

On Generalizing Trace Minimization

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January 23, 2021

Abstract

Ky Fan's trace minimization principle is extended along the line of the Brockett cost function $\text{tr}(DX^HAX)$ in X on the Stiefel manifold, where D of an apt size is positive definite. Specifically, we investigate $\inf_X \text{tr}(DX^HAX)$ subject to $X^HBX = I_k$ or $J_k = \text{diag}(\pm 1)$. We establish conditions under which the infimum is finite and when it is finite, analytic solutions are obtained in terms of the eigenvalues and eigenvectors of the matrix pencil $A - \lambda B$, where B is possibly indefinite and singular, and D is also possibly indefinite.

Key words. Ky Fan's trace minimization principle, positive semi-definite matrix pencil, eigenvalue, eigenvector, Brockett cost function.

AMS subject classifications. Primary 15A18. Secondary 15A22, 65F15.

1 Introduction

Quadratic optimization problems with matrix arguments are drawing tremendous attentions lately in data science, and they often involve traces of certain quadratic forms, for example, the trace ratio maximization problem from the linear discriminant analysis (LDA) [13, 20, 25, 26, 27, 28], the correlation maximization from the canonical correlation analysis (CCA) and its variants [7, 8, 12, 24, 29]. Some formulations admit analytical solutions in terms of matrix eigenvalue/singular value decompositions, but most don't. Among those that do admit analytical solutions, the most well-known one is perhaps Ky Fan's trace minimization principle [11, p.248]

$$\min_{X^HX=I_k} \text{tr}(X^HAX) = \sum_{i=1}^k \lambda_i, \quad (1.1)$$

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where $\text{trace}(\cdot)$ is the trace of a square matrix, I_k is the $k \times k$ identity matrix, and $A \in \mathbb{C}^{n \times n}$ is Hermitian and its eigenvalues are denoted by λ_i ($i = 1, 2, \dots, n$) and arranged in the ascending order:

$$\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n. \quad (1.2)$$

Moreover for any minimizer X_{\min} of (1.1), i.e., $\text{tr}(X_{\min}^H A X_{\min}) = \sum_{i=1}^k \lambda_i$, its columns span A 's invariant subspace associated with the first k eigenvalues λ_i , $i = 1, 2, \dots, k$.

The result (1.1) can be straightforwardly extended to

$$\min_{X^H B X = I_k} \text{tr}(X^H A X) = \sum_{i=1}^k \lambda_i, \quad (1.3)$$

where $A, B \in \mathbb{C}^{n \times n}$ are Hermitian and B is positive definite, and now λ_i are the eigenvalues of matrix pencil $A - \lambda B$ and ordered as in (1.2). Essentially, (1.3) is no more general than (1.1). In fact, upon substitutions: $X \leftarrow B^{1/2} X$ and $A \leftarrow B^{-1/2} A B^{-1/2}$, (1.3) reduces to (1.1). A nontrivial extension of (1.1), similar in form to (1.3), is [14, 17]

$$\inf_{X^H B X = J_k} \text{tr}(X^H A X) = \sum_{i=1}^{k_+} \lambda_i^+ - \sum_{i=1}^{k_-} \lambda_i^- \quad (1.4)$$

for a positive semi-definite matrix pencil¹ $A - \lambda B$, where λ_i^\pm are finite eigenvalues of $A - \lambda B$ and are arranged in the order as

$$\lambda_{n_-}^- \leq \dots \leq \lambda_1^- \leq \lambda_1^+ \leq \dots \leq \lambda_{n_+}^+,$$

n_- and n_+ are the numbers of negative and positive eigenvalues of B , respectively, and

$$0 \leq k_\pm \leq n_\pm, \quad k = k_+ + k_-, \quad J_k = \begin{bmatrix} I_{k_+} & \\ & -I_{k_-} \end{bmatrix} \in \mathbb{C}^{k \times k}. \quad (1.5)$$

Recently, Liu, So, and Wu [18] laboriously analyzed how to solve

$$\min_{X^H X = I_k} \text{tr}(D X^H A X) \quad (1.6)$$

by numerical optimization techniques, where $A \in \mathbb{C}^{n \times n}$ and $D \in \mathbb{C}^{k \times k}$ are Hermitian but D may be indefinite. Its objective function $\text{tr}(D X^H A X)$ in X on the Stiefel manifold $\{X \in \mathbb{R}^{n \times k} : X^H X = I_k\}$ is known as the *Brockett cost function* in the case when D is diagonal and positive semi-definite, and optimizing it has often been used as an illustrative example for optimization on the Stiefel manifold [1, p.80], [5, 6].

Our goal in this paper is to go beyond the Brockett cost function to investigate, as an extension of (1.1),

$$\inf_{X^H B X = I_k \text{ (or } -I_k)} \text{tr}(D X^H A X), \quad (1.7)$$

¹ $A, B \in \mathbb{C}^{n \times n}$ are Hermitian and there exists $\lambda_0 \in \mathbb{R}$ such that $A - \lambda_0 B$ is positive semi-definite [17, Definition 1.1].

where both B and D are possibly indefinite. Our first main result is an analytical solution to (1.7) for positive definite B (for which only $X^H B X = I_k$ can be used as a constraint) in terms of the eigen-decompositions of D and matrix pencil $A - \lambda B$ and the solution lends itself to be computed by more efficient numerical linear algebra techniques [2, 3, 9, 16]. In particular, this result yields an elegant solution to the widely studied (1.6) [1, 18]. Our second main result is for a more general setting that B is indefinite and possibly singular and $A - \lambda B$ is a positive semi-definite matrix pencil. We show that the infimum in (1.7) is finite if and only if D positive semi-definite and establish analytical solutions to it when the infimum is finite.

Note that whether D is diagonal or not is inconsequential so long that it is Hermitian and the constraint is either $X^H B X = I_k$ or $X^H B X = -I_k$ because we can always perform an eigen-decomposition $D = Q \Omega Q^H$ to get

$$\min_{X^H B X = \pm I_k} \operatorname{tr}(D X^H A X) = \min_{\tilde{X}^H B \tilde{X} = \pm I_k} \operatorname{tr}(\Omega \tilde{X}^H A \tilde{X}),$$

where X and \tilde{X} are related by $\tilde{X} = XQ$, Q is unitary and Ω is diagonal of eigenvalues. So far, we have been focusing on “minimization”, but these formulations admit straightforward restatements for “maximization” by simply considering $-A$ instead.

The rest of this paper is organized as follows. We state our main results for (1.7) in section 2 for positive definite B (and with $X^H B X = I_k$) and in section 3 for the more general setting that B is genuinely indefinite. The proofs for the main results are presented in sections 4 and 5, respectively. We draw our conclusion in section 6.

Notation. Throughout this paper, $\mathbb{C}^{n \times m}$ is the set of all $n \times m$ complex matrices, $\mathbb{C}^n = \mathbb{C}^{n \times 1}$, and $\mathbb{C} = \mathbb{C}^1$. \mathbb{R} is set of all real numbers. I_n (or simply I if its dimension is clear from the context) is the $n \times n$ identity matrix. For a matrix $X \in \mathbb{C}^{m \times n}$, $\mathcal{N}(X) = \{x \in \mathbb{C}^n : Xx = 0\}$ and $\mathcal{R}(X) = \{Xx : x \in \mathbb{C}^n\}$ are the null space and the range of X , respectively. X^H is the conjugate transpose of a vector or matrix. $A \succ 0$ ($A \succeq 0$) means that A is Hermitian positive (semi-)definite, and $A \prec 0$ ($A \preceq 0$) if $-A \succ 0$ ($-A \succeq 0$).

2 Positive Definite B

Throughout this section and section 4, $A, B \in \mathbb{C}^{n \times n}$ and $D \in \mathbb{C}^{k \times k}$ are Hermitian and B is positive definite. Then $A - \lambda B$ admits the following eigen-decomposition

$$U^H A U = \Lambda \equiv \operatorname{diag}(\lambda_1, \lambda_2, \dots, \lambda_n), \quad U^H B U = I_n, \quad (2.1)$$

where λ_i are the eigenvalues of $A - \lambda B$ and are, without loss of generality, arranged in the ascending order as in (1.2), and $U = [u_1, u_2, \dots, u_n]$ is the eigenvector matrix and unitary: $Au_i = \lambda_i B u_i$ for all i and $U^H U = I_n$. Let the eigen-decomposition of D be

$$Q^H D Q = \Omega \equiv \operatorname{diag}(\omega_1, \omega_2, \dots, \omega_k), \quad (2.2a)$$

where $Q \in \mathbb{C}^{k \times k}$ is unitary and, without loss of generality,

$$\omega_1 \geq \dots \geq \omega_\ell \geq 0 \geq \omega_{\ell+1} \geq \dots \geq \omega_k. \quad (2.2b)$$

The case $\ell = 0$ or $\ell = k$ corresponds to when D has no positive eigenvalues, i.e., $D \preceq 0$, or no nonnegative eigenvalues, i.e., $D \succeq 0$, respectively.

Our main result of this section is Theorem 2.1 below.

Theorem 2.1. *Suppose that $A, B \in \mathbb{C}^{n \times n}$ and $D \in \mathbb{C}^{k \times k}$ are Hermitian and B is positive definite, admitting the eigen-decompositions in (2.1) and (2.2). Then*

$$\min_{X^H B X = I_k} \text{tr}(D X^H A X) = \sum_{i=1}^{\ell} \omega_i \lambda_i + \sum_{i=\ell+1}^k \omega_i \lambda_{i+n-k}. \quad (2.3)$$

Furthermore, any minimizer X_{opt} has the following characterizations:

- (a) *If D is nonsingular, then $\mathcal{R}(X_{\text{opt}} Q)$ is the eigenspace of $A - \lambda B$ [21, p.303], associated with the ℓ smallest and $k - \ell$ largest eigenvalues of $A - \lambda B$. If also all ω_i are distinct, then*

$$(X_{\text{opt}} Q)^H A X_{\text{opt}} Q = \text{diag}(\underbrace{\lambda_1, \lambda_2, \dots, \lambda_{\ell}}_{\ell}, \underbrace{\lambda_{n-k+\ell+1}, \dots, \lambda_n}_{k-\ell}).$$

- (b) *Suppose that D is possibly singular and has ℓ_+ positive eigenvalues and ℓ_- negative eigenvalues, and let $\hat{Q} \in \mathbb{C}^{k \times (\ell_+ + \ell_-)}$ be the one from Q by keeping its first ℓ_+ and last ℓ_- columns. Then $\mathcal{R}(X_{\text{opt}} \hat{Q})$ is the eigenspace of $A - \lambda B$ associated with its ℓ_+ smallest and ℓ_- largest eigenvalues. If also the nonzero eigenvalues of D are distinct, then*

$$(X_{\text{opt}} \hat{Q})^H A X_{\text{opt}} \hat{Q} = \text{diag}(\underbrace{\lambda_1, \lambda_2, \dots, \lambda_{\ell_+}}_{\ell_+}, \underbrace{\lambda_{n-\ell_-+1}, \dots, \lambda_n}_{\ell_-}).$$

There are a couple of remarks in order. Firstly, the minimization extracts out the extreme eigenvalues of $A - \lambda B$. Secondly, if all ω_i are distinct and nonzero, then the columns of $X_{\text{opt}} Q$ are the associated eigenvectors. Thirdly, if D does have 0 as some of its eigenvalues, then in the notation of Theorem 2.1(b), those eigenvalues 0 can be matched to any λ_i ($\ell_+ + 1 \leq i \leq n - \ell_-$), other things being equal, to still yield the same objective value as the optimal one in the right-hand side of (2.3). Fourthly, upon replacing A by $-A$, we obtain immediately the following corollary.

Corollary 2.1. *Under the conditions of Theorem 2.1*

$$\max_{X^H B X = I_k} \text{tr}(D X^H A X) = \sum_{i=1}^{\ell} \omega_i \lambda_{n+1-i} + \sum_{i=\ell+1}^k \omega_i \lambda_{k-i+1}. \quad (2.4)$$

Furthermore, any maximizer X_{opt} has the following characterizations:

- (a) *If D is nonsingular, then $\mathcal{R}(X_{\text{opt}} Q)$ is the eigenspace of $A - \lambda B$ associated with the $k - \ell$ smallest and ℓ largest eigenvalues of $A - \lambda B$. If also all ω_i are distinct, then*

$$(X_{\text{opt}} Q)^H A X_{\text{opt}} Q = \text{diag}(\underbrace{\lambda_n, \lambda_{n-1}, \dots, \lambda_{n+1-\ell}}_{\ell}, \underbrace{\lambda_{k-\ell}, \dots, \lambda_1}_{k-\ell}).$$

- (b) Suppose that D is possibly singular and has ℓ_+ positive eigenvalues and ℓ_- negative eigenvalues, and let $\widehat{Q} \in \mathbb{C}^{k \times (\ell_+ + \ell_-)}$ be the one from Q by keeping its first ℓ_- and last ℓ_+ columns. Then $\mathcal{R}(X_{\text{opt}}\widehat{Q})$ is the eigenspace of $A - \lambda B$ associated with its ℓ_- smallest and ℓ_+ largest eigenvalues. If also the nonzero eigenvalues of D are distinct, then

$$(X_{\text{opt}}\widehat{Q})^H A X_{\text{opt}}\widehat{Q} = \text{diag}(\underbrace{\lambda_n, \lambda_{n-1}, \dots, \lambda_{n+1-\ell_+}}_{\ell_+}, \underbrace{\lambda_{\ell_-}, \dots, \lambda_1}_{\ell_-}).$$

The proof of Theorem 2.1 occupies a few pages and is deferred to section 4.

3 Genuinely Indefinite B

Throughout this section and section 5, $A - \lambda B \in \mathbb{C}^{n \times n}$ is a positive semi-definite matrix pencil, i.e., A and B are Hermitian and there exists $\lambda_0 \in \mathbb{R}$ such that $A - \lambda_0 B \succeq 0$, and B is genuinely indefinite in the sense that B has both positive and negative eigenvalues. We are interested in (1.7):

$$\inf \text{tr}(DX^H AX) \quad \text{subject to either } X^H B X = I_k \text{ or } X^H B X = -I_k. \quad (1.7)$$

After presenting our main results for it, we will discuss the more generally constraint $X^H B X = J_k$, where J_k is as given in (1.5).

Before we investigate (1.7), we review some of the related concepts and results about a positive semi-definite matrix pencil $A - \lambda B$ [17]. Let the integer triplet (n_+, n_0, n_-) be the *inertia* of B , meaning B has n_+ positive, n_0 0, and n_- negative eigenvalues, respectively. Necessarily

$$r := \text{rank}(B) = n_+ + n_-. \quad (3.1)$$

We say $\mu \neq \infty$ is a *finite eigenvalue* of $A - \lambda B$ if

$$\text{rank}(A - \mu B) < \max_{\lambda \in \mathbb{C}} \text{rank}(A - \lambda B), \quad (3.2)$$

and $x \in \mathbb{C}^n$ is a corresponding *eigenvector* if $0 \neq x \notin \mathcal{N}(A) \cap \mathcal{N}(B)$ satisfies

$$Ax = \mu Bx, \quad (3.3)$$

or equivalently, $0 \neq x \in \mathcal{N}(A - \mu B) \setminus (\mathcal{N}(A) \cap \mathcal{N}(B))$. It is known [17] that a *positive semi-definite pencil* $A - \lambda B$ has only $r = \text{rank}(B)$ finite eigenvalues all of which are real. Denote these finite eigenvalues by λ_i^\pm ordered as

$$\lambda_{n_-}^- \leq \dots \leq \lambda_1^- \leq \lambda_1^+ \leq \dots \leq \lambda_{n_+}^+. \quad (3.4)$$

It has been proved that for all i, j

$$\lambda_i^- \leq \lambda_0 \leq \lambda_j^+. \quad (3.5)$$

As in section 2, let D have its eigen-decomposition given by (2.2):

$$Q^H D Q = \Omega \equiv \text{diag}(\omega_1, \omega_2, \dots, \omega_k), \quad \omega_1 \geq \omega_2 \geq \dots \geq \omega_k.$$

Our main result of the section is Theorem 3.1 below.

Theorem 3.1. *Suppose that $A, B \in \mathbb{C}^{n \times n}$ and $D \in \mathbb{C}^{k \times k}$ are Hermitian, $A \neq 0$ and B is genuinely indefinite, $k \leq n_+$, and the matrix pencil $A - \lambda B$ is positive semi-definite. Then*

$$\inf_{X^H B X = I_k} \operatorname{tr}(D X^H A X) > -\infty$$

if and only if $D \succeq 0$, in which case

$$\inf_{X^H B X = I_k} \operatorname{tr}(D X^H A X) = \sum_{i=1}^k \omega_i \lambda_i^+. \quad (3.6)$$

The infimum can be attained, when $A - \lambda B$ is diagonalizable, by X such that the columns of XQ are the eigenvectors of $A - \lambda B$ associated with its eigenvalues λ_i^+ for $1 \leq i \leq k$, respectively.

Our proof of this theorem is rather involved and will be given in section 5. Apply Theorem 3.1 to the matrix pencil $A - (-\lambda)(-B)$, we immediately conclude the following corollary.

Corollary 3.1. *Suppose the conditions of Theorem 3.1, except now $k \leq n_-$. Then*

$$\inf_{X^H B X = -I_k} \operatorname{tr}(D X^H A X) > -\infty$$

if and only if $D \succeq 0$, in which case

$$\inf_{X^H B X = -I_k} \operatorname{tr}(D X^H A X) = - \sum_{i=1}^k \omega_i \lambda_i^-. \quad (3.7)$$

The infimum can be attained, when $A - \lambda B$ is diagonalizable, by X such that the columns of XQ are the eigenvectors of $A - \lambda B$ associated with its eigenvalues λ_i^- for $1 \leq i \leq k$, respectively.

Combining Theorem 3.1 and Corollary 3.1, we present a result for the more general constraint $X^H B X = J_k$, whose proof is deferred to section 5 as well.

Corollary 3.2. *Suppose that $A, B \in \mathbb{C}^{n \times n}$ and $D_{\pm} \in \mathbb{C}^{k_{\pm} \times k_{\pm}}$ are Hermitian, $A \neq 0$ and B is genuinely indefinite, $k_{\pm} \leq n_{\pm}$, and the matrix pencil $A - \lambda B$ is positive semi-definite. Let*

$$J_k = \begin{bmatrix} I_{k_+} & \\ & -I_{k_-} \end{bmatrix}, \quad D = \begin{matrix} k_+ & k_- \\ k_- & \end{matrix} \begin{bmatrix} D_+ & \\ & D_- \end{bmatrix},$$

and denote by $\omega_1^+ \geq \dots \geq \omega_{k_+}^+$ and $\omega_1^- \geq \dots \geq \omega_{k_-}^-$ the eigenvalues of D_+ and D_- , respectively. If $D_{\pm} \succeq 0$, then

$$\inf_{X^H B X = J_k} \operatorname{tr}(D X^H A X) = \sum_{i=1}^{k_+} \omega_i^+ \lambda_i^+ - \sum_{i=1}^{k_-} \omega_i^- \lambda_i^-. \quad (3.8)$$

The infimum can be attained when $A - \lambda B$ is diagonalizable.

One comment that we would like to emphasize about the conditions of Corollary 3.2 is that matrix D has to take the same block-diagonal structure as J_k . Our next example shows that if D doesn't have the same block-diagonal structure as J_k , the infimum may not be able to be expressed simply as some sum of the products of the eigenvalues between D and $A - \lambda B$. The example involves a fair amount of complicated computation and can be skipped in the first reading.

Consider, given μ and δ such that $0 < \delta < \frac{1}{\mu} < 1 < \mu$,

$$A = \begin{bmatrix} 1 & \\ & \mu \end{bmatrix}, B = \begin{bmatrix} 1 & \\ & -1 \end{bmatrix}, J_2 = B,$$

$$\Omega = \begin{bmatrix} 1 & \\ & \delta \end{bmatrix} \succ 0, Q = \begin{bmatrix} \sqrt{1-\sigma^2} & -\sigma \\ \sigma & \sqrt{1-\sigma^2} \end{bmatrix}, D = Q^H \Omega Q \succ 0,$$

where $0 \neq \sigma \in (-1, 1)$. $A - \lambda B$ is positive definite pencil because $A - 0 \cdot B = A \succ 0$. The two eigenvalues of $A - \lambda B$ are $\lambda_1^- = -\mu$, $\lambda_1^+ = 1$. D doesn't have the same block structure as J_2 if $\sigma \neq 0$. We will show that

$$\inf_{X^H B X = J_2} \text{tr}(D X^H A X) < \min\{1 + \delta\mu, \mu + \delta\} = 1 + \delta\mu, \quad (3.9)$$

implying that the infimum cannot be simply expressed as any of the two possible sums of products: $1 + \delta\mu$ and $\mu + \delta$, between the eigenvalues of $A - \lambda B$ and of D .

To see (3.9), we restrict X to those Y :

$$Y = \begin{bmatrix} \sqrt{1+\tau^2} & \\ \tau & \sqrt{1+\tau^2} \end{bmatrix}, \quad \tau \in [0, +\infty).$$

It can be verified that $Y^H B Y = J_2$. In order to show (3.9), it suffices to show that $f(\sigma, \tau) := \text{tr}(D Y^H A Y) < 1 + \delta\mu$ for some (σ, τ) . We have

$$\begin{aligned} f(\sigma, \tau) &= \text{tr}(D Y^H A Y) = \text{tr}(Q^H \Omega Q Y^H A Y) \\ &= \text{tr} \left(\begin{bmatrix} 1 - \sigma^2 + \delta\sigma^2 & (\delta - 1)\sigma\sqrt{1 - \sigma^2} \\ (\delta - 1)\sigma\sqrt{1 - \sigma^2} & \sigma^2 + \delta(1 - \sigma^2) \end{bmatrix} \begin{bmatrix} (1 + \tau^2) + \mu\tau^2 & (1 + \mu)\tau\sqrt{1 + \tau^2} \\ (1 + \mu)\tau\sqrt{1 + \tau^2} & \tau^2 + \mu(1 + \tau^2) \end{bmatrix} \right) \\ &= (1 - \sigma^2 + \delta\sigma^2) \cdot [(1 + \tau^2) + \mu\tau^2] + 2 \cdot (\delta - 1)\sigma\sqrt{1 - \sigma^2} \cdot (1 + \mu)\tau\sqrt{1 + \tau^2} \\ &\quad + [\sigma^2 + \delta(1 - \sigma^2)] \cdot [\tau^2 + \mu(1 + \tau^2)] \\ &= 1 + \delta\mu - \sigma^2(1 - \delta)(1 - \mu) + \tau^2(1 + \delta)(1 + \mu) + 2(\delta - 1)(1 + \mu)\tau\sigma\sqrt{1 - \sigma^2}\sqrt{1 + \tau^2} \\ &= 1 + \delta\mu + (1 + \delta)(1 + \mu) \left[\tau^2 - \gamma\nu\sigma^2 - 2\gamma\tau\sigma\sqrt{1 - \sigma^2}\sqrt{1 + \tau^2} \right], \end{aligned}$$

where for the last equality, we set $\gamma := \frac{1-\delta}{1+\delta} \in (\frac{\mu-1}{\mu+1}, 1)$ and $\nu := \frac{1-\mu}{1+\mu} \in (-1, 0)$. In particular, $0 < -\nu < \gamma < 1$. We calculate the partial derivatives:

$$\frac{1}{2} \frac{\partial f(\sigma, \tau)}{\partial \tau} = (1 + \delta)(1 + \mu) \left[\tau - \gamma \left(\sqrt{1 + \tau^2} + \tau \frac{\tau}{\sqrt{1 + \tau^2}} \right) \sigma \sqrt{1 - \sigma^2} \right]$$

$$\begin{aligned}
&= (1 + \delta)(1 + \mu) \left[\tau - \gamma \frac{1 + 2\tau^2}{\sqrt{1 + \tau^2}} \sigma \sqrt{1 - \sigma^2} \right], \\
\frac{1}{2} \frac{\partial f(\sigma, \tau)}{\partial \sigma} &= (1 + \delta)(1 + \mu) \left[-\gamma \nu \sigma - \gamma \tau \sqrt{1 + \tau^2} \left(\sqrt{1 - \sigma^2} + \sigma \frac{-\sigma}{\sqrt{1 - \sigma^2}} \right) \right] \\
&= -(1 + \delta)(1 + \mu) \gamma \left[\nu \sigma + \tau \sqrt{1 + \tau^2} \frac{1 - 2\sigma^2}{\sqrt{1 - \sigma^2}} \right].
\end{aligned}$$

The stationary points (σ, τ) of f satisfy

$$\frac{1}{2} \frac{\partial f(\sigma, \tau)}{\partial \tau} = 0, \quad \frac{1}{2} \frac{\partial f(\sigma, \tau)}{\partial \sigma} = 0. \quad (3.10)$$

It can be seen that $\tau = 0 \iff \sigma = 0$ from the system (3.10). For $\tau \sigma \neq 0$, (3.10) yields

$$\frac{\tau \sqrt{1 + \tau^2}}{1 + 2\tau^2} = \gamma \sigma \sqrt{1 - \sigma^2}, \quad \tau \sqrt{1 + \tau^2} = -\frac{\nu \sigma \sqrt{1 - \sigma^2}}{1 - 2\sigma^2},$$

or, equivalently

$$(1 + 2\tau^2)(1 - 2\sigma^2) = \frac{-\nu}{\gamma}, \quad \frac{\tau^2(1 + \tau^2)}{1 + 2\tau^2} = -\gamma \nu \frac{\sigma^2(1 - \sigma^2)}{1 - 2\sigma^2}. \quad (3.11)$$

The first equation in (3.11) yields

$$\tau^2 = -\frac{1}{2} \left[\frac{\nu}{\gamma(1 - 2\sigma^2)} + 1 \right], \quad (3.12)$$

and plug it into the second equation in (3.11) to get

$$\begin{aligned}
0 &= \gamma \nu \sigma^2(1 - \sigma^2) + \frac{-\gamma}{\nu} (1 - 2\sigma^2)^2 \frac{-1}{4} \left[\frac{\nu}{\gamma(1 - 2\sigma^2)} + 1 \right] \left[1 - \frac{\nu}{\gamma(1 - 2\sigma^2)} \right] \\
&= \gamma \nu \sigma^2(1 - \sigma^2) + \frac{\gamma}{4\nu} \left[(1 - 2\sigma^2)^2 - \frac{\nu^2}{\gamma^2} \right] \\
&= \frac{1}{4\gamma\nu} \left[\gamma^2 - \nu^2 - 4\gamma^2(1 - \nu^2)\sigma^2 + 4\gamma^2(1 - \nu^2)\sigma^4 \right], \\
&= \frac{\gamma(1 - \nu^2)}{\nu} \left[\frac{\gamma^2 - \nu^2}{4\gamma^2(1 - \nu^2)} - \sigma^2 + \sigma^4 \right].
\end{aligned} \quad (3.13)$$

Since $(-1)^2 - 4 \frac{\gamma^2 - \nu^2}{4\gamma^2(1 - \nu^2)} = \frac{\nu^2(1 - \gamma^2)}{\gamma^2(1 - \nu^2)} > 0$, solving (3.13) for σ^2 gives

$$\sigma^2 = \frac{1}{2} \left(1 \pm \sqrt{1 - \frac{\gamma^2 - \nu^2}{\gamma^2(1 - \nu^2)}} \right) = \frac{1}{2} \left(1 \pm \sqrt{\frac{\nu^2(1 - \gamma^2)}{\gamma^2(1 - \nu^2)}} \right),$$

which yields $1 - 2\sigma^2 = \mp \left| \frac{\nu}{\gamma} \right| \sqrt{\frac{1 - \gamma^2}{1 - \nu^2}}$ and $1 + 2\tau^2 = \pm \text{sign}(\gamma\nu) \sqrt{\frac{1 - \nu^2}{1 - \gamma^2}}$ by (3.12). Since $1 + 2\tau^2 > 0$, we conclude

$$1 + 2\tau^2 = \sqrt{\frac{1 - \nu^2}{1 - \gamma^2}}, \quad 1 - 2\sigma^2 = -\frac{\nu}{\gamma} \sqrt{\frac{1 - \gamma^2}{1 - \nu^2}}.$$

Hence stationary points (σ_*, τ_*) are determined by

$$\tau_*^2 = \frac{1}{2} \left(\sqrt{\frac{1-\nu^2}{1-\gamma^2}} - 1 \right) > 0, \quad \sigma_*^2 = \frac{1}{2} \left(\frac{\nu}{\gamma} \sqrt{\frac{1-\gamma^2}{1-\nu^2}} + 1 \right) \in (0, 1), \quad (3.14)$$

giving two stationary points (σ_*, τ_*) :

$$\tau_* = \sqrt{\frac{1}{2} \left(\sqrt{\frac{1-\nu^2}{1-\gamma^2}} - 1 \right)}, \quad \sigma_*^\pm = \pm \sqrt{\frac{1}{2} \left(\frac{\nu}{\gamma} \sqrt{\frac{1-\gamma^2}{1-\nu^2}} + 1 \right)}. \quad (3.15)$$

The values of f at these stationary points are

$$\begin{aligned} f(\sigma_*^\pm, \tau_*) &= 1 + \delta\mu + \frac{1}{2}(1 + \delta)(1 + \mu) \times \\ &\quad \left[\nu\gamma - 1 + \sqrt{\frac{1-\nu^2}{1-\gamma^2}} - \nu^2 \sqrt{\frac{1-\gamma^2}{1-\nu^2}} \mp \gamma \sqrt{\left(1 - \frac{\nu^2}{\gamma^2} \frac{1-\gamma^2}{1-\nu^2}\right) \left(1 - \frac{1-\nu^2}{1-\gamma^2}\right)} \right] \\ &= 1 + \delta\mu + \frac{1}{2}(1 + \delta)(1 + \mu) \times \\ &\quad \left[\nu\gamma - 1 + \sqrt{\frac{1-\nu^2}{1-\gamma^2}} - \nu^2 \sqrt{\frac{1-\gamma^2}{1-\nu^2}} \mp \sqrt{\frac{(\nu^2 - \gamma^2)^2}{(1-\nu^2)(1-\gamma^2)}} \right] \\ &\quad (\text{let } \eta = \sqrt{\frac{1-\gamma^2}{1-\nu^2}}) \\ &= 1 + \delta\mu + \frac{1}{2}(1 + \delta)(1 + \mu) \left[\nu\gamma - 1 + \frac{1}{\eta} - \nu^2\eta \mp \frac{\nu^2 - \gamma^2}{(1-\nu^2)\eta} \right] \\ &= 1 + \delta\mu + \frac{1}{2}(1 + \delta)(1 + \mu) \left[\nu\gamma - 1 + (1-\nu^2)\eta + \frac{1-\eta^2}{\eta} \mp \frac{\eta^2 - 1}{\eta} \right] \\ &= 1 + \delta\mu + \frac{1}{2}(1 + \delta)(1 + \mu) \left[\nu\gamma - 1 + \sqrt{(1-\gamma^2)(1-\nu^2)} + \frac{1-\eta^2}{\eta} (1 \pm 1) \right] \\ &= 1 + \delta\mu + \frac{1}{2}(1 + \delta)(1 + \mu) \left[-2 \frac{\delta + \mu - 2\sqrt{\delta\mu}}{(1 + \delta)(1 + \mu)} + \frac{1-\eta^2}{\eta} (1 \pm 1) \right]. \end{aligned}$$

It can be seen that $f(\sigma_*^-, \tau_*) < f(0, 0)$ because $\delta + \mu - 2\sqrt{\delta\mu} = (\sqrt{\delta} - \sqrt{\mu})^2 > 0$. This verifies (3.9).

4 Proof of Theorem 2.1

We start with three lemmas as preparation. We will need a result from majorization [4, 11]. Given two sets of real numbers $\{\alpha_i\}_{i=1}^m$ and $\{\beta_i\}_{i=1}^m$, we say that $\{\beta_i\}_{i=1}^m$ *majorizes* $\{\alpha_i\}_{i=1}^m$ if

$$\sum_{i=1}^j \alpha_i^\downarrow \leq \sum_{i=1}^j \beta_i^\downarrow, \quad \text{for } j = 1, 2, \dots, m$$

with equality holds for $j = m$, where $\{\alpha_i^\downarrow\}_{i=1}^m$ is from re-ordering $\{\alpha_i\}_{i=1}^m$ in the decreasing order, i.e.,

$$\alpha_1^\downarrow \geq \alpha_2^\downarrow \geq \cdots \geq \alpha_m^\downarrow$$

(similarly for $\{\beta_i^\downarrow\}_{i=1}^m$). We also use notation α_i^\uparrow obtained from re-ordering $\{\alpha_i\}_{i=1}^m$ as well but in the increasing order.

Lemma 4.1. *Let $\gamma_1 \geq \gamma_2 \geq \cdots \geq \gamma_m$. If $\{\beta_i\}_{i=1}^m$ majorizes $\{\alpha_i\}_{i=1}^m$, then*

$$\sum_{i=1}^m \gamma_i \beta_i^\uparrow \leq \sum_{i=1}^m \gamma_i \alpha_i \leq \sum_{i=1}^m \gamma_i \beta_i^\downarrow. \quad (4.1)$$

Furthermore, if all γ_i are distinct, then the first inequality becomes an equality if and only if $\alpha_i = \beta_i^\uparrow$ for all i . Similarly, if all γ_i are distinct, then the second inequality becomes an equality if and only if $\alpha_i = \beta_i^\downarrow$ for all i .

The first part of the lemma is exactly the same as [15, Lemma 2.3], except that here it is not required that all $\gamma_i \geq 0$. The second part on the inequalities becoming equalities was not explicitly stated there, but it follows from the proof there straightforwardly. This lemma likely appeared elsewhere but an explicit reference is hard to find. As a corollary, we have

$$\sum_{i=1}^m \gamma_i \beta_i^\uparrow \leq \sum_{i=1}^m \gamma_i \beta_i \leq \sum_{i=1}^m \gamma_i \beta_i^\downarrow$$

because clearly $\{\beta_i\}_{i=1}^m$ majorizes $\{\beta_i\}_{i=1}^m$ itself.

Proof of Lemma 4.1. Without loss of generality, we may assume $\gamma_m > 0$; otherwise we can always pick a scalar ξ such that $\gamma_m + \xi \geq 0$, and let

$$\tilde{\gamma}_i := \gamma_i + \xi > 0 \quad \text{for } 1 \leq i \leq m.$$

By assumption, we have $\sum_{i=1}^m \alpha_i = \sum_{i=1}^m \beta_i = \sum_{i=1}^m \beta_i^\uparrow = \sum_{i=1}^m \beta_i^\downarrow =: \eta$, and thus

$$\sum_{i=1}^m \gamma_i \beta_i^\uparrow = -\xi \eta + \sum_{i=1}^m \tilde{\gamma}_i \beta_i^\uparrow, \quad \sum_{i=1}^m \gamma_i \alpha_i = -\xi \eta + \sum_{i=1}^m \tilde{\gamma}_i \alpha_i, \quad \sum_{i=1}^m \gamma_i \beta_i^\downarrow = -\xi \eta + \sum_{i=1}^m \tilde{\gamma}_i \beta_i^\downarrow.$$

It suffices to prove the lemma for $\tilde{\gamma}_1 \geq \tilde{\gamma}_2 \geq \cdots \geq \tilde{\gamma}_m > 0$, instead.

The argument below up to (4.3) appears in the proof of [15, Lemma 2.3]. It is repeated here for the purpose of arguing when the equality signs in (4.1) are attained. Suppose $\gamma_1 \geq \gamma_2 \geq \cdots \geq \gamma_m > 0$ and set

$$p_j = \sum_{i=1}^j \beta_i^\uparrow, \quad s_j = \sum_{i=1}^j \alpha_i, \quad t_j = \sum_{i=1}^j \beta_i^\downarrow, \quad p_0 = s_0 = t_0 = 0.$$

Since $\{\beta_i\}_{i=1}^m$ majorizes $\{\alpha_i\}_{i=1}^m$, we have

$$p_j \leq s_j \leq t_j, \quad p_m = s_m = t_m$$

and thus

$$\begin{aligned}
\sum_{i=1}^m \gamma_i \alpha_i &= \sum_{i=1}^m (s_i - s_{i-1}) \gamma_i \\
&= \sum_{i=1}^m s_i \gamma_i - \sum_{i=2}^m s_{i-1} \gamma_i \\
&= s_m \gamma_m + \sum_{i=1}^{m-1} s_i (\gamma_i - \gamma_{i+1}) \\
&\leq t_m \gamma_m + \sum_{i=1}^{m-1} t_i (\gamma_i - \gamma_{i+1}) \\
&= \sum_{i=1}^m \gamma_i \beta_i^\downarrow, \tag{4.2}
\end{aligned}$$

$$\begin{aligned}
\sum_{i=1}^m \gamma_i \alpha_i &= s_m \gamma_m + \sum_{i=1}^{m-1} s_i (\gamma_i - \gamma_{i+1}) \\
&\geq p_m \gamma_m + \sum_{i=1}^{m-1} p_i (\gamma_i - \gamma_{i+1}) \\
&= \sum_{i=1}^m \gamma_i \beta_i^\uparrow, \tag{4.3}
\end{aligned}$$

as required. To figure out when any of the inequality in the lemma is an equality, we look at (4.2), for an example. We notice that there is only one inequality sign during the derivation in (4.2). In order for the inequality to become an equality, assuming all γ_i are distinct, we will have to have $s_i = t_i$ for all i and consequently, $\alpha_i = \beta_i^\downarrow$ for all i . \square

The next two lemmas relate the diagonal entries of a Hermitian matrix with its eigenvalues.

Lemma 4.2 ([4, Exercise II.1.12, p.35]). *The multiset of the diagonal entries of a Hermitian matrix is majorized by the multiset of its eigenvalues.*

Lemma 4.3. *For a Hermitian matrix, if the multiset of its diagonal entries is the same as the multiset of its eigenvalues, then it is diagonal.*

Proof. This lemma is probably known, but we could not find a reference to it. For completeness, we provide a quick proof. Let $A = [a_{ij}] \in \mathbb{C}^{n \times n}$ be such a Hermitian matrix with eigenvalues $\{\lambda_i\}_{i=1}^n$. By the assumption,

$$\|A\|_F^2 = \sum_{i,j=1}^n |a_{ij}|^2 = \sum_{i=1}^n |\lambda_i|^2 = \sum_{i=1}^n |a_{ii}|^2,$$

where $\|A\|_F$ denotes the Frobenius norm of A . Hence $|a_{ij}|^2 = 0$ for all $i \neq j$, as expected. \square

Now we are ready to prove Theorem 2.1.

Proof of Theorem 2.1. Recall the eigen-decomposition (2.1) with (1.2) for $A - \lambda B$ and the eigen-decomposition (2.2) for D . Consider first that D is nonsingular, i.e., all $\omega_i \neq 0$.

Introducing

$$Y = U^{-1}XQ \quad \Rightarrow \quad X = UYQ^H, \quad (4.4)$$

we find that the left-hand side of (2.3) can be transformed to

$$\min_{X^H B X = I_k} \operatorname{tr}(DX^H A X) = \min_{Y^H Y = I_k} \operatorname{tr}(\Omega Y^H \Lambda Y),$$

and any minimizer of one yield a minimizer of the other according to (4.4).

For any given $Y \in \mathbb{C}^{n \times k}$ with $Y^H Y = I_k$, denote the eigenvalues of $Y^H \Lambda Y$ by

$$\mu_1 \leq \mu_2 \leq \cdots \leq \mu_k,$$

where we suppress the dependency of μ_i on Y for clarity. Cauchy's interlacing inequalities say that

$$\lambda_{i+n-k} \geq \mu_i \geq \lambda_i \text{ for all } 1 \leq i \leq k. \quad (4.5)$$

Denote the diagonal entries of $Y^H \Lambda Y$ by $(Y^H \Lambda Y)_{ii}$ for $i = 1, 2, \dots, k$, and let α_i be the reordering of $(Y^H \Lambda Y)_{ii}$ in the increasing order, i.e.,

$$\alpha_1 \leq \alpha_2 \leq \cdots \leq \alpha_k.$$

Evidently, $\{(Y^H \Lambda Y)_{ii}\}_{i=1}^k$ is majorized by $\{\alpha_i\}_{i=1}^k$ because they are the same up to a permutation. By Lemma 4.2, $\{\alpha_i\}_{i=1}^k$ is majorized by $\{\mu_i\}_{i=1}^k$. We have

$$\begin{aligned} \operatorname{tr}(\Omega Y^H \Lambda Y) &= \sum_{i=1}^k \omega_i (Y^H \Lambda Y)_{ii} \quad (\text{use Lemma 4.1}) \\ &\geq \sum_{i=1}^k \omega_i \alpha_i \quad (\text{use Lemma 4.1}) \\ &\geq \sum_{i=1}^k \omega_i \mu_i \\ &= \sum_{i=1}^{\ell} \omega_i \mu_i + \sum_{i=\ell+1}^k \omega_i \mu_i \quad (\text{use (4.5)}) \\ &\geq \sum_{i=1}^{\ell} \omega_i \lambda_i + \sum_{i=\ell+1}^k \omega_i \lambda_{i+n-k}, \end{aligned} \quad (4.6)$$

Since Y is arbitrary, we have

$$\min_{Y^H Y = I_k} \operatorname{tr}(\Omega Y^H \Lambda Y) \geq \sum_{i=1}^{\ell} \omega_i \lambda_i + \sum_{i=\ell+1}^k \omega_i \lambda_{i+n-k}. \quad (4.7)$$

It is not too hard to find a particular Y such that $\text{tr}(\Omega Y^H A Y)$ is equal to the right-hand side of (4.7). Therefore we have (2.3).

Suppose now all ω_i are distinct and Y_{opt} is a minimizer. We must have

$$\begin{aligned} \text{tr}(\Omega Y_{\text{opt}}^H A Y_{\text{opt}}) &= \sum_{i=1}^k \omega_i (Y_{\text{opt}}^H A Y_{\text{opt}})_{ii} \\ &= \sum_{i=1}^k \omega_i \alpha_i \end{aligned} \quad (4.8)$$

$$= \sum_{i=1}^k \omega_i \mu_i \quad (4.9)$$

$$= \sum_{i=1}^{\ell} \omega_i \lambda_i + \sum_{i=\ell+1}^k \omega_i \lambda_{i+n-k}, \quad (4.10)$$

where $\alpha_1 \leq \alpha_2 \leq \dots \leq \alpha_k$ are the reordering of $(Y_{\text{opt}}^H A Y_{\text{opt}})_{ii}$, and $\mu_1 \leq \mu_2 \leq \dots \leq \mu_k$ are the eigenvalues of $Y_{\text{opt}}^H A Y_{\text{opt}}$. For the equalities in (4.8) – (4.10) to hold, we must have for all i

$$\begin{aligned} (Y_{\text{opt}}^H A Y_{\text{opt}})_{ii} &= \alpha_i = \mu_i = \lambda_i \quad \text{for } 1 \leq i \leq \ell, \\ (Y_{\text{opt}}^H A Y_{\text{opt}})_{ii} &= \alpha_i = \mu_i = \lambda_{n-k+i} \quad \text{for } \ell+1 \leq i \leq k, \end{aligned}$$

and $Y_{\text{opt}}^H A Y_{\text{opt}} = \text{diag}(\alpha_1, \alpha_2, \dots, \alpha_k) = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_\ell, \lambda_{n-k+\ell+1}, \dots, \lambda_n)$. Now use the relation (4.4) to conclude the proof for the case when D is nonsingular.

Return to the case when D is singular, i.e., some of its eigenvalues $\omega_i = 0$. Let \widehat{Q} be as the one defined in item (b) and \widehat{Q}_\perp be the columns of Q not in \widehat{Q} . The eigen-decomposition (2.2) of D can be rewritten as

$$D = [\widehat{Q}, \widehat{Q}_\perp] \begin{bmatrix} \widehat{\Omega} & 0 \\ 0 & 0 \end{bmatrix} [\widehat{Q}, \widehat{Q}_\perp]^H,$$

where $\widehat{\Omega} = \text{diag}(\omega_1, \dots, \omega_{\ell_+}, \omega_{k-\ell_++1}, \dots, \omega_k)$ of all nonzero eigenvalues of D . It can be verified that

$$\text{tr}(D X^H A X) = \text{tr}(\widehat{\Omega} \widehat{Y}^H A \widehat{Y}), \quad (4.11)$$

where $\widehat{Y} = X \widehat{Q}$, given X . If $X^H B X = I_k$, then $Y^H B Y = \widehat{Q}^H X^H B X \widehat{Q} = \widehat{Q}^H \widehat{Q} = I_{\ell_++\ell_-}$. On the other hand, given $\widehat{Y} \in \mathbb{C}^{n \times (\ell_++\ell_-)}$ such that $Y^H B Y = I_{\ell_++\ell_-}$, we can expand it to $Y = [\widehat{Y}, \widehat{Y}_c] \in \mathbb{C}^{n \times k}$ such that $Y^H B Y = I_k$ and then let $X = Y [\widehat{Q}, \widehat{Q}_\perp]^H$ for which it can be seen that (4.11) holds. This proves

$$\min_{X^H B X = I_k} \text{tr}(D X^H A X) = \min_{\widehat{Y}^H B \widehat{Y} = I_{\ell_++\ell_-}} \text{tr}(\widehat{\Omega} \widehat{Y}^H A \widehat{Y}), \quad (4.12)$$

and a maximizer for one leads to the maximizer for the other. The right-hand side of (4.12) is a minimization problem belonging to the case of nonsingular D that we just dealt with. \square

5 Proof of Theorem 3.1

In preparing for the proof of Theorem 3.1, we may assume, without loss of generality, that $A \succeq 0$; Otherwise, noticing

$$\operatorname{tr}(DX^HAX) = \operatorname{tr}(DX^H(A - \lambda_0 B)X) + \lambda_0 \operatorname{tr}(D), \quad (5.1)$$

we may consider $\operatorname{tr}(DX^H(A - \lambda_0 B)X)$, instead.

In what follows, suppose that $A \succeq 0$.

By [17, Lemma 3.8], $A - \lambda B$ admits an eigen-decomposition as follows. There exists a nonsingular matrix $U \in \mathbb{C}^{n \times n}$ such that

$$U^H A U = \begin{array}{c} n_+ - m_0 \\ n_- - m_0 \\ 2m_0 \\ n_0 \end{array} \begin{bmatrix} n_+ - m_0 & n_- - m_0 & 2m_0 & n_0 \\ \Lambda_+ & & & \\ & -\Lambda_- & & \\ & & \Lambda_b & \\ & & & \Lambda_\infty \end{bmatrix} =: \begin{array}{c} r \\ n_0 \end{array} \begin{bmatrix} \Lambda_r & \\ & \Lambda_\infty \end{bmatrix} =: \Lambda \succeq 0, \quad (5.2a)$$

$$U^H B U = \begin{array}{c} n_+ - m_0 \\ n_- - m_0 \\ 2m_0 \\ n_0 \end{array} \begin{bmatrix} n_+ - m_0 & n_- - m_0 & 2m_0 & n_0 \\ I_{n_+ - m_0} & & & \\ & -I_{n_- - m_0} & & \\ & & J_b & \\ & & & 0 \end{bmatrix} =: \begin{array}{c} r \\ n_0 \end{array} \begin{bmatrix} J_r & \\ & J_\infty \end{bmatrix} =: J_n, \quad (5.2b)$$

where $0 \leq m_0 \leq \min\{n_+, n_-\}$, and²

$$U = \begin{array}{c} n_+ - m_0 \\ n_- - m_0 \\ 2m_0 \\ n_0 \end{array} \begin{bmatrix} U_+ & U_- & U_b & U_\infty \end{bmatrix} =: \begin{array}{c} r \\ n_0 \end{array} \begin{bmatrix} U_r & U_\infty \end{bmatrix}, \quad (5.2c)$$

$$\Lambda_+ = \operatorname{diag}(\lambda_{m_0+1}^+, \dots, \lambda_{n_+}^+), \quad \Lambda_- = \operatorname{diag}(\lambda_{n_-}^-, \dots, \lambda_{m_0+1}^-), \quad (5.2d)$$

$$\Lambda_0 = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, \quad F_2 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad (5.2e)$$

$$J_b = \operatorname{diag}(\underbrace{F_2, \dots, F_2}_{m_0}), \quad \Lambda_b = \operatorname{diag}(\underbrace{\Lambda_0, \dots, \Lambda_0}_{m_0}), \quad \Lambda_\infty \succeq 0. \quad (5.2f)$$

Both Λ in (5.2a) and J_n in (5.2b) are diagonal if $m_0 = 0$, i.e., in the absence of blocks Λ_b , J_b , and U_b . For the case, we say that $A - \lambda B$ is *diagonalizable*. It can be seen from (5.2) that the finite eigenvalues of $A - \lambda B$ are given by

$$\lambda_{n_-}^- \leq \dots \leq \lambda_{m_0+1}^- \leq \underbrace{0 = \dots = 0}_{m_0} = \underbrace{0 = \dots = 0}_{m_0} \leq \lambda_{m_0+1}^+ \leq \dots \leq \lambda_{n_+}^+,$$

which, compared to (3.5), implies $\lambda_{m_0}^- = \dots = \lambda_1^- = 0 = \lambda_1^+ = \dots = \lambda_{m_0}^+$, and they come from $\Lambda_b - \lambda J_b$.

²Recall the simplification due to (5.1). In general, Λ_0 in (5.2e) takes the form $\begin{bmatrix} 0 & \lambda_0 \\ \lambda_0 & 1 \end{bmatrix}$, and thus $\lambda_{m_0}^- = \dots = \lambda_1^- = \lambda_0 = \lambda_1^+ = \dots = \lambda_{m_0}^+$.

Letting $Y = U^{-1}XQ$, we can transform (1.7) for the case $X^H B X = I_k$ into

$$\inf_{X^H B X = I_k} \operatorname{tr}(D X^H A X) = \inf_{Y^H J_n Y = I_k} \operatorname{tr}(\Omega Y^H \Lambda Y), \quad (5.3)$$

where $k \leq n_+$. The next two lemmas will be needed in our later proof.

Lemma 5.1 ([23, Corollary 5.12]). *Let $J_n = \operatorname{diag}(I_{n_+}, -I_{n_-})$ and $n = n_+ + n_-$. Any vector set u_1, \dots, u_k satisfying $u_i^H J_n u_j = \pm \delta_{ij}$ for $i, j = 1, \dots, k$ can be complemented to a basis $\{u_1, \dots, u_n\}$ of \mathbb{C}^n satisfying $u_i^H J_n u_j = \pm \delta_{ij}$ for $i, j = 1, \dots, n$, where δ_{ij} is the Kronecker delta which is 1 for $i = j$ and 0 otherwise, and the numbers of 1 and -1 among $u_i^H J_n u_i$ for $1 \leq i \leq n$ are n_+ and n_- , respectively.*

Lemma 5.2 ([23, Example 6.3]). *Let $J_n = \operatorname{diag}(I_{n_+}, -I_{n_-})$. A matrix X satisfies $X^H J_n X = J_n$ if and only if it is of the form*

$$X = \begin{bmatrix} (I_{n_+} + W W^H)^{1/2} & W \\ W^H & (I_{n_-} + W^H W)^{1/2} \end{bmatrix} \begin{bmatrix} V_+ \\ V_- \end{bmatrix}, \quad (5.4)$$

where $V_+ \in \mathbb{C}^{n_+ \times n_+}$ and $V_- \in \mathbb{C}^{n_- \times n_-}$ are unitary, and $W \in \mathbb{C}^{n_+ \times n_-}$.

Lemma 5.1 can also be found in many classical monographs, e.g., [19, 10], and Lemma 5.2 can be found in [22, 14], where (5.4) is called a (hyperbolic) *polar decomposition* of X . Now we are ready to present our proof.

Proof of Theorem 3.1. First we deal with the case when **the matrix B is singular**, i.e.,

$n_0 > 0$ in (5.2). Partition $Y = \begin{matrix} r \\ n_0 \end{matrix} \begin{bmatrix} Y_r \\ Y_\infty \end{bmatrix}$, and then

$$\begin{aligned} \inf_{Y^H J_n Y = I_k} \operatorname{tr}(\Omega Y^H \Lambda Y) &= \inf_{Y_r^H J_r Y_r = I_k} [\operatorname{tr}(\Omega Y_r^H \Lambda_r Y_r) + \operatorname{tr}(\Omega Y_\infty^H \Lambda_\infty Y_\infty)] \\ &= \inf_{Y_r^H J_r Y_r = I_k} \operatorname{tr}(\Omega Y_r^H \Lambda_r Y_r) + \inf_{Y_\infty} \operatorname{tr}(\Omega Y_\infty^H \Lambda_\infty Y_\infty). \end{aligned} \quad (5.5)$$

We will examine the two terms in (5.5) separately. Constraint $Y^H J_n Y = I_k$ yields $Y_r^H J_r Y_r = I_k$, leaving $Y_\infty \in \mathbb{C}^{n_0 \times k}$ arbitrary. Restricting Y_∞ to a rank-1 matrix xy^H , we find

$$\begin{aligned} \inf_{Y_\infty} \operatorname{tr}(\Omega Y_\infty^H \Lambda_\infty Y_\infty) &\leq \inf_{\operatorname{rank}(Y_\infty) \leq 1} \operatorname{tr}(\Omega Y_\infty^H \Lambda_\infty Y_\infty) \\ &= \inf_{y, x} \operatorname{tr}(\Omega x y^H \Lambda_\infty y x^H) \\ &= \inf_{y, x} (x^H \Omega x)(y^H \Lambda_\infty y). \end{aligned}$$

There are three cases.

1. $\Omega \not\geq 0$ and $\Lambda_\infty \neq 0$: we have $\inf_{y, x} (x^H \Omega x)(y^H \Lambda_\infty y) = -\infty$, which leads to that the second infimum in (5.5) is $-\infty$.

2. $\Omega \not\geq 0$ and $A_\infty = 0$: we have $Y_\infty^H A_\infty Y_\infty = 0$, which leads to that the second infimum in (5.5) is 0. But our later proof for nonsingular B shows that for the case the first infimum in (5.5) is $-\infty$.
3. $\Omega \succeq 0$: we have $Y_\infty^H A_\infty Y_\infty \succeq 0$, and $\text{tr}(\Omega Y_\infty^H A_\infty Y_\infty) \geq 0$ and $\text{tr}(\Omega Y_\infty^H A_\infty Y_\infty) = 0$ for $Y_\infty = 0$, which leads to that the second infimum in (5.5) is 0.

The first infimum in (5.5): $\inf_{Y_r^H J_r Y_r = I_k} \text{tr}(\Omega Y_r^H A_r Y_r)$, falls into the case when **the matrix B is nonsingular**, which we are about to investigate.

Suppose now that B is nonsingular, i.e., $n_0 = 0$ in (5.2).

Consider first that $m_0 = 0$, namely **the pencil $A - \lambda B$ is also diagonalizable**. Then $J_n = \text{diag}(I_{n_+}, -I_{n_-})$. Since $Y^H J_n Y = I_k$, by Lemma 5.1 we can complement Y to $\tilde{Y} = [Y \ Y_c] \in \mathbb{C}^{n \times n}$ such that $\tilde{Y}^H J_n \tilde{Y} = J_n$. By Lemma 5.2, \tilde{Y} has a hyperbolic polar decomposition

$$\tilde{Y} = \begin{bmatrix} (I_{n_+} + \tilde{\Sigma} \tilde{\Sigma}^H)^{1/2} & \tilde{\Sigma} \\ \tilde{\Sigma}^H & (I_{n_-} + \tilde{\Sigma}^H \tilde{\Sigma})^{1/2} \end{bmatrix} \begin{bmatrix} \tilde{V}_+ & \\ & \tilde{V}_- \end{bmatrix}, \quad (5.6)$$

where $\tilde{V}_+ \in \mathbb{C}^{n_+ \times n_+}$ and $\tilde{V}_- \in \mathbb{C}^{n_- \times n_-}$ are unitary, and $\tilde{\Sigma} \in \mathbb{C}^{n_+ \times n_-}$. Let $\tilde{\Sigma} = W_+ \Sigma W_-^H$ be the singular value decomposition of $\tilde{\Sigma}$, where

$$\Sigma = \begin{bmatrix} \Sigma_0 \\ 0 \end{bmatrix} \text{ if } n_+ \geq n_-, \quad \text{or } \Sigma = [0 \ \Sigma_0] \text{ if } n_+ < n_-.$$

Hence plug $\tilde{\Sigma} = W_+ \Sigma W_-^H$ into (5.6) to turn $\tilde{Y} = W S V^H$, where

$$W = \begin{matrix} n_+ \\ n_- \end{matrix} \begin{bmatrix} W_+ & \\ & W_- \end{bmatrix}, \quad V = \begin{matrix} n_+ \\ n_- \end{matrix} \begin{bmatrix} V_+ & \\ & V_- \end{bmatrix} := \begin{matrix} n_+ \\ n_- \end{matrix} \begin{bmatrix} \tilde{V}_+^H W_+ & \\ & \tilde{V}_-^H W_- \end{bmatrix}, \quad (5.7a)$$

and

$$\begin{aligned} S &= \begin{bmatrix} (I_{n_+} + \Sigma \Sigma^H)^{1/2} & \Sigma \\ \Sigma^H & (I_{n_-} + \Sigma^H \Sigma)^{1/2} \end{bmatrix} \\ &= \begin{bmatrix} (I + \Sigma_0^2)^{1/2} & 0 & \Sigma_0 \\ 0 & I_{|n_+ - n_-|} & 0 \\ \Sigma_0 & 0 & (I + \Sigma_0^2)^{1/2} \end{bmatrix}. \end{aligned} \quad (5.7b)$$

Noticing $Y = \tilde{Y} I_{n;k}$ where $I_{n;k} = \begin{bmatrix} I_k \\ 0 \end{bmatrix} \in \mathbb{C}^{n \times k}$, we have from (5.3)

$$\begin{aligned} \inf_{Y^H J_n Y = I_k} \text{tr}(\Omega Y^H A Y) &= \inf_{\tilde{Y}^H J_n \tilde{Y} = J_n} \text{tr}(\Omega I_{n;k}^H \tilde{Y}^H A \tilde{Y} I_{n;k}) \\ &= \inf_{\substack{\Sigma_0 \succeq 0 \text{ diagonal} \\ V_+, V_-, W_+, W_- \text{ unitary}}} \text{tr}(I_{n;k} \Omega I_{n;k}^H V S W^H A W S V^H) \end{aligned}$$

$$= \inf_{\substack{\Sigma_0 \geq 0 \text{ diagonal} \\ V_+, V_-, W_+, W_- \text{ unitary}}} \text{tr}(\tilde{\Omega}_V S \Lambda_W S), \quad (5.8)$$

where $\tilde{\Omega}_V = V^H I_{n;k} \Omega I_{n;k}^H V$ and $\Lambda_W = W^H \Lambda W$. Use (5.7a) to see

$$\tilde{\Omega}_V = \begin{matrix} & n_+ & n_- \\ n_+ & \tilde{\Omega}_{+,V} & \\ n_- & & 0 \end{matrix}, \quad \Lambda_W = \begin{matrix} & n_+ & n_- \\ n_+ & \Lambda_{+,W} & \\ n_- & & -\Lambda_{-,W} \end{matrix},$$

where $\tilde{\Omega}_+ = \begin{matrix} & k & n_+ - k \\ k & \Omega & \\ n_+ - k & & 0 \end{matrix}$, $\tilde{\Omega}_{+,V} = V_+^H \tilde{\Omega}_+ V_+$, $\Lambda_{+,W} = W_+^H \Lambda_+ W_+$, and $\Lambda_{-,W} = W_-^H \Lambda_- W_-$. As a result, $\text{tr}(\tilde{\Omega}_V S \Lambda_W S)$ can be given by

$$\begin{aligned} & \text{tr} \left(\begin{bmatrix} \tilde{\Omega}_{+,V} & \\ & 0 \end{bmatrix} \begin{bmatrix} (I_{n_+} + \Sigma \Sigma^H)^{1/2} & \Sigma \\ \Sigma^H & (I_{n_-} + \Sigma^H \Sigma)^{1/2} \end{bmatrix} \begin{bmatrix} \Lambda_{+,W} & \\ & \Lambda_{-,W} \end{bmatrix} \begin{bmatrix} (I_{n_+} + \Sigma \Sigma^H)^{1/2} & \Sigma \\ \Sigma^H & (I_{n_-} + \Sigma^H \Sigma)^{1/2} \end{bmatrix} \right) \\ &= \text{tr} \left(\begin{bmatrix} \tilde{\Omega}_{+,V} (I_{n_+} + \Sigma \Sigma^H)^{1/2} & \tilde{\Omega}_{+,V} \Sigma \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \Lambda_{+,W} (I_{n_+} + \Sigma \Sigma^H)^{1/2} & \Lambda_{+,W} \Sigma \\ \Lambda_{-,W} \Sigma^H & \Lambda_{-,W} (I_{n_-} + \Sigma^H \Sigma)^{1/2} \end{bmatrix} \right) \\ &= \text{tr}(\tilde{\Omega}_{+,V} [(I_{n_+} + \Sigma \Sigma^H)^{1/2} \Lambda_{+,W} (I_{n_+} + \Sigma \Sigma^H)^{1/2} - \Sigma \Lambda_{-,W} \Sigma^H]). \end{aligned}$$

The last infimum in (5.8) becomes

$$\begin{aligned} & \inf_{\substack{\Sigma_0 \geq 0 \text{ diagonal} \\ V_+, V_-, W_+, W_- \text{ unitary}}} \text{tr}(\tilde{\Omega}_V S \Lambda_W S) \\ &= \inf_{\substack{\Sigma_0 \geq 0 \text{ diagonal} \\ V_+, W_+, W_- \text{ unitary}}} \text{tr}(\tilde{\Omega}_{+,V} [(I_{n_+} + \Sigma \Sigma^H)^{1/2} \Lambda_{+,W} (I_{n_+} + \Sigma \Sigma^H)^{1/2} - \Sigma \Lambda_{-,W} \Sigma^H]). \quad (5.9) \end{aligned}$$

This infimum is $-\infty$ if $\Omega \not\geq 0$. In fact, suppose $\tilde{\Omega}_+ x_+ = \omega_k x_+$ where $\omega_k < 0$, and x_+ is a unit eigenvector. Construct $\hat{V}_+ = [x_+ \ V_+, c] \in \mathbb{C}^{n_+ \times n_+}$ that is unitary. Thus, upon restrictions $V_+ = \hat{V}_+$, $W_+ = I$, $W_- = I$, $\Sigma_0 = \text{diag}(\sigma, 0, \dots, 0)$, we have by (5.9)

$$\begin{aligned} & \inf_{\substack{\Sigma_0 \geq 0 \text{ diagonal} \\ V_+, V_-, W_+, W_- \text{ unitary}}} \text{tr}(\tilde{\Omega}_V S \Lambda_W S) \leq \inf_{\sigma} \text{tr}(\hat{V}_+^H \tilde{\Omega}_+ \hat{V}_+ [\Lambda_+ + \sigma^2 (\lambda_{n_+}^+ - \lambda_{n_-}^-) e_1 e_1^H]) \\ &= \inf_{\sigma} \sigma^2 (\lambda_{n_+}^+ - \lambda_{n_-}^-) \text{tr}(\hat{V}_+^H \tilde{\Omega}_+ \hat{V}_+ e_1 e_1^H) + \text{tr}(\hat{V}_+^H \tilde{\Omega}_+ \hat{V}_+ \Lambda_+) \\ &= \inf_{\sigma} \sigma^2 (\lambda_{n_+}^+ - \lambda_{n_-}^-) (e_1^H \hat{V}_+^H \tilde{\Omega}_+ \hat{V}_+ e_1) + \text{tr}(\hat{V}_+^H \tilde{\Omega}_+ \hat{V}_+ \Lambda_+) \\ &= \inf_{\sigma} \sigma^2 (\lambda_{n_+}^+ - \lambda_{n_-}^-) (x_+^H \tilde{\Omega}_+ x_+) + \text{tr}(\hat{V}_+^H \tilde{\Omega}_+ \hat{V}_+ \Lambda_+) \\ &= \inf_{\sigma} \sigma^2 (\lambda_{n_+}^+ - \lambda_{n_-}^-) \omega_k + \text{tr}(\hat{V}_+^H \tilde{\Omega}_+ \hat{V}_+ \Lambda_+) \\ &= -\infty, \end{aligned}$$

as long as $\Lambda_+ \neq 0$ or $\Lambda_- \neq 0$, which is equivalent to $A \neq 0$, where e_1 is the first column of the identity matrix.

So far, we have shown that if $\Omega \not\geq 0, A \neq 0$, the infimum is $-\infty$, for any positive semi-definite pencil $A - \lambda B$ with B genuinely indefinite, except the case $A - \lambda B$ is not diagonalizable, to which we will return.

In what follows, suppose that $\Omega \succeq 0$. Then

$$\begin{aligned} & \inf_{\substack{\Sigma_0 \succeq 0 \text{ diagonal} \\ V_+, V_-, W_+, W_- \text{ unitary}}} \text{tr}(\tilde{\Omega}_{+,V}[(I + \Sigma \Sigma^H)^{1/2} \Lambda_{+,W}(I + \Sigma \Sigma^H)^{1/2} - \Sigma \Lambda_{-,W} \Sigma^H]) \\ &= \inf_{V_\pm, W_\pm \text{ unitary}} \inf_{\Sigma_0 \succeq 0 \text{ diagonal}} \text{tr}(\tilde{\Omega}_{+,V}[(I + \Sigma \Sigma^H)^{1/2} \Lambda_{+,W}(I + \Sigma \Sigma^H)^{1/2} - \Sigma \Lambda_{-,W} \Sigma^H]). \end{aligned} \quad (5.10)$$

Note that $\tilde{\Omega}_{+,V}, \Lambda_{+,W}, -\Lambda_{-,W}$ are positive semi-definite. In the following, we will show that the ‘‘infimum’’ in (5.10) is $\sum_{i=1}^k \omega_i \lambda_i^+$ and is attained at $\Sigma = 0$.

Firstly, since $\tilde{\Omega}_{+,V} \succeq 0$ and $\Sigma(-\Lambda_{-,W})\Sigma^H \succeq 0$, we have by Theorem 2.1

$$\text{tr}(-\tilde{\Omega}_{+,V} \Sigma \Lambda_{-,W} \Sigma^H) = \text{tr}(\Sigma(-\Lambda_{-,W})\Sigma^H) \geq 0. \quad (5.11)$$

Secondly, we claim that

$$\text{tr}(\tilde{\Omega}_{+,V}(I + \Sigma \Sigma^H)^{1/2} \Lambda_{+,W}(I + \Sigma \Sigma^H)^{1/2}) \geq \sum_{i=1}^k \omega_i \lambda_i^+. \quad (5.12)$$

Denote the eigenvalues of $(I + \Sigma \Sigma^H)^{1/2} \Lambda_{+,W}(I + \Sigma \Sigma^H)^{1/2}$ by $\delta_1 \leq \delta_2 \leq \dots \leq \delta_{n_+}$. By Ostrowski’s theorem [11, p.283], we know

$$\lambda_i^+ \leq \delta_i \leq (1 + \|\Sigma\|_2^2) \lambda_i^+ \quad \text{for } 1 \leq i \leq n_+, \quad (5.13)$$

where $\|\Sigma\|_2$ is the spectral norm of Σ . Let $I_{n_+;k} = \begin{bmatrix} I_k \\ 0 \end{bmatrix} \in \mathbb{C}^{n_+ \times k}$. We have

$$\begin{aligned} & \text{tr}(\tilde{\Omega}_{+,V}(I + \Sigma \Sigma^H)^{1/2} \Lambda_{+,W}(I + \Sigma \Sigma^H)^{1/2}) \\ &= \text{tr}(V_+^H I_{n_+;k} \Omega I_{n_+;k}^H V_+ (I + \Sigma \Sigma^H)^{1/2} \Lambda_{+,W}(I + \Sigma \Sigma^H)^{1/2}) \\ &= \text{tr}(\Omega (V_+^H I_{n_+;k})^H (I + \Sigma \Sigma^H)^{1/2} \Lambda_{+,W}(I + \Sigma \Sigma^H)^{1/2} (V_+^H I_{n_+;k})) \\ &\geq \sum_{i=1}^k \omega_i \delta_i \quad (\text{by Theorem 2.1}) \\ &\geq \sum_{i=1}^k \omega_i \lambda_i^+, \end{aligned} \quad (5.14)$$

where we have used (5.13) in the last step. This is (5.12). It is not hard to see that the equality in (5.14) is attained at $\Sigma = 0$ and appropriately chosen V_+ and W_+ . Combining (5.9), (5.10), (5.11), and (5.12) completes the proof of the theorem for the case when $A - \lambda B$ is diagonalizable.

Consider now that $m_0 > 0$, namely **the pencil $A - \lambda B$ is not diagonalizable**. We perturb $A - \lambda B$ to $(A + \varepsilon E) - \lambda B$ with $\varepsilon > 0$, where

$$E = U^{-H} \text{diag}(0, 0, E_b, 0) U^{-1}, \quad E_b = \text{diag}(\underbrace{E_0, \dots, E_0}_{m_0}), \quad E_0 = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}.$$

Clearly $(A + \varepsilon E) \succeq 0$ and the pencil is diagonalizable. Letting $\varepsilon \rightarrow 0^+$ leads to the desired result, based on the case for diagonalizable $A - \lambda B$. \square

Proof of Corollary 3.2. Partition $X = [X_+ \ X_-]$, and let $D_{\pm} = Q_{\pm} \Omega_{\pm} Q_{\pm}^H$ be the eigen-decompositions of D_+ and D_- , respectively. First consider the case that $A - \lambda B$ is diagonalizable. We have

$$\begin{aligned} \min_{X^H B X = J_k} \text{tr}(D X^H A X) &= \min_{\substack{X_{\pm}^H B X_{\pm} = \pm I_{k_{\pm}} \\ X_+^H B X_- = 0}} \text{tr}(D_+ X_+^H A X_+ + D_- X_-^H A X_-) \\ &\geq \min_{X_+^H B X_+ = I_{k_+}} \text{tr}(D_+ X_+^H A X_+) + \min_{X_-^H B X_- = -I_{k_-}} \text{tr}(D_- X_-^H A X_-) \\ &= \sum_{i=1}^{k_+} \omega_i^+ \lambda_i^+ - \sum_{i=1}^{k_-} \omega_i^- \lambda_i^-, \end{aligned}$$

of which the last equality holds by making the columns of $X_{\pm} Q_{\pm}$ be the eigenvectors of $A - \lambda B$ associated with its eigenvalues λ_i^{\pm} for $1 \leq i \leq k_{\pm}$, respectively. This proves (3.8).

For the case that $A - \lambda B$ is not diagonalizable, (3.8) also holds, by using the same technique at the end of the proof of Theorem 3.1 above. \square

6 Conclusion

Previously, the classical Ky Fan's trace minimization principle on $\min_{X^H X = I_k} \text{tr}(X^H A X)$ for a Hermitian matrix A has been extended to about

$$\begin{aligned} \min_{X^H B X = I_k} \text{tr}(X^H A X) &\quad \text{for positive definite } B, \text{ or more generally} \\ \inf_{X^H B X = J_k} \text{tr}(X^H A X) &\quad \text{for genuinely indefinite } B, \end{aligned}$$

where J_k is diagonal with diagonal entries ± 1 . The extension for a positive definite B is rather straightforward, but quite complicated when B is genuinely indefinite [14, 17]. In fact, the infimum can be $-\infty$ for the last case.

Our extensions in this paper are along the line of the Brockett cost function: $\text{tr}(D X^H A X)$ in X satisfying $X^H X = I_k$, when D is Hermitian and positive semi-definite. Specifically, we present elegant analytic solutions, in terms of eigenvalues and eigenvectors of matrix pencil $A - \lambda B$, to

$$\min_{X^H B X = I_k} \text{tr}(D X^H A X) \quad \text{for positive definite } B, \quad (6.1)$$

$$\inf_{X^H B X = J_k} \text{tr}(D X^H A X) \quad \text{for genuinely indefinite } B, \quad (6.2)$$

where D is no longer assumed to be positive semi-definite. It is shown that the infimum in (6.2) is finite if and only if D is positive semi-definite. Our analytic solutions are concise and our algebraic technique compares favorably to previously laborious effort for the case $B = I$ via the usual optimization technique [18].

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