} = (-O_1^T K_1)_{ij} = 0, \quad i, j = 1, \dots, k,$$

$$(K_2^T O_1)_{ij} = (O_1^T K_2)_{ij} = \begin{cases} 1, & \text{if } (i, j) \in \{(1, 1), \dots, (c, c)\}, \\ 0, & \text{otherwise} \end{cases}$$

implying the relations in (B.3). □

Though covered in the proof, we still want to show two special cases of c . If $c = 0$, then $O = 0$ and, hence, we can choose any $K_* \in \text{OrSp}(2k)$. If $c = k$, i.e., X_0 is a minimizer, then $O_1 = I$. In this case, we can take, for example, $K_* = J_{2k}$.

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