Introducing Discrepancy Values of Matrices with Application to Bounding Norms of Commutators

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Abstract

We introduce discrepancy values, quantities inspired by the notion of the spectral spread of Hermitian matrices. We define them as the discrepancy between two consecutive Ky-Fan-like seminorms. As a result, discrepancy values share many properties with singular values and eigenvalues, yet are substantially different to merit their own study. We describe key properties of discrepancy values, and establish several tools such as representation theorems, majorization inequalities, convex formulations, etc., for working with them. As an important application, we illustrate the role of discrepancy values in deriving tight bounds on the norms of commutators.

1 Introduction

Eigenvalues and singular values are fundamental objects associated with linear transformations; their importance across all of science and engineering hardly needs an introduction [12]. A lesser-known, but important quantity based on eigenvalues is spectral spread, defined for an $n \times n$ Hermitian matrix $A$ as

$$\text{spr}^+(A) := (\lambda_i(A) - \lambda_{n-i+1}(A))_{i=1,2,\ldots,\lfloor n/2 \rfloor},$$

where the eigenvalues $\lambda_i$ are ordered decreasingly. The spectral spread was introduced in [14] as a measure of the dispersion of the eigenvalues of Hermitian matrices; it is a vector extension of the better known spread of Hermitian operators [7], which is equal to the greatest eigenvalue minus the smallest eigenvalue of the Hermitian matrix. Spectral spread derives its importance from a class of useful inequalities it satisfies, see e.g., [16, 17, 18]. But its definition is limited to Hermitian matrices and for general square (complex) matrices there is no clear analog.

One could define the spectral spread for the general matrix $A$ as an extension of the notion of the spread of square matrices [19]: $\text{spd}(A) := \max_{i,j} |\lambda_i(A) - \lambda_j(A)|$. After finding the spread, we repeatedly remove the two indices that maximize the spread, find the spread of the remaining eigenvalues, and insert it in a vector. When $A$ is a Hermitian matrix, the obtained vector is equivalent to 1.1. However, for non-Hermitian matrices, this quantity does not enjoy many nice properties that the spectral spread of a Hermitian function possesses. Therefore, we need to find an alternative analog that satisfies all the nice properties of the spectral spread.

We motivate, propose, and analyze an analog that is defined for general square matrices: namely, discrepancy values, which we define as the discrepancy between consecutive Ky-Fan-like seminorms (see Def. 3.1). We will show that discrepancy values can be essentially thought of as two copies of spectral spread. Alternatively, they can also be thought of as a (vector-valued) cost of approximating linear operators via scalar multiples of the identity, a topic of some importance—see e.g., [8, 20, 2].

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1.1 Outline of paper and main contributions

We first define discrepancy values (Definition 3.1) in Section 3; next, we elucidate their connections with Ky-Fan norms (Theorems 4.1, 4.3), singular values (Proposition 4.7, and inequality (4.15)), and principal angles between subspaces (Theorem 4.21) in Section 4. Through several results we explore invariances and majorization inequalities satisfied by discrepancy values while underscoring their analogy with spectral spread (see e.g., Corollary 4.18).

In Section 5 we apply our results on discrepancy values to study commutators, a subject that has received extensive interest [13, 9, 11, 15, 22, 21, 20]. Specifically, we obtain tight bounds on norms of commutators using discrepancy values (Corollaries 5.2, 5.6), and determine when two Hermitian matrices with fixed eigenvalues are maximally non-commutative (Theorem 5.12). Thereafter, in Section 6, we propose approaches for calculating discrepancy values via semi-definite programming (see e.g., Equation (6.5)). We conclude with a discussion about the extension of our results to compact operators on Hilbert spaces, and with a conjecture that posits a stronger majorization inequality involving commutators and discrepancy values (Conjecture 7.1).

2 Notation and Preliminaries

Bold letters denote vectors and matrices, both of which are assumed to be complex unless specified otherwise. The vectors $\sigma(A)$ and $\lambda(A)$ respectively denote singular values and eigenvalues of $A$. We assume that the singular values of any matrix, and eigenvalues of Hermitian matrices are ordered decreasingly. Let $I_n$ be the $n \times n$ identity; and $J_n$ the exchange matrix that has ones on its antidiagonal and zeros elsewhere; $1_k$ is a vector with $k$ ones, followed by $n-k$ zeros. For $x \in \mathbb{R}^n$, $x^\dagger$ is the vector with coordinates arranged nonincreasingly. The Schatten norm of an $n \times n$ matrix $A$ is defined by $\|A\|_p := (\sum_{i=1}^n \sigma_i^p(A))^{1/p}$, for $p \geq 1$, while its Ky-Fan norms are defined as $\|A\|_{(k)} := \sum_{i=1}^k \sigma_i(A)$, for $k = 1, \ldots, n$. Ky-Fan norms enjoy the following maximal formulation:

$$\|A\|_{(k)} = \max \left\{ \left| \sum_{i=1}^k \langle Ax_i, y_i \rangle \right| : \{x_i\}_{j=1}^k \text{ o.n., } \{y_i\}_{j=1}^k \text{ o.n.} \right\},$$

(2.1)

where `o.n.' means that the set of vectors $\{x_i\}_{j=1}^k$ is orthonormal.

An $n \times r$ matrix $A$ is called an isometry if $A^*A = I_r$, for some $r \leq n$, and a partial isometry of order $k \leq n = r$ if $A = BC^*$ where $B \in \mathbb{C}^n \times k$ and $C \in \mathbb{C}^n \times k$ are both isometries. Recall that a norm $\| \cdot \|$ is unitarily invariant if $\|A\| = \|UAV\|$ for all unitary matrices $U, V$. In the sequel, we use $\| \cdot \|$ to denote such norms. Both Schatten and Ky-Fan norms are unitarily invariant.

Finally, recall that for $x, y \in \mathbb{R}^n$, we say that $x$ is weakly majorized by $y$, denoted $x \prec_w y$, if the following set of inequalities hold:

$$\sum_{i=1}^k x_i^j \leq \sum_{i=1}^k y_i^j, \quad \text{for } k = 1, \ldots, n.$$

Moreover, $y$ majorizes $x$, denoted $x \prec y$, when the equality $\sum_{i=1}^n x_i = \sum_{i=1}^n y_i$ also holds. Many fundamental majorization inequalities are known for eigenvalues and singular values; for instance for two square matrices $A$ and $B$ it is known that

$$\sigma(A + B) \prec_w \sigma(A) + \sigma(B), \quad \text{and} \quad \sigma(AB) \prec_w \sigma(A)\sigma(B),$$

where $\sigma(A)\sigma(B)$ is the entrywise product of the vectors of the singular values. We refer the readers to [1, 3, 5, 10, 12, 24], for a deeper study of these topics.
3 Definition of discrepancy values

Now we are ready to introduce discrepancy values. We need to first introduce a new class of seminorms that are obtained via an innocuous-looking modification to the Ky-Fan norm (2.1): namely, an additional partial-orthogonality constraint \( \sum_j \langle x_j, y_j \rangle = 0 \). Why we consider the constraint in (3.1), and what ramifications it has will unravel in the subsequent sections.

**Definition 3.1.** Let \( A \in \mathbb{C}^{n \times n} \), we define its \( k \)-th discrepancy seminorm as

\[
\|A\|_{\delta(k)}^\delta := \max_{\{x_i\}_{i=1}^k \text{ o.n.}} \left| \sum_{i=1}^k \langle Ax_i, y_i \rangle \right|, \text{ s.t. } \sum_{j=1}^k \langle x_j, y_j \rangle = 0, \text{ for } 1 \leq k \leq n. \tag{3.1}
\]

Further, let \( \|A\|_{\delta,(0)} = 0 \). Using (3.1) we define the \( k \)-th discrepancy value of \( A \) as

\[
\delta_k(A) := \|A\|_{\delta,(k)}^\delta - \|A\|_{\delta,(k-1)}^\delta. \tag{3.2}
\]

Clearly, \( \|A\|_{\delta,(k)}^\delta \leq \|A\|_{\delta,(k)} \); equivalently, writing \( \delta(A) := (\delta_1(A), \ldots, \delta_n(A)) \) (decreasingly sorted), we obtain \( \delta(A) \prec_s \sigma(A) \). Moreover, \( \sigma_1(A) \geq \delta_1(A) \geq \delta_2(A) \geq \cdots \geq \delta_n(A) \geq 0 \). But unlike singular values, there may not exist two sets of orthonormal vectors \( \{x_i\} \) and \( \{y_i\} \) such that \( x_i \perp y_i \) and \( \delta_i(A) = |\langle Ax_i, y_i \rangle| \). Nevertheless, we will call the vectors \( x_i \) and \( y_i \) in (3.1), the left and right discrepancy vectors.

Before proceeding to our main results, let us note down more compact forms for the discrepancy seminorms and Ky-Fan norms.

**Proposition 3.2.** For an arbitrary \( n \times n \) matrix \( A \), we have the following:

\[
\|A\|_{(k)} = \max_{M \in P_k(n)} \text{ Re tr}(AM), \tag{3.3}
\]

\[
\|A\|_{\delta,(k)}^\delta = \max_{M \in \mathcal{P}_k(n)} \text{ Re tr}(AM), \tag{3.4}
\]

where \( \mathcal{P}_k(n) := \{ X \in \mathbb{C}^{n \times n} : X = VU^* U^* U = I_k, V^* V = I_k \} \) is the set of \( n \times n \) partial isometries of rank \( k \), and \( \mathcal{P}^{(0)}_k(n) := \{ X \in \mathbb{C}^{n \times n} : X = VU^* U^* V = I_k, \text{ tr}(X) = 0 \} \) is the set of \( n \times n \) traceless partial isometries of rank \( k \).

**Proof.** Given a positive integer \( k \leq n \), the set

\[
\left\{ \sum_{j=1}^k \langle Ax_i, y_i \rangle : \{x_j\}_{j=1}^k \text{ o.n.}, \{y_j\}_{j=1}^k \text{ o.n.}, \sum_{j=1}^k \langle x_j, y_j \rangle = 0 \right\}
\]

forms a circle in the complex plane whose center is located at the origin. To observe this fact, note that we can multiply each vector in the set \( \{y_j\}_{j=1}^k \) with \( e^{i\theta} \) and do not violate the conditions of the set while rotating the value of \( \sum_{j=1}^k \langle Ax_i, y_i \rangle \) arbitrarily in the complex plane. Therefore, we can replace the modulus in the definitions of \( \|\cdot\|_{(k)} \) and \( \|\cdot\|_{\delta,(k)}^\delta \) with the real part of the complex number. Thus,

\[
\|A\|_{(k)} = \max_{\|x_i\| = \|y_i\| = 1, \sum_{j=1}^k \langle x_j, y_j \rangle = 0} \text{ Re } \sum_{i=1}^k \langle Ax_i, y_i \rangle = \max_{U^* U = I_k, V^* V = I_k} \text{ Re tr}(AVU^*),
\]

\[
\|A\|_{\delta,(k)}^\delta = \max_{\|x_i\| = \|y_i\| = 1, \sum_{j=1}^k \langle x_j, y_j \rangle = 0} \text{ Re } \sum_{i=1}^k \langle Ax_i, y_i \rangle = \max_{U^* U = I_k, V^* V = I_k, \text{ tr}(U^* V) = 0} \text{ Re tr}(AVU^*).
\]

Setting \( M = VU^* \) we obtain the desired result. \( \square \)
From the definition of discrepancy values, the following invariances are immediate.

**Proposition 3.3** (invariances of discrepancy). Let \( A \in \mathbb{C}^{n \times n} \). Discrepancy values display the following invariances:

- (Unitary conjugation): \( \delta(UAU^*) = \delta(A) \), for all unitary matrix \( U \).
- (Conjugate transpose): \( \delta(A^*) = \delta(A) \).
- (Phase): \( \delta(e^{i\theta}A) = \delta(A) \), for all \( \theta \in [0, 2\pi) \).
- (Shift): \( \delta(A - \alpha I_n) = \delta(A) \), for all \( \alpha \in \mathbb{C} \).

## 4 Main results

In this section, we study fundamental properties of discrepancy values that should be of broader interest. We first take a closer look at discrepancy seminorms and their relation to Ky-Fan norms in Section 4.1. Then, in Section 4.2 we uncover the precise relation between discrepancy values and spectral spread of Hermitian matrices. In Section 4.3, we discuss special classes of matrices that have zero-one discrepancy values, and in analogy with singular values, we also advance the notion of “discrepancy rank.” Basic majorization inequalities and a generalization to direct sums of matrices are covered in Sections 4.4 and 4.5, respectively.

### 4.1 Discrepancy seminorms and Ky-Fan norms

We develop a more thorough connection between discrepancy seminorms and Ky-Fan norms. We will need the following simple observation.

**Lemma 1.** For any two \( n \times m \) isometries \( U, V \), where \( n \geq m \), there exists a \( n \times n \) unitary matrix \( Q \) such that \( QU = V \).

**Proof.** Immediate upon noting that we can write \( U = R_n \times n \left[ \begin{array}{c} I_m \\ 0_{(n-m) \times m} \end{array} \right] \), for an appropriate unitary matrix \( R \). \( \square \)

The first main result of this section is Theorem 4.1 that shows how Ky-Fan norms can be realized via maximal discrepancy seminorms of unitarily transformed matrices.

**Theorem 4.1.** For the square matrix \( A \), we have

\[
\|A\|_{(k)} = \max_{Q \in U(n)} \|AQ\|_{(k)},
\]

where \( U(n) \) denotes the set of \( n \times n \) unitary matrices.

**Proof.** We want to show that \( \max_{Q \in U(n)} \sum_{i=1}^{k} \delta_i(AQ) = \|A\|_{(k)} \). Trivially, \( \delta(AQ) \prec_w \sigma(A) \) for any unitary \( Q \); i.e., \( \max_{Q \in U(n)} \sum_{i=1}^{k} \delta_i(AQ) \leq \|A\|_{(k)} \). Using the variational formula (3.4) of discrepancy seminorms and noting that \( \delta(R^*AR) = \delta(A) \) for any unitary matrix \( R \), we see that the RHS of (4.1) equals

\[
\max_{Q,R \in U(n)} \max_{U^*U = I_k, V^*V = I_k} \Re \text{tr} \left( A(QV)(RU)^* \right). \tag{4.2}
\]
Also, by the variational formula for Ky-Fan norms, the LHS of (4.1) is
\[
\max_{M^* M = I_k \atop N^* N = I_k} \Re \text{tr}(ANM^*). \tag{4.3}
\]
Assume that the optimum of (4.3) occurs at \( \hat{M} \) and \( \hat{N} \). By Lemma 1, for isometries \( U \) and \( V \) there exist \( Q, R \in U(n) \) such that \( \hat{N} = QV \) and \( \hat{M} = RU \). Hence, \( \max_{Q \in U(n)} \sum_{i=1}^{k} \delta_i(AQ) \geq \|A\|_{(k)} \), which concludes the proof.

Proposition 3.2 provides a maximal representation for discrepancy seminorms. Now we want to provide a minimal representation. This dual representation reveals another aspect of the connection between discrepancy seminorms and Ky-Fan norms. Before mentioning the relationship, let us state two results.

**Lemma 2.** The set \( P_k(n) \) is the set of extreme points of the compact convex set \( \text{Conv}(P_k(n)) := \{ X \in \mathbb{C}^{n \times n} : \|X\|_{(1)} \leq 1, \|X\|_{(n)} \leq k \} \). Similarly, the set \( P^0_k(n) \) is the set of extreme points of the compact convex set \( \text{Conv}(P^0_k(n)) := \{ X \in \mathbb{C}^{n \times n} : \|X\|_{(1)} \leq 1, \|X\|_{(n)} \leq k, \text{tr}(X) = 0 \} \).

Lemma 2, together with representations (3.3) and (3.4) implies that
\[
\|A\|_{(k)} = \max_{M \in \text{Conv}(P_k(n))} \Re \text{tr}(AM) \tag{4.4}
\]
\[
\|A\|_{(k)}^\delta = \max_{M \in \text{Conv}(P^0_k(n))} \Re \text{tr}(AM), \tag{4.5}
\]
since the cost is linear and we replaced the sets \( P_k(n), P^0_k(n) \) with their convex hulls.

**Theorem 4.2** (Sion’s minimax theorem). Let \( X \) be a compact convex subset of a linear topological space and \( Y \) a convex subset of a linear topological space. If \( f \) is a real-valued function on \( X \times Y \) such that \( f(x, \cdot) \) is upper semicontinuous and quasi-convex on \( Y \) for any \( x \in X \) and \( f(\cdot, y) \) is lower semicontinuous and quasi-convex on \( X \) for any \( y \in Y \), then we have
\[
\min_{x \in X} \sup_{y \in Y} f(x, y) = \sup_{y \in Y} \min_{x \in X} f(x, y). \tag{4.6}
\]

The announced minimal representation is noted in Theorem 4.3.

**Theorem 4.3.** Let \( A \in \mathbb{C}^{n \times n} \). For \( 1 \leq k \leq n \), we have the variational formula
\[
\|A\|_{(k)}^\delta = \min_{\alpha \in \mathbb{C}} \|A - \alpha I_n\|_{(k)}. \tag{4.7}
\]

**Proof.** Using representation (4.5) for the discrepancy seminorm, we have
\[
\|A\|_{(k)}^\delta = \max_{M \in \text{Conv}(P^0_k(n))} \Re \text{tr}(AM) = \max_{M \in \text{Conv}(P_k(n))} \min_{\alpha \in \mathbb{C}} \Re \text{tr}(AM) - \Re \text{tr}(M) = \min_{\alpha \in \mathbb{C}} \max_{M \in \text{Conv}(P_k(n))} \Re \text{tr}((A - \alpha I_n)M) = \min_{\alpha \in \mathbb{C}} \|A - \alpha I_n\|_{(k)}, \tag{4.8}
\]
where the second equality follows since \( \text{Conv}(P^0_k(n)) \) is the intersection of the traceless matrices with \( \text{Conv}(P_k(n)) \). The third equality follows by Sion’s minimax theorem, while the last equality follows from the maximal representation (4.4). \qed
In words, Theorem 4.3 shows that discrepancy values can be thought of as a vector-valued extension of the (spectral norm) distance of a linear operator to a scalar multiple of the identity; i.e., a vector-extension of the following observation

$$\delta_1(A) = \min_{\alpha \in \mathbb{C}} \sigma_1(A - \alpha I_n) = \max_{\|x\| = \|y\| = 1} |\langle Ax, y \rangle|.$$  \hspace{1cm} (4.9)

The problem of projecting a linear operator onto the subspace of scalar linear operators has been investigated in the literature (see [2, 8]). Finally, the two relations between discrepancy seminorms and Ky-Fan norms imply the following identity.

**Corollary 4.4.** Using Lemma 4.1 and Theorem 4.3, we have the equality

$$\max_{U \in U(n)} \min_{\alpha \in \mathbb{C}} \|A - \alpha U\|_{(k)} = \|A\|_{(k)}.$$  \hspace{1cm} (4.10)

### 4.2 Discrepancy values for Hermitian matrices

Now we can illustrate the connection between discrepancy values and the spectral spread of Hermitian matrices. When \(A\) is Hermitian, we can solve the optimization problem (4.7) in closed form and get

$$\delta_{2k-1}(A) = \delta_{2k}(A) = |\lambda_k(A) - \lambda_{n-k+1}(A)|/2 \text{ for } k = 1, \ldots, [n/2].$$  \hspace{1cm} (4.11)

Moreover, if \(n\) is odd, then \(\delta_n(A)\) would be zero. On the other hand, in Def. 3.1, for a Hermitian matrix with eigenvectors \(v_1, v_2, \ldots, v_n\) corresponding to the non-increasing eigenvalues, we can check that the vectors \(x_{2k-1} = (-v_k + v_{n-k+1})/\sqrt{2}\) and \(y_{2k-1} = (-v_k - v_{n-k+1})/\sqrt{2}\) for the odd terms, and \(x_{2k} = y_{2k-1}\) and \(y_{2k} = x_{2k-1}\) for the even terms are maximizers in problem 3.1. More compactly, for a Hermitian matrix \(A\) we have the (vector) equality

$$\delta(A) = \frac{|\lambda_k(A) - \lambda_{k}'(A)|}{2}. \hspace{1cm} (4.12)$$

**Remark 4.5.** The discrepancy value of Hermitian matrices is invariant w.r.t. a particular transformation. We call this invariance looseness or slackness. It states that if we fix the outer eigenvalues, we can shift the inner eigenvalues, and the discrepancy values remain the same so long as we do not cross the fixed eigenvalues. We are going to exploit this property later in this paper.

The interlacing property for Hermitian matrices implies the stability of discrepancy values under perturbation.

**Proposition 4.6** (Interlacing theorem). Let \(A\) be a Hermitian matrix of order \(n\), and \(B\) be a principal submatrix of \(A\). Using the Cauchy interlacing theorem we obtain \(\delta_1(A) = \delta_2(A) \geq \delta_1(B) = \delta_2(B) \geq \delta_3(A) = \delta_4(A) \geq \delta_3(B) = \delta_4(B) \geq \ldots\

Finally, we note the following: for an \(n \times n\) Hermitian matrix \(A\), when \(n\) is even, the spectral spread of the direct sum \(A \oplus A\) is related to the discrepancy values via

$$\delta(A) = \text{spr}^+(A \oplus A)/2,$$  \hspace{1cm} (4.13)

while for odd \(n\), \(\delta(A)\) has an extra zero at the end of the vector \(\text{spr}^+(A \oplus A)/2\).

### 4.3 Important classes of matrices based on their discrepancy values

We know that unitary matrices have unit singular values, while partial isometries have zero and one as their singular values, and both matrices play an important role in the characterization of singular values. We believe that to understand discrepancy values better, we need to understand the equivalent classes of matrices associated with them. We explore below the structure of matrices with unit discrepancy values and discuss matrices with or zero and one discrepancy values. Before that, we need some tools.
Proposition 4.7. For $A \in \mathbb{C}^{n \times n}$, we have $\delta(A) = \sigma(A)$ if and only if it has the singular value decomposition $A = U\Sigma V^*$, with $U, V \in \mathbb{U}(n)$ and $\text{Diag}(U^*V) = 0$; i.e., $\langle u_i, v_i \rangle = 0$ for $i = 1, \ldots, n$.

Proof. The “if” part follows trivially by the definition of discrepancy values. We first prove the “only if” for full-rank matrices with unique singular values; in this case, the singular vectors are unique up to multiplication by $e^{i\theta}$. We then have

$$\max_{\|x_{11}\|=\|y_{11}\|=1} |\langle Ax_{11}, y_{11} \rangle| = \max_{\|u_{11}\|=\|v_{11}\|=1} |\langle Au_{11}, v_{11} \rangle|.$$  

Therefore, it must be the case that the optimizers $u_{11}^* = e^{i\theta}x_{11}$ and $v_{11}^* = e^{i\phi}y_{11}$; i.e., $\langle u_{11}, v_{11}^* \rangle = 0$. Next, we have the equality

$$\max_{\|x_{12}\|=\|y_{12}\|=1} \left| \langle Ax_{12}, y_{12} \rangle + \langle Ax_{22}, y_{22} \rangle \right| = \max_{\|u_{12}\|=\|v_{12}\|=1} \left| \langle Au_{12}, v_{12} \rangle + \langle Au_{22}, v_{22} \rangle \right|,$$

which implies that $\langle u_{12}^*, v_{12}^* \rangle + \langle u_{22}^*, v_{22}^* \rangle = 0$. On the other hand, we know that $u_{12}^* = e^{i\phi}u_{11}$ and $v_{12}^* = e^{i\phi}v_{11}$; thus $\langle u_{22}, v_{22}^* \rangle = 0$. The general result follows inductively. For matrices with repeated singular values or zero singular values, not all possible singular value decompositions of $A$ have the property that $\text{Diag}(U^*V) = 0$, but a decomposition with such property belongs to the set of possible singular value decompositions of that matrix. 

Remark 4.8. In other words, matrices of the form $A = \sum_{i=1}^n \delta_i X_i + \alpha I_n$ have discrepancy values equal to $\delta_i$, where $\delta_i \geq 0$, and when $X_i$ are nilpotent rank-1 isometries and mutually orthogonal; i.e., $\langle X_i, X_j \rangle = 0$.

Corollary 4.9. If $A = U\Sigma V^* + \alpha I_n$, where $U$ and $V$ are unitary matrices with $\text{tr}(U^*V) = 0$, then $\delta_1(A) = 1$.

Proof. It follows by the fact that there exists a unitary matrix $Q$ such that for $U = UQ$ and $V = VQ$ we have $\text{Diag}(U^*V) = 0$ and $A = U\Sigma V^* + \alpha I_n$.

Corollary 4.10. The singular values and the discrepancy values of matrices of the form $B = QAQ^*$, where $A$ is an antidiagonal matrix and $Q$ unitary, are equal to the absolute value of the anti-diagonal entries of $A$.

We next note a concrete setting where discrepancy values equal singular values.

Proposition 4.11. For a $2n \times 2n$ Hamiltonian matrix $H$, we have

$$\delta(H) = \sigma(H).$$

Proof. We know that any Hamiltonian matrix can be represented as the multiplication of $J = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}$ and a symmetric matrix. Thus, we have $H = JQAQ^*$. Let $A = \Sigma D$ where $D$ is just a diagonal matrix with $\pm 1$ entries. In the singular value decomposition of $H = U\Sigma V^*$ we have $\mu = JQ$ and $V = QD$. To show that $\text{Diag}(DQ^* JQ) = 0$ one only needs to prove $\text{Diag}(Q^* JQ) = 0$, which is immediate after recognizing that $\delta(Q^* JQ) = \sigma(Q^* JQ)$.

Remark 4.12. The same argument can be used to prove that the singular and discrepancy values of the multiplication of $J$ and any normal matrix are equal.

Let us adopt the notation $\Psi(n)$ to refer to the set of $n \times n$ matrices with unit discrepancy values. Theorem 4.13 states that this class is equivalent to the scalar shifts of traceless unitary matrices.

Theorem 4.13. A square matrix belongs to $\Psi(n)$ if and only if it has the form $M - \alpha I_n$, where $M$ is unitary and $\text{tr} M = 0$, while $\alpha$ an arbitrary complex number.
Proof. We already proved in Corollary 4.9 that \( M - \alpha I_n \in \Psi(n) \) when \( M \) is a traceless unitary matrix. By the definition of discrepancy values, there exists \( \hat{\alpha} \) such that \( \sigma_1(A - \hat{\alpha} I_n) = \delta_1(A) = 1 \), and \( \sigma_1(A - \hat{\alpha} I_n) + \sigma_2(A - \hat{\alpha} I_n) \geq \delta_1(A) + \delta_2(A) = 2 \). Therefore, \( \sigma_2(A - \hat{\alpha} I_n) \geq 1 \), but we assumed that \( \sigma_2(A - \hat{\alpha} I_n) \leq \delta_1(A - \hat{\alpha} I_n) \); hence \( \sigma_2(A - \hat{\alpha} I_n) = \delta_2(A) = 1 \). Using the same argument we can show that \( \sigma_k(A - \hat{\alpha} I_n) = \delta_k(A) = 1 \), for \( 1 \leq k \leq n \). Finally, by proposition 4.7 we know that matrix \( A - \hat{\alpha} I_n \) has a decomposition \( UV^* \) where \( \text{Diag}(U^*V) = 0 \).

In other words, a matrix is in \( \Psi(n) \) iff for some \( \alpha \) its eigenvalues satisfy \( |\lambda_i - \alpha| = 1 \) and \( \sum_{i=1}^{n} |\lambda_i| = 0 \), which always has roots for \( n \geq 2 \). Thus, \( \Psi(n) \) is not empty.

Before studying the class of matrices with zero or one discrepancy values, let us define the notion of \textit{discrepancy-rank}.

**Definition 4.14.** Let \( A \in \mathbb{C}^{n \times n} \). We define \textit{discrepancy-rank} of \( A \) as

\[
\delta^k(A) := \text{the number of non-zero entries of } \delta(A).
\]

One can verify that \( \delta^k(A) = r(A - \hat{\alpha} I_n) \) where \( \hat{\alpha} = \arg\min_{\alpha \in \mathbb{C}} \|A - \alpha I_n\|_{(n)} \). We can also see that \( \delta^k(A) = 0 \) iff \( A = \alpha I_n \) for a complex number \( \alpha \). And \( \delta^k(A) = 1 \) iff \( A = \beta uv^* + \alpha I_n \) for some (complex) \( \alpha \) and \( \beta \), and orthogonal unit vectors \( u \) and \( v \).

**Definition 4.15.** Let \( \Psi_k(n) \) denote the set of \( n \times n \) matrices with discrepancy-rank \( k \) with unit non-zero discrepancy values (i.e. \( \delta_i = 1 \) for \( i = 1, \ldots, k \)).

Now we want to explore the relation between \( \Psi_k(n) \) and the set \( \mathcal{P}_k^0(n) \). Note that \( \mathcal{P}_k^0(n) \neq \Psi_k(n) \); for instance, consider \( M = \text{Diag}([1, 3, 4]) \) which belongs to \( \Psi_2(3) \) but not to \( \mathcal{P}_2^0(3) \). However, we can state the following inclusion:

**Lemma 3.** \( \mathcal{P}_k^0(n) \subset \Psi_k(n) \).

**Proof.** Consider a matrix \( M \in \mathcal{P}_k^0(n) \). Observe that \( \|M\|_{\delta}^k = k \) by using the left and right singular vectors of \( M \) as the vectors \( x \) and \( y \) in (3.1). On the other hand, we know that \( \delta(M) \prec_w 1_k \). Therefore, the only possibility is that \( \delta(M) = 1_k \).

### 4.4 Basic majorization inequalities

A plethora of majorization inequalities for singular values exists in the literature. In this part, we investigate some majorization results for discrepancy values. We also see that the discrepancy values satisfy many of the majorization bounds known for the spectral spread of Hermitian matrices, which underscores our claim that discrepancy values are a true generalization of spectral spread. First, let us state two trivial inequalities.

**Proposition 4.16.** For \( n \times n \) matrices \( A \) and \( B \), one has

1. \( |\delta(A) - \delta(B)| \prec_w \delta(A \pm B) \prec_w \delta(A) + \delta(B) \).
2. \( \delta(A) \prec_w \sigma(A) \).

Now let us look at some non-trivial inequalities. The first one is about the pinching of matrices (see e.g., Problem II.5.5 in [5] for the definition). A similar inequality holds for singular values, see [7].

---

1. or any scalar shift of it.
Proposition 4.17. Let $A$ be any square matrix and $C(A)$ denote a pinching, and $L(A) = A - C(A)$ an anti-pinching of this matrix. Then, we have

$$\delta(C(A)) \prec_w \delta(A)$$
$$\delta(L(A)) \prec_w \delta(A).$$

Proof. We only prove the first inequality; the second one is similar. Since $C(A)$ is a pinching, there exists a unitary $U$ (see [7]) such that $C(A) = \frac{1}{2}(A + UAU^*).$ Thus,

$$\sum_{i=1}^{k} \delta_i(C(A)) = \frac{1}{2} \sum_{i=1}^{k} \delta_i(A + UAU^*) \leq \sum_{i=1}^{k} \delta_i(A). \quad (4.13)$$

Corollary 4.18. For any $n \times n$ matrices $A_1, A_2, A_3, A_4$, we have

$$\sigma\left(\begin{bmatrix} 0 & A_2 \\ A_1 & 0 \end{bmatrix}\right) = \delta\left(\begin{bmatrix} 0 & A_2 \\ A_1 & 0 \end{bmatrix}\right) \prec_w \delta\left(\begin{bmatrix} A_3 & A_2 \\ A_1 & A_4 \end{bmatrix}\right).$$

Proof. Assume that $A_1$ and $A_2$ have the singular value decompositions $A_1 = U_1 \Sigma_1 V_1^*$ and $A_2 = U_2 \Sigma_2 V_2^*$, then we have

$$\begin{bmatrix} 0 & A_2 \\ A_1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & U_2 \\ U_1 & 0 \end{bmatrix} \Sigma_1 \begin{bmatrix} 0 & 0 \\ 0 & \Sigma_2 \end{bmatrix} \begin{bmatrix} V_1 & 0 \\ 0 & V_2 \end{bmatrix}^*$$

Note that $Q$ and $R$ are unitary matrices and $\text{Diag}(Q^*R) = 0$; therefore by Proposition 4.7 we have the equality. The weak majorization follows by Proposition 4.17.

Remark 4.19. One can recover the non-commutative AM-GM inequality [6] from Corollary 4.18. This corollary implies that for any square matrices $A$ and $B$,

$$\sigma\left(\begin{bmatrix} 0 & AB^* \\ BA^* & 0 \end{bmatrix}\right) \prec_w \delta\left(\begin{bmatrix} A & 0 \\ B & 0 \end{bmatrix}\right).$$

Using the fact that for $2n \times 2n$ positive definite matrix $X$ we have $2\delta_{2i-1}(X) \leq \sigma_i(X)$, for $i = 1, \ldots, n$, we get the inequality

$$2\sigma_{2i-1}\left(\begin{bmatrix} 0 & AB^* \\ BA^* & 0 \end{bmatrix}\right) \leq \sigma_i\left(\begin{bmatrix} A^*A + B^*B & 0 \\ 0 & 0 \end{bmatrix}\right),$$

which implies that for $i = 1, \ldots, n$,

$$2\sigma_i(AB^*) \leq \sigma_i(A^*A + B^*B).$$

Corollary 4.18 improves and generalizes Inequality (8) in [17] that studies spectral spread. Moreover, it also implies that

Corollary 4.20. For an isometry $S \in \mathbb{C}^{n \times k}$ and arbitrary matrix $X$ we have

$$\sigma(S^*XS) \prec_w \delta(X)|_{\min(k,n-k)}$$

where $S_\perp$ is an isometry whose range is orthogonal to the range of $S$. 

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Using Corollary 4.20 we can provide an easy proof to a known upper-bound on the principal angles \( \Theta(S, T) \) between two subspaces \( S \) and \( T \). For a detailed discussion regarding the principal angles between subspaces, we refer the readers to [18], in which this upper bound was first discovered.

**Theorem 4.21** (Theorem 2.15 in [18]). Given the Hermitian matrix \( X \), the principal angles between \( k \)-dimensional subspaces \( S \subset \mathbb{C}^n \) and \( T = e^{iX}S \subset \mathbb{C}^n \) satisfy

\[
\Theta(S, T) \approx_w \delta(X)_{\min(k,n-k)},
\]

where \( \delta(X)_{\vert k} \) denotes a \( k \)-dimensional vector with the first \( k \) entries of \( \delta(X) \).

**Proof.** Define \( T(t) = e^{itX}S \). We have \( T(0) = S \) and \( T(1) = T \). By the triangle inequality for principal angles we have

\[
\Theta(S, T) \approx_w \sum_{j=0}^{m-1} \Theta\left( T\left( \frac{j}{m} \right), T\left( \frac{j+1}{m} \right) \right) = \sum_{j=0}^{m-1} \arcsin \left( \sigma(S^*e^{iX}S_\perp) \right)
\]

\[
= m \arcsin \left( \sigma(S^*e^{iX}S_\perp) \right) \quad (4.14)
\]

\[
\rightarrow \sigma(S^*XS_\perp)
\]

\[
\approx_w \delta(X)_{\min(k,n-k)},
\]

where the last majorization follows by Corollary 4.20. The limit can be justified by L’Hospital’s rule and the continuity of singular values. \( \square \)

Finally, we propose two inequalities that shed further light on the relationship between discrepancy values and singular values.

**Lemma 4.** For the \( n \times n \) Hermitian matrix \( X \) we have the majorization

\[
\delta(e^{iX}) \approx_w \sigma(X).
\]

**Proof.** We first show that \( \delta(e^{iX}) \approx_w \int_0^1 \delta(iXe^{itX})dt \). Then, using the fact that \( \delta(e^{itX}) \approx_w \sigma(X) \) we have \( \delta(e^{iX}) \approx_w \int_0^1 \sigma(X)dt = \sigma(X) \). To prove the former inequality, first define \( f(t) = e^{itX} \). Then, consider the series

\[
e^{iX} = I_n - \sum_{j=1}^{m-1} f\left( \frac{i}{m} \right) - f\left( \frac{i+1}{m} \right).
\]

Consequently, upon applying \( \delta(\cdot) \) to both sides, we obtain

\[
\delta(e^{iX}) \approx_w \sum_{j=1}^{m-1} \delta\left( f\left( \frac{i}{m} \right) - f\left( \frac{i+1}{m} \right) \right).
\]

If we let \( m \) goes to infinity the RHS would converge to \( \int_0^1 \delta\left( \frac{df(t)}{dt} \right)dt \). Finally, use the fact that \( df(t)/dt = iXe^{itX} \). \( \square \)

**Corollary 4.22.** For any square matrix \( A \), let \( |A| = (A^*A)^{1/2} \). Then, we have

\[
\delta(e^{i|A|}) \approx_w \sigma(A).
\]

We also have another similar relationship between the discrepancy of the absolute values of a matrix and the discrepancy of the matrix. For any matrix \( A \),

\[
\delta(|A|) = \frac{||\sigma(A) - \sigma^*(A)||}{2} \approx_w \delta(A).
\]

(4.15)

To prove inequality (4.15), we need the following statement:
Proposition 4.23. Let $P$ be Hermitian positive definite, $Q$ be unitary. Then,
$$\delta(P) \preceq_w \delta(QP).$$

Proof. It suffices to show that for any diagonal matrix with non-negative entries $\Lambda$ and unitary matrix $Q$ we have
$$\delta(\Lambda) \preceq_w \delta(Q\Lambda).$$

Note that $\sigma(\Lambda) - |\alpha| \sigma(Q) \preceq_w \sigma(\Lambda - \alpha Q)$; hence for any unitary matrix $Q$, we have $\min_{\alpha \in \mathbb{R}^+} \|\Lambda - \alpha I\| \leq \min_{\alpha \in \mathbb{C}} \|\Lambda - \alpha Q\|$, which implies the desired inequality. \hfill $\Box$

4.5 Discrepancy values of direct sums

Below, we briefly discuss discrepancy values of the direct sum of matrices. These results would particularly become useful when comparing the results for discrepancy values with ones for the spread of Hermitian matrices. Inspired by the minimal representation of the discrepancy seminorm, we introduce for $A, B \in \mathbb{C}^{n \times n}$, the generalization
$$\frac{\sum_{i=1}^k \delta(A, B) := \min_{\alpha \in \mathbb{C}} \frac{\|A - \alpha I_n\|_{(i)} + \|B - \alpha I_n\|_{(i)}}{2}}{4.16}.$$  

Note that $\delta(A, Q^*AQ) = \delta(A)$, for any unitary matrix $Q$, and $2\delta(A, 0) = \sigma(A)$.

Proposition 4.24. Let $A, B \in \mathbb{C}^{n \times n}$. The following majorization holds:
$$(\delta(A, B), \delta(A, B)) \preceq_w \delta(A \oplus B).$$

Proof. First note that for any $x, y \in \mathbb{R}^n$, we have
$$\left(\frac{x^1 + y^1}{2}, \frac{x^1 + y^1}{2}\right) \preceq_w (x, y)^\downarrow.$$

Then for any scalar $\alpha$, we have
$$\left(\frac{\sigma(A - \alpha I_n)^\downarrow + \sigma(B - \alpha I_n)^\downarrow}{2}, \frac{\sigma(A - \alpha I_n)^\downarrow + \sigma(B - \alpha I_n)^\downarrow}{2}\right) \preceq_w \sigma(A \oplus B - \alpha I_n)^\downarrow.$$

The result follows by minimizing the RHS of the above inequality w.r.t. $\alpha$. \hfill $\Box$

For the sequel, we need to introduce an averaging operator on vectors. Assume that $x \in \mathbb{R}^{kn}$, where $k$ and $n$ are some positive integers. Then, define $\mu_k(x) \in \mathbb{R}^n$ by
$$\mu_k(x) := \left[\begin{array}{c}
\frac{x_1 + \cdots + x_k}{k} \\
\frac{x_{k+1} + \cdots + x_{2k}}{k} \\
\vdots \\
\frac{x_{kn-k+1} + \cdots + x_{kn}}{k}
\end{array}\right].$$

Using the operator $\mu_k$ we can restate (4.17) as $\delta(A, B) \preceq_w \mu_2(\delta(A \oplus B))$, or restate the connection between the spectral spread of a Hermitian matrix $A \in M_n$ with even $n$ and discrepancy values as $\mu_2(\delta(A)) = \text{spr}^+(A)/2$. Therefore, for Hermitian matrices $A$ and $B$, we have $\delta(A, B) \preceq_w \text{spr}^+(A \oplus B)/2$. The averaging operator allows us to write discrepancy of direct sums of a matrix with itself via the discrepancy of the individual matrix. Indeed, we have the following:
**Lemma 5.** Let $A$ be $n \times n$ matrix. Then

$$\mu_k\left(\delta\left(\underbrace{A \oplus \cdots \oplus A}_{k}\right)\right) = \delta(A).$$

**Proof.** Note that

$$\min_{a \in \mathbb{C}} \left\| \underbrace{A \oplus \cdots \oplus A}_{k} - aI_n \right\|_{(km)} = \min_{a \in \mathbb{C}} \left\| (A - aI_n) \oplus \cdots \oplus (A - aI_n) \right\|_{(km)} = k \min_{a \in \mathbb{C}} \|A - aI_n\|_{(m)},$$

for $m = 1, \ldots, n$. Hence we have the desired result. \hfill \Box

We can similarly prove this lemma if matrices $A$ are arbitrarily replaced by $A^*$. 

### 5 Application: bounding norms of commutators

In this section, our main goal is to employ the tools developed so far to bound the Ky-Fan norms of commutators. We first note an obvious invariance of the **generalized commutator** $AX - XB$ under shifts: for any $a \in \mathbb{C}$ and square matrices $A, B, X$, we have

$$\left( A - aI_n \right)X - X\left( B - aI_n \right) = AX - XB. \tag{5.1}$$

An special case of this invariance is $[A, B] = [A, B - aI_n]$, where $[\cdot, \cdot]$ denotes the usual commutator (Lie bracket). We will use invariance (5.1) together with properties of discrepancy values to amplify existing majorization inequalities such as $\sigma([A, B]) \prec_\sigma 2\sigma(A)\sigma(B)$, and to achieve sharp bounds for similar objects. Our first result is:

**Lemma 6.** For square matrices $A, B$, and any partial isometry $X$ we have

$$\sigma(AX - XB) \prec_\sigma 2\delta(A, B)\sigma(X).$$

**Proof.** Using invariance (5.1), we know that

$$\sum_{i=1}^k \sigma_i(AX - XB) \leq \sum_{i=1}^k (\sigma_i(A - aI) + \sigma_i(B - aI))\sigma_i(X)$$

for any $a \in \mathbb{C}$. Now we minimize the RHS for any $k = 1, \ldots, n$. Considering the fact that $\sigma_i(X)$ is either 1 or 0, we get the desired result. \hfill \Box

Next, we propose a decomposition that enables us to extend the above lemma.

**Lemma 7.** Any square matrix $A$ has the following decomposition

$$A = \sum_{i=1}^n \alpha_i X_i, \tag{5.2}$$

where $X_i$ is a rank-$i$ isometry; i.e., with $i$ non-zero singular values equal to one. And, $\sum_{i=2}^n \alpha_i = \sigma_2, \ldots, \alpha_n = \sigma_n$.

**Proof.** Consider the singular value decomposition $A = \sum_{i=1}^n \sigma_i x_i y_i^*$, and then use summation by parts. Thus, we can rewrite $A$ as follows:

$$A = (\sigma_1 - \sigma_2)x_1 y_1^* + (\sigma_2 - \sigma_3)(x_1 y_1^* + x_2 y_2^*) + \cdots + \sigma_n(x_1 y_1^* + \cdots + x_n y_n^*).$$

Now let $\alpha_i = \sigma_i - \sigma_{i+1}$ and $X_i = x_1 y_1^* + \cdots + x_i y_i^*$, completing the proof. \hfill \Box
Observe that if matrix $A$ in Lemma 7 is positive definite, then each $X_i$ is an orthogonal projection. We are ready to now present the first main result of this section.

**Theorem 5.1.** For $n \times n$ square matrices $A$, $B$, and $X$ we have

$$
\sigma(AX - XB) \preceq_w 2\delta(A, B)\sigma(X).
$$

**Proof.** Using Lemma 7 to obtain the decomposition $X = \sum_{i=1}^n \alpha_i X_i$, we have

$$
\sigma(AX - XB) = \sigma\left(\sum_{i=1}^n \alpha_i (AX_i - X_iB)\right)
\preceq_w \sum_{i=1}^n \alpha_i \sigma(AX_i - X_iB)
\preceq_w 2\delta(A, B)\sum_{i=1}^n \alpha_i \sigma(X_i)
= 2\delta(A, B)\sigma(X),
$$

where the first majorization follows upon noting that $\alpha_i \geq 0$, and the second majorization from Lemma 6. \hfill \Box

Theorem 5.1 provides an extension to a related inequality for the spectral spread proved in [17, inequality (11)]; using $\delta(A, A) = \delta(A)$, we have the following:

**Corollary 5.2.** For the $n \times n$ square matrices $A$ and $B$ we have

$$
\sigma\left([B, A]\right) \preceq_w 2\delta(B)\sigma(A).
$$

**Remark 5.3.** If either $A$ or $B$ belongs to $\Psi_k(n)$ (i.e., it only has discrepancy values zero or one) then we can tighten (5.5) to obtain $\sigma([B, A]) \preceq_w 2\delta(B)\delta(A)$.

**Corollary 5.4.** For $n \times n$ square matrices $A$ and $B$, we have the inequalities

$$
\sigma(AX - XB) \preceq_w 2\mu_2\left(\delta(A \oplus B)\right)\sigma(X),
\sigma(A - B) \preceq_w 2\delta(A, B) \preceq_w 2\mu_2\left(\delta(A \oplus B)\right).
$$

If $A$ and $B$ are Hermitian then $2\mu_2(\delta(A \oplus B)) = \text{Spr}^+(A \oplus B)$, and the resulting inequality has been previously shown for spectral spread [17, inequality (9)]. If $A$ and $B$ are positive definite, then considering the fact that $\delta_{2i-1}(A \oplus B) \leq \sigma_i(A \oplus B)$, the above corollary implies that $\sigma_i(AX - XB) \leq \sigma_i(A \oplus B)\sigma_i(X)$, for $i = 1, \ldots, n$. Moreover, for Hermitian matrices, decomposition (5.2) can be refined as follows.

**Lemma 8.** Any Hermitian matrix $A$ has the decomposition

$$
A = \omega Y + \sum_{i=1}^n \beta_i X_i = \omega Y + (\delta_1 - \delta_2)X_1 + (\delta_2 - \delta_3)X_2 + \cdots + \delta_n X_n,
$$

where $\sum_{i=1}^n \beta_i = \delta_k(A)$, and $\delta(X_i)$ is a zero-one vector with $k$ ones, $\omega$ is a complex scalar, and $\delta(Y) = 0$.

Note that the last two conditions imply that $\sum_{i=1}^n \delta(X_i)\beta_i = \delta(A)$. We now employ the slackness of discrepancy values of Hermitian matrices to prove the claim.
Proof. Note that for the Hermitian matrix $A$ we have $\beta_{2k-1} = 0$ since $\delta_{2k-1} = \delta_{2k}$ for $k = 1, \ldots, \left\lfloor \frac{n}{2} \right\rfloor$. First, we can verify that for $A = \text{Diag}(\lambda(A))$ we have

$$
A = (\delta_2 - \delta_3) \text{Diag} \left( \begin{bmatrix} \frac{\alpha_3 - \alpha_2}{\delta_2 - \delta_3} & \cdots & \frac{\alpha_3 - \alpha_2}{\delta_2 - \delta_3} & -1 \end{bmatrix} \right)
+ (\delta_4 - \delta_5) \text{Diag} \left( \begin{bmatrix} 1, 1, \frac{\alpha_5 - \alpha_4}{\delta_4 - \delta_5}, \cdots, \frac{\alpha_5 - \alpha_4}{\delta_4 - \delta_5}, -1, -1 \end{bmatrix} \right)
+ \cdots + \delta_{n-1} \text{Diag} \left( \begin{bmatrix} 1, \cdots, 1, -1, \cdots, -1 \end{bmatrix} \right) + \alpha_1 (I + O),
$$

where we assume that $\alpha_1 = \alpha_2 = \frac{\lambda_1 + \lambda_n}{2}$, $\alpha_3 = \alpha_4 = \frac{\lambda_2 + \lambda_{n-1}}{2}$, and $\delta_1 = \delta_2 = \frac{\lambda_1 - \lambda_n}{2}$, $\delta_3 = \delta_4 = \frac{\lambda_2 - \lambda_{n-1}}{2}, \cdots$. Matrix $O$ is zero when $n$ is even, otherwise only its central entry is nonzero, and we have $\delta(Y) = 0$. To show that $\delta(X_2) = 1_2$, $\delta(X_4) = 1_4$, \cdots, we need to prove that

$$
|\alpha_i - \alpha_{i-1}| \leq |\delta_i - \delta_{i-1}|
$$

for all odd $i$ greater than or equal to 3. For brevity, we only prove this claim for one case; the other cases follow similarly. We need to show that $|\alpha_3 - \alpha_2| \leq |\delta_3 - \delta_2|$, which is equivalent to

$$
| (\lambda_1 - \lambda_2) - (\lambda_{n-1} - \lambda_n) | \leq |(\lambda_1 - \lambda_2) + (\lambda_{n-1} - \lambda_n)|.
$$

This claim follows immediately after recognizing that $\lambda_1 - \lambda_2 \geq 0$ and $\lambda_{n-1} - \lambda_n \geq 0$. Finally, the claim of the theorem follows because

$$A = Q(A) = (\delta_2 - \delta_3)QX_2Q^* + (\delta_4 - \delta_5)QX_4Q^* + \cdots + \delta_{n-1}QX_{n-1}Q^* + \alpha_1 QYQ^*,
$$

and because discrepancy values are invariant under unitary similarity transforms. \hfill\Box

With these tools, we are ready to prove the second main result of this section. In particular, Theorem 5.5 fixes one matrix to be Hermitian and proves the majorization inequality (5.7) that is tighter than its counterpart implied by Theorem 5.1.

**Theorem 5.5.** For the $n \times n$ square matrix $B$ and Hermitian matrix $A$ we have

$$
\sigma([A, B]) \prec_w 2\delta(A)\delta(B).
$$

(5.7)

Proof. Decomposing $A$ as per Lemma 8, we have

$$
\sigma([B, A]) = \sigma \left( B, \omega Y + \sum_{i=1}^n \beta_i X_i \right)
\prec_w \omega |\sigma([B, Y]) + \sum_{i=1}^n \beta_i |\sigma([B, X_i])
\prec_w 2\delta(B) \sum_{i=1}^n \beta_i \delta(X_i)
= 2\delta(B) \delta(A),
$$

where the first majorization follows by the fact that $\beta_i \geq 0$, and the second majorization from Corollary 5.2, and the fact that $\delta(Y) = 0$. \hfill\Box

In fact we can amplify this theorem to a slightly stronger statement:

**Corollary 5.6.** For an $n \times n$ matrix $A$ and a normal matrix $B$ whose eigenvalues lie on a straight line in the complex plane, we have $\sigma([B, A]) \prec_w 2\delta(B)\delta(A)$. 14
Let us now focus on one special case of inequality (5.7) where one of the matrices is an orthogonal projection; i.e., \( P = P^* = P^2 \). This case uncovers a useful inequality between singular and discrepancy values that is known for the spectral spread.

**Corollary 5.7.** Let \( A \) be an arbitrary \( n \times n \) matrix, and \( P \) be an orthogonal projection of rank \( r \). Then for \( 1 \leq k \leq n \) and \( q = \min\{2r, 2n - 2r\} \), we have

\[
\| [A, P] \|_k \leq \min(\min(q,k), k) \sum_{i=1}^{\delta_i(A)}.
\]

**Corollary 5.8.** Given \( X \in \mathbb{C}^{n \times n} \) and an orthogonal projection \( P \), we have

\[
\sigma(PX(I_n - P)) \preceq_w \delta(X).
\] (5.8)

**Proof.** The claim follows from \( \sigma(PX(I_n - P)) \preceq_w \sigma([P, X]) \), which holds since the singular values of \([P, X]\) include all the nonzero singular values of \( PX(I_n - P) \).

Inequality (5.8) was previously known for the spectral spread of self-adjoint operators. Here we show that it holds for arbitrary square matrices. Following the proof of Theorem 4.14 in [17], the majorization (5.8) implies the following inequality:

\[
\sigma(AXB^*) \preceq_w \delta \left( (A^*A + B^*B)^{1/2}X(A^*A + B^*B)^{1/2} \right),
\] (5.9)

where \( A, B \) and \( X \) are arbitrary square matrices.

### 5.1 Maximally non-commutative Hermitian matrices

In this section, we use the majorization bounds derived in the previous part, together with Fan’s dominance theorem to solve some optimization problems. These results indicate that the inequalities are sharp. We begin by recalling Fan’s celebrated dominance theorem.

**Theorem 5.9** (Fan’s dominance theorem). Let \( A, B \in \mathbb{C}^{m \times n} \). Then, \( \| A \| \leq \| B \| \) for any unitarily invariant norm on \( \mathbb{C}^{m \times n} \) if and only if \( \sigma(A) \preceq_w \sigma(B) \).

The diameter of the unitary orbit of a matrix \( A \in \mathbb{C}^{n \times n} \) w.r.t. the \( k^{th} \) Ky-Fan norm is defined by the following optimization problem:

\[
d_k(A) := \max_{U, V \in U(n)} \| VAV^* - UAU^* \|_k.
\] (5.10)

By inequality (5.3), we know that \( d_k(A) \leq 2\| A \|_k^\delta \). Importantly, for Hermitian matrices we can show that this bound is tight.

**Proposition 5.10** (Generalization of Theorem 1.2 in [8]). Let \( A \) be a Hermitian matrix, then \( d_k(A) = 2\| A \|_k^\delta \).

**Proof.** Let \( A \) have the eigenvalue decomposition \( A = Q\Lambda Q^* \), such that the eigenvalues are in nonincreasing order, and \( Q^*UQ \) is the exchange matrix. Then,

\[
\| A - UAU^* \|_k = \| \Lambda - (Q^*UQ)\Lambda(Q'UQ)^* \|_k = \sum_{i=1}^{k} |\lambda_i - \lambda_{n-i+1}|^\delta.
\]
A special case of inequality (5.7) states that for Hermitian $A$ and $B$, we have

$$\sigma([A, B]) \leq \sqrt{\frac{\lambda_1(A) - \lambda_1^t(A)\|\lambda_1^t(B) - \lambda_1^t(B)\|}{2}}.$$  \hfill (5.11)

Before proving that this inequality is sharp (it also implies that inequality (5.7) is sharp), let us define a family of rotation matrices.

**Definition 5.11.** We define the rotation matrix $R_n(\theta)$ for even and odd $n$ as

$$
\begin{bmatrix}
\cos \theta & 0 & \ldots & 0 & -\sin \theta \\
0 & \cos \theta & \ldots & 0 & -\sin \theta \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \ldots & \cos \theta & 0 \\
\sin \theta & 0 & \ldots & 0 & \cos \theta
\end{bmatrix}
\quad \text{and} \quad
\begin{bmatrix}
\cos \theta & 0 & \ldots & 0 & -\sin \theta \\
0 & \cos \theta & \ldots & 0 & -\sin \theta \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \ldots & \cos \theta & 0 \\
\sin \theta & 0 & \ldots & 0 & \cos \theta
\end{bmatrix},
$$

respectively, where the angle $\theta \in [0, 2\pi)$. This family of matrices can be viewed as the direct sum of two by two rotation matrices.

**Theorem 5.12.** Let $A, B$ be two Hermitian matrices with the eigenvalue decompositions $A = QAQ^*$ and $B = VDV^*$. Assume that $\Lambda = \text{Diag}([\lambda_1, \ldots, \lambda_n])$ and $D = \text{Diag}([d_1, \ldots, d_n])$ where $\lambda_1 \geq \cdots \geq \lambda_n$ and $d_1 \geq \cdots \geq d_n$. Then, we have

$$QR_n\left(\frac{\pi}{4}\right)V^* \in \arg\max_{U \in U(n)} \| [A, UB^*] \|.$$  \hfill (5.12)

**Proof.** Note that the matrix $\tilde{U} := QR_n\left(\frac{\pi}{4}\right)V^*$ is indeed unitary, and it is independent of the eigenvalues. At the maximum point, we have the equality

$$\sigma(A\tilde{U}B\tilde{U}^* - \tilde{U}B\tilde{U}^*A) = \sigma(\Lambda R_n DR_n^* - R_n\left(\frac{\pi}{4}\right)DR_n\left(\frac{\pi}{4}\right)^*\Lambda).$$

And the matrix $M = \Lambda R_n\left(\frac{\pi}{4}\right)DR_n\left(\frac{\pi}{4}\right)^* - R_n\left(\frac{\pi}{4}\right)DR_n\left(\frac{\pi}{4}\right)^*\Lambda$ is an anti-diagonal skew Hermitian matrix, hence $(MM^*)^{1/2}$ is diagonal with values

$$\sigma_i(M) = \frac{\lambda_i - \lambda_{n-i+1}}{2} ||d_i - d_{n-i+1}||, \quad \text{for } i = 1, \ldots, n.$$

From inequality (5.11), we know that these specific singular values majorize the singular values of $[A, UB^*]$ for an arbitrary unitary matrix $U$. Hence, by Fan dominance theorem $\tilde{U}$ is a maximizer of the above optimization problem.

One can interpret Theorem 5.12 as follows: two Hermitian matrices with fixed eigenvalues are maximally non-commutative when their eigenspaces are rotated $R_n\left(\frac{\pi}{4}\right)$ relative to each other. As an example, let represent the eigenvalues and eigenvectors of two $2 \times 2$ real positive definite matrices as two ellipses. This can be viewed as the linear transformation of a unit circle, when the transformation is represented by a positive definite matrix. We are allowed to rotate the matrices so that they become maximally non-commutative. The maximal configuration is illustrated in Fig. 1.

**5.2 Miscellaneous results**

We now briefly note (without proof) some additional results; we refer the interested reader to the longer version [23] of this work for proofs and more elaborate context motivating the noted results.

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Two $2 \times 2$ real positive definite matrices are maximally non-commutative when their corresponding eigenspaces have the above configuration relative to each other. Here, each ellipse represents a matrix. The length of the semi-axes of the ellipses are the eigenvalues of the positive definite matrix, and the directions of the semi-axes are the corresponding eigenvectors.

**Proposition 5.13.** For any square matrix $X \in \mathbb{C}^{n \times n}$, we have

$$
\sum_{i=1}^{k} \delta_i(X, X^*) = \min_{\alpha \in \mathbb{R}} \|X + \alpha I_n\|_2, \quad \sum_{i=1}^{k} \delta_i(-X, X^*) = \min_{\alpha \in \mathbb{R}} \|-X + \alpha I_n\|_2.
$$

They enable us obtaining majorization bounds for $\sigma(AB^* - BA)$ and $\sigma(AB^* + BA)$. We can generalize Corollary 5.2 as follows:

**Proposition 5.14.** Let $A_1, \ldots, A_k$ be square matrices of the same size. Then we have

$$
\sigma\left([A_1, [A_2, \ldots, [A_{k-1}, A_k]\ldots]\right) \prec_w 2^{k-1} \sigma(A_1)\delta(A_2)\ldots\delta(A_k).
$$

While if all $A_1, \ldots, A_k$ are Hermitian,

$$
\sigma\left([A_1, [A_2, \ldots, [A_{k-1}, A_k]\ldots]\right) \prec_w \frac{|\lambda^{\downarrow}(A_1) - \lambda^{\downarrow}(A_1)| \cdot \ldots \cdot |\lambda^{\downarrow}(A_k) - \lambda^{\uparrow}(A_k)|}{2}.
$$

Discrepancy values could be useful when there is a multiplicative scalar invariance.

**Theorem 5.15.** Let $A, B \in \mathbb{C}^{n \times n}$. Then,

$$
\sigma(e^A Be^{-A}) \prec_w \sigma(B) \exp(2\delta(A)),
$$

where $\exp(\cdot)$ denotes the elementwise exponential.

**Corollary 5.16.** Let $A$ be strictly positive definite, and $B \in \mathbb{C}^{n \times n}$. Then,

$$
\sigma(ABA^{-1}) \prec_w \sigma(B) \frac{\lambda^{\downarrow}(A)}{\lambda^{\uparrow}(A)}.
$$

These inequalities help us solve some spectral optimization problems, for instance:

**Corollary 5.17.** Let $A$ be a positive definite matrix and $B \in \mathbb{C}^{n \times n}$ the eigendecomposition $A = V \Lambda V^*$ and singular value decompositions $B = QDP^*$. Assume that $\Lambda = \text{Diag}([\lambda_1, \ldots, \lambda_n])$ and $D = \text{Diag}([d_1, \ldots, d_n])$ where $\lambda_1 \geq \cdots \geq \lambda_n$ and $d_1 \geq \cdots \geq d_n$. Then we have

$$
(V R_n(\frac{\pi}{4})Q^*, VR_n(\frac{\pi}{4})P^*) \in \arg\max_{U_1, U_2 \in U(n)} \|AU_1 BU_2^* A^{-1}\|.
$$

(5.13)
6 Calculation of discrepancy values

As shown earlier, for Hermitian $A$, we know the discrepancy values in closed form: $\delta_1(A), \delta_2(A) = |\lambda_1 - \lambda_2|, \delta_3(A), \delta_4(A) = \frac{|\lambda_3 - \lambda_4|}{2}, \ldots$. We can also find the discrepancy of some other types of matrices easily. Indeed, since $\delta(e^{i\theta}A) = \delta(A)$, and using the formula for discrepancy of Hermitian matrices, one can easily show the following simple yet intriguing result:

**Proposition 6.1.** For any normal matrix whose eigenvalues lie on a straight line in the complex plane and are symmetric about the origin we have $\delta(A) = \sigma(A)$.

**Corollary 6.2.** The singular and discrepancy values of a real skew-symmetric matrix are equal. Furthermore, if $A$ and $B$ are real symmetric matrices, we have

$$\delta([A, B]) = \sigma([A, B]).$$

### 6.1 Computing discrepancy for normal matrices

We know that $\delta(A^*) = \delta(A)$ and $\delta(U^* AU) = \delta(A)$ for any unitary matrix $U$; hence, if $A$ is a normal matrix with the eigenvalue decomposition $A = U^* \Lambda U$ then $\delta(A) = \delta(A)$. Consequently,

$$\sum_{i=1}^{k} \delta_i(A) = \min_{a \in \mathbb{C}} \max_{1 \leq i_1 < i_2 \leq n} \sum_{j=1}^{k} |\lambda_{i_j} - a|.$$  \hspace{1cm} (6.1)

Problem (6.1) can be reformulated as the second-order cone programming problem:

$$\sum_{i=1}^{k} \delta_i(A) = \min_{a \in \mathbb{C}, q \in \mathbb{R}, u \in \mathbb{R}^n} \left(1^T u + k q, 1^T u + k q, u \geq x - q 1_n, x \geq |\lambda - a 1_n|, u \geq 0, \right)$$  \hspace{1cm} (6.2)

where $| \cdot |$ denotes the element-wise modulus of a complex vector. The optimal objective function value of (6.2) equals $\sum_{i=1}^{k} \delta_i(A)$.

Notice that for any normal matrix $A$ we have $\delta_1(A) = \delta_2(A) = R$, where $R$ corresponds to the radius of the smallest circle containing all the eigenvalues; see Fig. 2. Also, we can see that the optimum $a$ which minimizes $\|A - a I_n\|_{(n)}$ is just the geometric median of the eigenvalues in the two-dimensional complex plane.

### 6.2 SDP representation for discrepancy seminorms

From Theorem 4.3, we know that $\|A\|_{(k)}^d = \min_{a \in \mathbb{C}} \|A - a I_n\|_{(k)}$, where the latter is a convex function in $a$. Hence, we can find $\delta(A)$ by employing a series of nonsmooth convex optimization methods. We propose below a more convenient way to compute the discrepancy values via semidefinite programming (SDP). To that end, recall that

$$\sum_{i=1}^{n} \delta_i(A) = \max_{U^* U = I_n, V^* V = I_n, \text{tr}(U^* V) = 0} \text{Re tr}(A V U^*).$$  \hspace{1cm} (6.3)

If we let $M = \begin{bmatrix} U^* & V \end{bmatrix}$ and $\mathcal{H}(A) = \begin{bmatrix} 0 & A \vline A^* \end{bmatrix}$, then using (6.3) we can write

$$\sum_{i=1}^{n} \delta_i(A) = \max_{M = \begin{bmatrix} I_n & K \vline K \end{bmatrix}, \text{tr}(K) = 0} \frac{1}{2} \text{Re tr} \left( \mathcal{H}(A) M \right).$$  \hspace{1cm} (6.4)
To derive SDP formulations for other $\sum_{j=1}^{k} \delta_j(A)$, we use the fact that for any Hermitian matrix $X$ with eigenvalues $\lambda_1(X) \geq \cdots \geq \lambda_n(X)$ we have (see [4])

$$t \geq \lambda_1(X) + \cdots + \lambda_k(X) \iff \exists (Z, s) : Z \succeq 0, Z + sI_{2n} \succeq X, t \geq \Re \left( \text{tr}(Z) + ks \right),$$

where $t$ is a non-negative real number, and $s \in \mathbb{C}$ and $Z$ can be complex valued in general. As a result, we have the following SDP formulation for the Ky-Fan norm:

$$\|A\|_{(k)} = \min_{Z \succeq 0, t \geq 0, s \in \mathbb{C}} t$$

$$\mathcal{H}(A) \leq Z + sI_{2n}, \quad t \geq \Re \left( \text{tr}(Z) + ks \right),$$

where $k = 1, \ldots, n$ and $Z$ is a $2n \times 2n$ complex matrix. We similarly also obtain

$$\|A\|_{(k)}^d = \min_{Z \succeq 0, t \geq 0, s, \alpha \in \mathbb{C}} t, \quad \left[ \begin{array}{cc} 0 & Z + sI_{2n} \\ A^* - \alpha I_n & A - \alpha I_n \end{array} \right] \succeq 0, \quad t \geq \Re \left( \text{tr}(Z) + ks \right)$$

where $k = 1, \ldots, n$ and $Z$ is a $2n \times 2n$ complex matrix. Note that if matrix $A$ is real, we can let $Z$ and other optimization variables be real.\(^2\)

\section{Discussion and extensions}

Most of the results proven in the previous sections can be extended to linear operators of the form $A + \gamma I$, where $A$ is a compact operator on Hilbert spaces, and $\gamma \in \mathbb{C}$. For any compact operator $A : H \to K$ between Hilbert spaces $H$ and $K$, we know that $A$ always has countably many non-negative singular values, among which $\sigma = 0$ is the only possible point of accumulation. For any finite $k$, the operator norm $\|A\|_{(k)}$ is finite, hence $\delta_k(A + \gamma I)$ is well-defined. Furthermore, if the rank of the operator is not finite, we have $\delta_k(A + \gamma I) \to 0$ as $k \to \infty$ regardless of the fact that $A$ belongs to the trace-class or not. This follows by the fact that $\|A + \gamma I\|_{(k)}^d \leq \|A\|_{(k)}$ for any finite $k \in \mathbb{N}$ and $\sigma_k \to 0$ as $k \to \infty$.

We end the paper with a conjecture on discrepancy values.

\(^2\)An implementation of this formulation is available at https://github.com/PouriaZ/Discrepancy
Conjecture 7.1. For the $n \times n$ square matrices $A$ and $B$ we have

$$\sigma([A, B]) \preceq_w 2\delta(A)\delta(B),$$

(7.1)

where $\delta(A)\delta(B)$ is the entrywise product of the vectors of the discrepancy values.

For the $2 \times 2$ matrix $A = [A_{ij}]$, for $i = 1, 2$, we can show that

$$\delta_i(A) = \frac{1}{\sqrt{2}} \left[ \frac{1}{2} (A_{11} - A_{22})^2 + A_{12}^2 + A_{21}^2 \pm |A_{12} - A_{21}| \sqrt{(A_{12} + A_{21})^2 + (A_{11} - A_{22})^2} \right]^{1/2}.$$

By inspection, one can verify that $\delta(A) = \sigma \left( A - \frac{A_{11} + A_{22}}{2} I_2 \right)$. Thus we have

$$\sigma([A, B]) = \sigma \left( \left[ A - \frac{A_{11} + A_{22}}{2} I_2, B - \frac{B_{11} + B_{22}}{2} I_2 \right] \right) \preceq_w 2\delta(A)\delta(B).$$

Therefore the conjecture is true for any two by two matrices. Furthermore, the conjecture has been proven for some general cases in this paper (see Remark 5.3 and Corollary 5.6). However, the conjecture in its full generality is an open problem.

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A The X decomposition for Hermitian matrices

In this part, we propose a decomposition for the Hermitian matrices based on their discrepancy values and vectors. First, let us introduce a family of matrices.

Definition A.1 (X matrices). We call a square matrix which is allowed to have nonzero entries only on the main diagonal, or on the anti-diagonal, an X matrix (or star matrix).

Remark A.2. The set of X matrices are unitarily similar to matrices of the form $B_1 \oplus B_2 \oplus \cdots \oplus B_n$, where $B_i$ are two by two matrices, plus one scalar if it has odd dimensionality.

Let the notations $CX(a_1, \ldots, a_n)(b_1, \ldots, b_n)$ and $CX(a_1, \ldots, a_n)(c)(b_1, \ldots, b_n)$ denote the following centrosymmetric X matrices, respectively:

\[
\begin{bmatrix}
  a_1 & 0 & \ldots & 0 & b_1 \\
  0 & \ddots & \ddots & \ddots & \vdots \\
  \vdots & a_n & \ddots & \ddots & \ddots \\
  b_n & \ddots & \ddots & \ddots & \ddots \\
  b_1 & \ldots & 0 & \ddots & 0 \\
\end{bmatrix},
\]

\[
\begin{bmatrix}
  a_1 & 0 & \ldots & 0 & b_1 \\
  0 & \ddots & \ddots & \ddots & \vdots \\
  \vdots & a_n & \ddots & \ddots & \ddots \\
  c & \ddots & \ddots & \ddots & \ddots \\
  b_n & \ddots & \ddots & \ddots & \ddots \\
  b_1 & \ldots & 0 & \ddots & 0 \\
\end{bmatrix}.
\]

Proposition A.3 (X decomposition). Any $n \times n$ Hermitian matrix $A$ can be decomposed as $A = UXV^*$, where $X$ is a centrosymmetric X matrix; moreover, $U$ and $V$ are unitary matrices such that $U^*V = J_n$, the exchange matrix.

Proof. Let $R_n(\cdot)$ be the $n \times n$ orthogonal matrix defined in 5.11, then using the eigenvalue decomposition of $A$ we have

$A = Q\Lambda Q^* = QR_n(\frac{\pi}{4})(R_n(\frac{\pi}{4})^* \Lambda J_n R_n(\frac{\pi}{4})^*)(QJ_n R_n(\frac{\pi}{4})^*)^*$.

Now let $U = QR_n(\frac{\pi}{4})$, $V = QJ_n R_n(\frac{\pi}{4})^*$, and $X = R_n(\frac{\pi}{4})^* \Lambda J_n R_n(\frac{\pi}{4})^*$. One can easily verify all the conditions in the proposition are satisfied. \qed

In the previous proposition, we can show that the columns of $U$ and $V$ are vectors $x_i$ and $y_i$ in the definition of $\delta$ in 3.1. Also if $n$ is an even number we have

$X = CX(\delta_1(A), \delta_3(A), \ldots)(a^*_1(A), a^*_3(A), \ldots),$

and otherwise we have

$X = CX(\delta_1(A), \delta_3(A), \ldots)(a^*_n(A), a^*_1(A), a^*_3(A), \ldots),$

where $\delta_i(A) = (\lambda_i - \lambda_{n-i+1})/2$ and $a^*_i(A) = (\lambda_i + \lambda_{n-i+1})/2$. 

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