POSITIVE DEFINITE MATRICES AND THE S-DIVERGENCE*

SUVRIT SRA†

Abstract. Positive definite matrices abound in a dazzling variety of applications. This ubiquity can be in part attributed to their rich geometric structure: positive definite matrices form a self-dual convex cone whose strict interior is a Riemannian manifold. The manifold view is endowed with a "natural" distance function while the conic view is not. Nevertheless, drawing motivation from the conic view, we introduce the S-Divergence as a "natural" distance-like function on the open cone of positive definite matrices. We motivate the S-divergence via a sequence of results that connect it to the Riemannian distance. In particular, we show that (a) this divergence is the square of a distance; and (b) that it has several geometric properties similar to those of the Riemannian distance, though without being computationally as demanding. The S-Divergence is even more intriguing: although nonconvex, we can still compute matrix means and medians using it to global optimality. We complement our results with some numerical experiments illustrating our theorems and our optimization algorithm for computing matrix medians.

Key words. Bregman matrix divergence; Log Determinant; Stein Divergence; Jensen-Bregman divergence; matrix geometric mean; matrix median; nonpositive curvature

1. Introduction. Hermitian positive definite (HPD) matrices are a noncommutative generalization of positive reals. They abound in a multitude of applications and exhibit attractive geometric properties—e.g., they form a differentiable Riemannian (also Finslerian) manifold [10,33] that is a well-studied example of a manifold of non-positive curvature [17, Ch.10]. HPD matrices possess even more structure: (i) they embody a canonical higher-rank symmetric space [51]; and (ii) their closure forms a closed, self-dual convex cone.

The convex conic view enjoys great importance in convex optimization [6, 43, 44] and in nonlinear Perron-Frobenius theory [40]; symmetric spaces are important in algebra, analysis [32, 39, 51], and optimization [43, 52]; while the manifold view (Riemannian or Finslerian) plays diverse roles—see [10, Ch.6] and [46].

The manifold view is equipped with a with a "natural" distance function while the conic view is not. Nevertheless, drawing motivation from the convex conic view, we introduce the *S-Divergence* as a "natural" distance-like function on the open cone of positive definite matrices. Indeed, we prove a sequence of results connecting the S-Divergence to the Riemannian distance. Most importantly, we show that (a) this divergence is the square of a distance; and (b) that it has several geometric properties in common with the Riemannian distance, without being numerically as demanding. This builds an informal link between the manifold and conic views of HPD matrices.

1.1. Background and notation. We begin by fixing notation. The letter \mathcal{H} denotes some Hilbert space, usually just \mathbb{C}^n . The inner product between two vectors x and y in \mathcal{H} is $\langle x, y \rangle := x^*y$ (x^* denotes 'conjugate transpose'). The set of $n \times n$ Hermitian matrices is denoted as \mathbb{H}_n . A matrix $A \in \mathbb{H}_n$ is called *positive definite* if

$$\langle x, Ax \rangle > 0$$
 for all $x \neq 0$, also written as $A > 0$. (1.1)

The set of all positive definite (henceforth positive) matrices is denoted by \mathbb{P}_n . We say A is positive semidefinite if $\langle x, Ax \rangle \geq 0$ for all x; denoted $A \geq 0$. The inequality

^{*}A small fraction of an initial version of this work was presented at the Advances in Neural Information Processing Systems (NIPS) 2012 conference—see [48].

[†]Parts of this paper were written during my stay at Carnegie Mellon University; the initial version was prepared while I was at the Max Planck Institute for Intelligent Systems, Tübingen, Germany.

 $A \geq B$ is the usual Löwner order and means $A - B \geq 0$. The Frobenius norm of a matrix $X \in \mathbb{C}^{m \times n}$ is defined as $||X||_{\mathcal{F}} = \sqrt{\operatorname{tr}(X^*X)}$; and ||X|| denotes the operator 2-norm. Let f be an analytic function on \mathbb{C} ; for a matrix A with eigendecomposition $A = U\Lambda U^*$, f(A) equals $Uf(\Lambda)U^*$ with $f(\Lambda) = \operatorname{Diag}[f(\lambda_1), \ldots, f(\lambda_n)]$.

The set \mathbb{P}_n is a well-studied differentiable Riemannian manifold, with the Riemannian metric given by the differential form $ds = ||A^{-1/2}dAA^{-1/2}||_{\mathrm{F}}$. This metric induces the *Riemannian distance* (see e.g., [10, Ch. 6]):

$$\delta_R(X,Y) := \|\log(Y^{-1/2}XY^{-1/2})\|_{\mathcal{F}} \quad \text{for} \quad X,Y > 0,$$
 (1.2)

and where $\log(\cdot)$ denotes the matrix logarithm.

A counterpart to the distance (1.2) was formally introduced in [48] under the name S-Divergence¹; this divergence is defined as

$$\delta_S^2(X,Y) := \log \det \left(\frac{X+Y}{2}\right) - \frac{1}{2} \log \det(XY) \quad \text{for} \quad X,Y > 0. \tag{1.3}$$

Our definition above already writes δ_S^2 in anticipation of Theorem 3.1 that shows δ_S to be a metric. This paper suggests S-Divergence as an alternative to (1.2), and studies several of its properties that may also be of independent interest. The simplicity of (1.3) is one of the key reasons for using it as an alternative to (1.2): it is cheaper to compute, as is its derivative, and certain basic algorithms involving it run much faster than corresponding ones that use δ_R [48].

This line of thought actually originates in [24, 25], where for an image search task based on "nearest neighbors," δ_S^2 is used to measure nearness instead of δ_R , and is shown to yield large speedups without blighting the quality of search results. Although exact details of this image search are outside the scope of this paper, let us highlight below the two speedups that were crucial to [24, 25].

The first speedup is shown in the left panel of Fig. 1.1, which compares times taken to compute δ_S^2 and δ_R . For computing the latter, we used the dist.m function in the Matrix Means Toolbox (MMT)². The second, more dramatic speedup in shown in the right panel which shows time taken to compute the matrix means

$$GM_{\ell d} := \operatorname*{argmin}_{X>0} \sum\nolimits_{i=1}^m \delta_S^2(X,A_i), \quad \text{and} \quad GM := \operatorname*{argmin}_{X>0} \sum\nolimits_{i=1}^m \delta_R^2(X,A_i),$$

where (A_1, \ldots, A_m) are HPD matrices. For details on $GM_{\ell d}$ see Section 5; the geometric mean GM is also known as the "Karcher mean", and was computed using the MMT via the rich.m script which implements a state-of-the-art method [13,34].

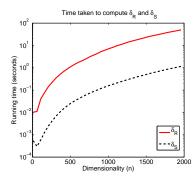
We mention here that other alternatives to δ_R are also possible, for instance the popular "log-Euclidean" distance [3], given by

$$\delta_{le}(X,Y) = \|\log X - \log Y\|_{F}.$$
 (1.4)

Notice that to compute δ_{le} we require two eigenvector decompositions; this makes it more expensive than δ_S^2 which requires only 3 Cholesky factorizations. Even though the matrix mean under δ_{le}^2 can be computed in closed form, its dependency on matrix logarithms and exponentials can make it slower than $GM_{\ell d}$. However, much more importantly, for the applications in [24, 25], δ_{le} and other alternatives to δ_R proved

¹It is a divergence because although nonnegative, definite, and symmetric, it is *not* a metric.

²Downloaded from http://bezout.dm.unipi.it/software/mmtoolbox/



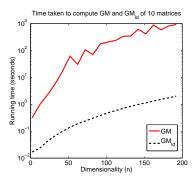


Fig. 1.1. Left: Time taken to compute δ_R and δ_S^2 . For δ_R , we used MMT's Schur factorization based implementation. The results are averaged over 10 runs to reduce variance. The plot indicates that δ_S^2 can be up to 50 times faster than δ_R . Right: Time taken to compute GM and $GM_{\ell d}$. The former was computed using the method of [13], while the latter was obtained via a fixed-point iteration. The differences are huge: $GM_{\ell d}$ can be obtained up to 1000 times faster! Even the slew of methods surveyed in [34] show similar or worse runtimes than those cited for δ_R above.

to be substantially less competitive than (1.3), so we limit our focus to δ_S^2 ; for more extensive empirical comparisons with other distances, we refer the reader to [24,25].

While our paper was under review (in 2011), we became aware of a concurrent paper of Chebbi and Moakher (CM) [21], who consider a one parameter family of divergences that generalize (1.3). Our work differs from CM in the following aspects:

- CM prove δ_S to be a distance only for commuting matrices. As per Remark 3.11, the commuting case essentially reduces to the scalar case. The noncommuting case is much harder, and was conjectured to be true in [21]. We propose and solve the general noncommuting case, independent of CM.
- We establish several theorems connecting δ_S^2 to the Riemannian distance δ_R . These connections have not been made either by CM or *elsewhere*.
- A question closely related to metricity of δ_S is whether the matrix

$$[\det(X_i + X_j)^{-\beta}]_{i,j=1}^m, \qquad X_1, \dots, X_m \in \mathbb{P}_n,$$

is positive semidefinite for every integer $m \geq 1$ and every scalar $\beta \geq 0$. CM considered special cases of this question. We provide a complete characterization of β necessary and sufficient for the above matrix to be semidefinite.

• CM analyze the "matrix-mean" $\min_{X>0} f(X) := \sum_i \delta_S^2(X, A_i)$, whose solution they obtain by solving $\nabla f(X) = 0$. CM's results essentially imply global optimality³; we provide two different proofs of this fact. One of our proofs is based of establishing *geodesic convexity* of the S-Divergence—a result that is also interesting because in our previous attempts [48, 49] we oversaw this property. In fact, we show (Theorem 4.4) that δ_S^2 is jointly geodesically convex.

Other contributions. The present paper substantially extends our initial work [48]; we outline below the key differences from [48].

• Due to lack of space proofs of the lemmas supporting Theorem 3.1 did not appear in [48]. In particular, proofs of Corollaries 3.5, 3.8 and Theorems 3.6, 3.7 are absent from [48] (these results are not difficult though).

³We thank a referee for alerting us to this fact, which ultimately follows from CM's uniqueness theorem and the observation that the cost function goes to $+\infty$ for both $X \to 0$ and $X \to \infty$ (see Sec. 5 for more details).

- None of our results on similarities between the Riemannian distance δ_R and δ_S are present in [48]. Although some of these results are mentioned in a summary table in [48], the full theorem statements as well as their proofs are absent. The concerned results are: Theorems 4.1, 4.5, 4.6, 4.7, 4.8, and 4.10.
- This paper uncovers a new result (previously unknown): δ_S^2 is jointly geodesically convex—Prop. 4.3 and Theorem 4.4 establish this remarkable fact.
- This paper proves several new "conic" contraction results for δ_S and δ_R . The appurtenant results are: Proposition 4.12, Corollary 4.13, Theorem 4.15, Corollary 4.16, Theorem 4.17, and Corollary 4.18.
- This paper proves bi-Lipschitz-like inequalities for δ_R and δ_S (Theorem 4.19).
- Finally, this paper studies the weighted matrix-medians problem:

$$\min_{X>0} \quad \sum_{i=1}^{m} w_i \delta_S(X, A_i), \qquad A_i \in \mathbb{P}_n, \text{ for } 1 \le i \le m.$$

This problem was also partially studied by [19], who presented an iterative method that was erroneously claimed to be a fixed-point iteration in the Thompson metric. We present a counterexample to illustrate this error, and rectify it by presenting different analysis that ensures convergence (see §6).

2. The S-Divergence. We proceed now to formally introduce the S-Divergence. We follow the viewpoint of Bregman divergences. Consider, thus, a differentiable strictly convex function $f: \mathbb{R} \to \mathbb{R}$; then, $f(x) \geq f(y) + f'(y)(x-y)$, with equality if and only if x = y. The difference between the two sides of this inequality defines the $Bregman\ Divergence^4$

$$D_f(x,y) := f(x) - f(y) - f'(y)(x - y). \tag{2.1}$$

The scalar divergence (2.1) can be extended to Hermitian matrices.

PROPOSITION 2.1. Let f be differentiable and strictly convex on \mathbb{R} ; let $X, Y \in \mathbb{H}_n$ be arbitrary. Then, we have the matrix Bregman Divergence:

$$D_f(X,Y) := \operatorname{tr} f(X) - \operatorname{tr} f(Y) - \operatorname{tr} (f'(Y)(X-Y)) \ge 0.$$
 (2.2)

By construction D_f is nonnegative, strictly convex in X, and zero if and only if X = Y. It is typically asymmetric, and may be viewed as a measure of dissimilarity.

EXAMPLE 2.2. Let $f(x) = \frac{1}{2}x^2$. Then, for $X \in \mathbb{H}_n$, $\operatorname{tr} f(X) = \frac{1}{2}\operatorname{tr}(X^2)$, with which (2.2) yields the squared Frobenius norm

$$D_f(X,Y) = \frac{1}{2} ||X - Y||_F^2.$$

If $f(x) = x \log x - x$ on $(0, \infty)$, then $\operatorname{tr} f(X) = \frac{1}{2} \operatorname{tr}(X \log X - X)$, and (2.2) yields the (unnormalized) von Neumann Divergence of quantum information theory [45]:

$$D_{vn}(X,Y) = \operatorname{tr}(X \log X - X \log Y - X + Y), \qquad X, Y \in \mathbb{P}_n.$$

For $f(x) = -\log x$ on $(0, \infty)$, $\operatorname{tr} f(X) = -\log \det(X)$, and we obtain the divergence

$$D_{\ell d}(X,Y) = \operatorname{tr}(Y^{-1}(X-Y)) - \log \det(XY^{-1}), \qquad X, Y \in \mathbb{P}_n,$$

⁴Bregman divergences over scalars and vectors have been well-studied; see e.g., [4, 18]. They are called divergences because they are not distances (though they often behave like squared distances, in a sense that can be made precise for certain choices of f [22]).

which is known as the LogDet Divergence [37], or more classically as Stein's loss [50].

The divergence $D_{\ell d}$ is of key importance to our paper, so we mention some additional noteworthy contexts where it occurs: (i) information theory [26], as the relative entropy between two multivariate gaussians with same mean; (ii) optimization, when deriving the famous Broyden-Fletcher-Goldfarb-Shanno (BFGS) updates [47]; (iii) matrix divergence theory [5, 28, 46]; (iv) kernel learning [37].

Despite the broad applicability of Bregman divergences, their asymmetry is sometimes undesirable. This drawback has leads us to consider symmetric divergences, among which the most popular is the "Jensen-Bregman" divergence⁵

$$S_f(X,Y) := D_f(X, \frac{X+Y}{2}) + D_f(\frac{X+Y}{2}, Y).$$
 (2.3)

This divergence has two attractive and perhaps more useful representations:

$$S_f(X,Y) = \frac{1}{2} \left(\operatorname{tr} f(X) + \operatorname{tr} f(Y) \right) - \operatorname{tr} f\left(\frac{X+Y}{2} \right),$$

$$S_f(X,Y) = \min_Z D_f(X,Z) + D_f(Y,Z).$$
(2.4)

$$S_f(X,Y) = \min_Z D_f(X,Z) + D_f(Y,Z). \tag{2.5}$$

Compare (2.2) with (2.4): both formulas define divergence as departure from linearity; the former uses derivatives, while the latter is stated using midpoint convexity. Representation (2.4) has an advantage over (2.2), (2.3), and (2.5), in that it does not need to assume differentiability of f.

The reader must have realized by now that the S-Divergence (1.3) is nothing but the symmetrized divergence (2.3) generated by $f(x) = -\log x$. Alternatively, the S-Divergence may be essentially viewed as the Jensen-Bregman divergence between two multivariate gaussians [26], or as the Bhattacharya distance between them [12].

Let us now list a few basic properties of S.

PROPOSITION 2.3. Let $\lambda(X)$ be the vector of eigenvalues of X, and $\operatorname{Eig}(X)$ be a diagonal matrix with $\lambda(X)$ as its diagonal. Let $A, B, C \in \mathbb{P}_n$. Then,

- (i) $\delta_S(I, A) = \delta_S(I, \operatorname{Eig}(A));$
- (ii) $\delta_S(A, B) = \delta_S(PAQ, PBQ)$, where $P, Q \in GL(n, \mathbb{C})$;
- (iii) $\delta_S(A, B) = \delta_S(A^{-1}, B^{-1});$
- (iv) $\delta_S^2(A \otimes B, A \otimes C) = n\delta_S^2(B, C)$; and
- $(v) \ \delta_S^2(A \oplus B, C \oplus D) = \delta_S^2(A, C) + \delta_S^2(B, D).$

Proof. (i) follows from the equality $\det(I+A) = \prod_i \lambda_i(I+A) = \prod_i (1+\lambda_i(A))$.

(ii) follows upon observing that

$$\frac{\det(PAQ + PBQ)}{[\det(PAQ)]^{1/2}[\det(PBQ)]^{1/2}} = \frac{\det(P) \cdot \det(A + B) \cdot \det(Q)}{\det(P) \cdot [\det(A)]^{1/2}[\det(B)]^{1/2} \cdot \det(Q)}.$$

(iii) follows upon noting

$$\frac{\det(A^{-1}+B^{-1})}{[\det(A^{-1})]^{1/2}[\det(B)^{-1}]^{1/2}} = \frac{\det(A)\cdot\det(A^{-1}+B^{-1})\cdot\det(B)}{[\det(A)]^{1/2}[\det(B)]^{1/2}}.$$

(iv) follows as $A \otimes B + A \otimes C = A \otimes (B + C)$, and $\det(A \otimes B) = \det(A)^n \det(B)^n$.

(v) is trivial since
$$det(A \oplus B) = det(A) det(B)$$
.

The most useful corollary to Prop. 2.3 is congruence invariance of δ_S . COROLLARY 2.4. Let A, B > 0, and let X be any invertible matrix. Then,

$$\delta_S(X^*AX, X^*BX) = \delta_S(A, B).$$

⁵This symmetrization has been largely studied only for divergences over scalars or vectors.

The next result reaffirms that $\delta_S^2(\cdot,\cdot)$ is a divergence, while showing that it enjoys some limited convexity and concavity.

PROPOSITION 2.5. Let A, B > 0. Then, (i) $\delta_S^2(A, B) \ge 0$ with equality if and only if A = B; (ii) for fixed B, $\delta_S^2(A, B)$ is convex in A for $A \le (1 + \sqrt{2})B$, while for $A \ge (1 + \sqrt{2})B$, it is concave.

Proof. Since δ_S^2 is a sum of Bregman divergences, property (i) follows from definition (2.3). Alternatively, note that $\det((A+B)/2) \geq [\det(A)]^{1/2} [\det(B)]^{1/2}$, with equality if and only if A=B. Part (ii) follows upon analyzing the Hessian $\nabla_A^2 \delta_S^2(A,B)$. This Hessian can be identified with the matrix

$$H := \frac{1}{2} (A^{-1} \otimes A^{-1}) - (A+B)^{-1} \otimes (A+B)^{-1}, \qquad (2.6)$$

where \otimes is the usual the Kronecker product. Matrix H is positive definite for $A \leq (1+\sqrt{2})B$ and negative definite for $A \geq (1+\sqrt{2})B$, which proves (ii).

Below we show that δ_S^2 is richer than a divergence: its square-root δ_S is actually a distance on \mathbb{P}_n . This is the first main result of our paper. Previous authors [21,24] conjectured this result but could not establish it, perhaps because both ultimately sought to map δ_S to a Hilbert space metric. This approach fails because HPD matrices do not form even a (multiplicative) semigroup, which renders the powerful theory of harmonic analysis on semigroups [7] inapplicable to δ_S . This difficulty necessitates a different path to proving metricity of δ_S , and this is the subject of the next section.

3. The δ_S metric. In this section we prove the following main theorem. THEOREM 3.1. Let δ_S be defined by (1.3). Then, δ_S is a metric on \mathbb{P}_n .

The proof of Theorem 3.1 depends on several results, which we first establish.⁶

DEFINITION 3.2 ([7, Def. 1.1]). Let \mathcal{X} be a nonempty set. A function $\psi : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is said to be *negative definite* if for all $x, y \in \mathcal{X}$, $\psi(x, y) = \psi(y, x)$, and the inequality

$$\sum_{i,j=1}^{n} c_i c_j \psi(x_i, x_j) \le 0,$$

holds for all integers $n \geq 2$, and subsets $\{x_i\}_{i=1}^n \subseteq \mathcal{X}, \{c_i\}_{i=1}^n \subseteq \mathbb{R} \text{ with } \sum_{i=1}^n c_i = 0.$ Theorem 3.3 ([7, Prop. 3.2, Ch. 3]). Let $\psi : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ be negative definite. Then, there is a Hilbert space $\mathcal{H} \subseteq \mathbb{R}^{\mathcal{X}}$ and a mapping $x \mapsto \varphi(x)$ from $\mathcal{X} \to \mathcal{H}$ such that one has the relation

$$\|\varphi(x) - \varphi(y)\|_{\mathcal{H}}^2 = \frac{1}{2}(\psi(x, x) + \psi(y, y)) - \psi(x, y). \tag{3.1}$$

Moreover, negative definiteness of ψ is necessary for such a mapping to exist.

Theorem 3.3 helps prove the triangle inequality for the scalar case.

Lemma 3.4. Define, the scalar version of \sqrt{S} as

$$\delta_s(x,y) := \sqrt{\log[(x+y)/(2\sqrt{xy})]}, \quad x, y > 0.$$

Then, δ_s satisfies the triangle inequality, i.e.,

$$\delta_s(x,y) \le \delta_s(x,z) + \delta_s(y,z)$$
 for all $x, y, z > 0$. (3.2)

⁶We note that a referee wondered whether the "metrization" results of [22, 23] could yield an alternative proof of Thm. 3.1. Unfortunately, those results rely very heavily on the commutativity and total-order available on \mathbb{R} , both of which are missing in \mathbb{P}_n . Indeed, for the commutative case, Lemma 3.4 alone suffices to prove that δ_S is a metric.

Proof. We show that $\psi(x,y) = \log((x+y)/2)$ is negative definite. Since $\delta_s^2(x,y) = \psi(x,y) - \frac{1}{2}(\psi(x,x) + \psi(y,y))$, Theorem 3.3 then immediately implies the triangle inequality (3.2). To prove that ψ is negative definite, by [7, Thm. 2.2, Ch. 3] we may equivalently show that $e^{-\beta\psi(x,y)} = \left(\frac{x+y}{2}\right)^{-\beta}$ is a positive definite function for $\beta > 0$, and x,y > 0. To that end, it suffices to show that the matrix

$$H = [h_{ij}] = [(x_i + x_j)^{-\beta}], \quad 1 \le i, j \le n,$$

is HPD for every integer $n \geq 1$, and positive numbers $\{x_i\}_{i=1}^n$. Now, observe that

$$h_{ij} = \frac{1}{(x_i + x_j)^{\beta}} = \frac{1}{\Gamma(\beta)} \int_0^\infty e^{-t(x_i + x_j)} t^{\beta - 1} dt,$$
 (3.3)

where $\Gamma(\beta) = \int_0^\infty e^{-t} t^{\beta-1} dt$ is the Gamma function. Thus, with $f_i(t) = e^{-tx_i} t^{\frac{\beta-1}{2}} \in L_2([0,\infty))$, we see that $[h_{ij}]$ equals the Gram matrix $[\langle f_i, f_j \rangle]$, whereby $H \geq 0$.

Using Lemma 3.4 obtain the following "Minkowski" inequality for δ_s . COROLLARY 3.5. Let $x, y, z \in \mathbb{R}^n_{++}$; and let $p \geq 1$. Then,

$$\left(\sum_{i} \delta_s^p(x_i, y_i)\right)^{1/p} \le \left(\sum_{i} \delta_s^p(x_i, z_i)\right)^{1/p} + \left(\sum_{i} \delta_s^p(y_i, z_i)\right)^{1/p}. \tag{3.4}$$

Proof. Lemma 3.4 implies that for positive scalars x_i , y_i , and z_i , we have

$$\delta_s(x_i, y_i) \le \delta_s(x_i, z_i) + \delta_s(y_i, z_i), \qquad 1 \le i \le n.$$

Exponentiate, sum, and invoke Minkowski's inequality to conclude (3.4).

Theorem 3.6. Let X, Y, Z > 0 be diagonal matrices. Then,

$$\delta_S(X,Y) \le \delta_S(X,Z) + \delta_S(Y,Z) \tag{3.5}$$

Proof. For diagonal matrices X and Y, it is easy to verify that $\delta_S^2(X,Y) = \sum_i \delta_s^2(X_{ii}, Y_{ii})$. Now invoke Corollary 3.5 with p = 2.

Next, we recall an important determinantal inequality for positive matrices.

THEOREM 3.7 ([9, Exercise VI.7.2]). Let A, B > 0. Let $\lambda^{\downarrow}(X)$ denote the vector of eigenvalues of X sorted in decreasing order; define $\lambda^{\uparrow}(X)$ likewise. Then,

$$\prod_{i=1}^{n} (\lambda_i^{\downarrow}(A) + \lambda_i^{\downarrow}(B)) \le \det(A+B) \le \prod_{i=1}^{n} (\lambda_i^{\downarrow}(A) + \lambda_i^{\uparrow}(B)). \tag{3.6}$$

COROLLARY 3.8. Let A, B > 0. Let $\operatorname{Eig}^{\downarrow}(X)$ denote the diagonal matrix with $\lambda^{\downarrow}(X)$ as its diagonal; define $\operatorname{Eig}^{\uparrow}(X)$ likewise. Then,

$$\delta_S(\operatorname{Eig}^{\downarrow}(A), \operatorname{Eig}^{\downarrow}(B)) \leq \delta_S(A, B) \leq \delta_S(\operatorname{Eig}^{\downarrow}(A), \operatorname{Eig}^{\uparrow}(B)).$$

Proof. Scale A and B by 2, divide each term in (3.6) by $\sqrt{\det(A)\det(B)}$, and note that $\det(X)$ is invariant to permutations of $\lambda(X)$; take logarithms to conclude.

The final result we need is well-known in linear algebra (we provide a proof). LEMMA 3.9. Let A > 0, and let B be Hermitian. There is a matrix P for which

$$P^*AP = I$$
, and $P^*BP = D$, where D is diagonal. (3.7)

Proof. Let $A = U\Lambda U^*$, and define $S = \Lambda^{-1/2}U$. The the matrix S^*U^*BSU is Hermitian; so let V diagonalize it to D. Set P = USV, to obtain

$$P^*AP = V^*S^*U^*U\Lambda U^*USV = V^*U^*\Lambda^{-1/2}\Lambda\Lambda^{-1/2}UV = I;$$

and by construction, it follows that $P^*BP = V^*S^*U^*BUSV = D$.

Accoutered with the above results, we can finally prove Theorem 3.1.

Proof. (Theorem 3.1). We need to show that δ_S is symmetric, nonnegative, definite, and that is satisfies the triangle inequality. Symmetry is obvious. Nonnegativity and definiteness were shown in Prop. 2.5. The only hard part is to prove the triangle inequality, a result that has eluded previous attempts [21,24].

Let X, Y, Z > 0 be arbitrary. From Lemma 3.9 we know that there is a matrix P such that $P^*XP = I$ and $P^*YP = D$. Since Z > 0 is arbitrary, and congruence preserves positive definiteness, we may write just Z instead of P^*ZP . Also, since $\delta_S(P^*XP, P^*YP) = \delta_S(X, Y)$ (see Prop. 2.3), proving the triangle inequality reduces to showing that

$$\delta_S(I, D) \le \delta_S(I, Z) + \delta_S(D, Z). \tag{3.8}$$

Consider now the diagonal matrices D^{\downarrow} and $\operatorname{Eig}^{\downarrow}(Z)$. Theorem 3.6 asserts

$$\delta_S(I, D^{\downarrow}) < \delta_S(I, \operatorname{Eig}^{\downarrow}(Z)) + \delta_S(D^{\downarrow}, \operatorname{Eig}^{\downarrow}(Z)).$$
 (3.9)

Prop. 2.3(i) implies that $\delta_S(I, D) = \delta_S(I, D^{\downarrow})$ and $\delta_S(I, Z) = \delta_S(I, \operatorname{Eig}^{\downarrow}(Z))$, while Corollary 3.8 shows that $\delta_S(D^{\downarrow}, \operatorname{Eig}^{\downarrow}(Z)) \leq \delta_S(D, Z)$. Combining these inequalities, we immediately obtain (3.8).

We now turn our attention to a connection of importance to machine learning and approximation theory: kernel functions related to δ_S . Indeed, some of connections (e.g., Theorem 3.10) have already been recently useful in computer vision [31].

3.1. Hilbert space embedding. Since δ_S is a metric, and Lemma 3.4 shows that for scalars, δ_S embeds isometrically into a Hilbert space, one may ask if $\delta_S(X,Y)$ also admits such an embedding. But as mentioned previously, it is the lack of such an embedding that necessitated a different route to metricity. Let us look more carefully at what goes wrong, and what kind of Hilbert space embeddability does δ_S^2 admit.

Theorem 3.3 implies that a Hilbert space embedding exists if and only if $\delta_S^2(X, Y)$ is a negative definite kernel; equivalently, if and only if the map (cf. Lemma 3.4)

$$e^{-\beta\delta_S^2(X,Y)} = \frac{\det(X)^\beta \det(Y)^\beta}{\det((X+Y)/2)^\beta},$$

is a positive definite kernel for $\beta > 0$. It suffices to check whether the matrix

$$H_{\beta} = [h_{ij}] = [\det(X_i + X_j)^{-\beta}], \quad 1 \le i, j \le m,$$
 (3.10)

is positive definite for every $m \geq 1$ and arbitrary HPD matrices $X_1, \ldots, X_m \in \mathbb{P}_n$.

Unfortunately, a quick numerical experiment reveals that H_{β} can be indefinite. A counterexample is given by the following positive definite matrices (m = 5, n = 2)

$$X_{1} = \begin{bmatrix} 0.1406 & 0.0347 \\ 0.0347 & 0.1779 \end{bmatrix}, \ X_{2} = \begin{bmatrix} 2.0195 & 0.0066 \\ 0.0066 & 0.2321 \end{bmatrix}, \ X_{3} = \begin{bmatrix} 1.0924 & 0.0609 \\ 0.0609 & 1.2520 \end{bmatrix},$$

$$X_{4} = \begin{bmatrix} 1.0309 & 0.8694 \\ 0.8694 & 1.2310 \end{bmatrix}, \ \text{and} \ X_{5} = \begin{bmatrix} 0.2870 & -0.4758 \\ -0.4758 & 2.3569 \end{bmatrix},$$

$$(3.11)$$

and by setting $\beta = 0.1$, for which $\lambda_{\min}(H_{\beta}) = -0.0017$. This counterexample destroys hopes of embedding the metric space (\mathbb{P}_n, δ_S) isometrically into a Hilbert space.

Although matrix (3.10) is not HPD in general, we might ask: For what choices of β is H_{β} HPD? Theorem 3.10 answers this question for H_{β} formed from symmetric real positive definite matrices, and characterizes the values of β necessary and sufficient for H_{β} to be positive definite. We note here that the case $\beta = 1$ was essentially treated in [27], in the context of semigroup kernels on measures.

THEOREM 3.10. Let X_1, \ldots, X_m be real symmetric matrices in \mathbb{P}_n . The $m \times m$ matrix H_β defined by (3.10) is positive definite, if and only if β satisfies

$$\beta \in \left\{ \frac{j}{2} : j \in \mathbb{N}, \text{ and } 1 \le j \le (n-1) \right\} \cup \left\{ \gamma : \gamma \in \mathbb{R}, \text{ and } \gamma > \frac{1}{2}(n-1) \right\}.$$
 (3.12)

Proof. We first prove the "if" part. Recall therefore, the Gaussian integral

$$\int_{\mathbb{R}^n} e^{-x^T X x} dx = \pi^{n/2} \det(X)^{-1/2}.$$

Define the map $f_i := \frac{1}{\pi^{n/4}} e^{-x^T X_i x} \in L_2(\mathbb{R}^n)$, where the inner-product is given by

$$\langle f_i, f_j \rangle := \frac{1}{\pi^{n/2}} \int_{\mathbb{R}^n} e^{-x^T (X_i + X_j) x} dx = \det(X_i + X_j)^{-1/2}.$$

Thus, it follows that $H_{1/2} \geq 0$. The Schur product theorem says that the elementwise product of two positive matrices is again positive. So, in particular H_{β} is positive whenever β is an integer multiple of 1/2. To extend the result to all β covered by (3.12), we invoke another integral representation: the multivariate Gamma function, defined as [42, §2.1.2]

$$\Gamma_n(\beta) := \int_{\mathbb{P}_n} e^{-\operatorname{tr}(A)} \det(A)^{\beta - (n+1)/2} dA, \quad \text{where } \beta > \frac{1}{2}(n-1).$$
 (3.13)

Let $f_i := ce^{-\operatorname{tr}(AX_i)} \in L_2(\mathbb{P}_n)$, for some constant c; then, compute the inner product

$$\langle f_i, f_j \rangle := c' \int_{\mathbb{P}_n} e^{-\operatorname{tr}(A(X_i + X_j))} \det(A)^{\beta - (n+1)/2} dA = \det(X_i + X_j)^{-\beta},$$

which exists if $\beta > \frac{1}{2}(n-1)$. Thus, $H_{\beta} \geq 0$ for all β defined by (3.12).

The converse is a deeper result grounded in the theory of symmetric cones. Specifically, since \mathbb{P}_n is a symmetric cone, and $1/\det(X)$ is decreasing on this cone, an appeal to [30, Thm. VII.3.1] yields the only if part of our claim.

REMARK 3.11. Let \mathcal{X} be a set of HPD matrices that commute with each other. Then, (\mathcal{X}, δ_S) can be isometrically embedded into a Hilbert space. This claim follows because a commuting set of matrices can be simultaneously diagonalized, and for diagonal matrices, $\delta_S^2(X,Y) = \sum_i \delta_s^2(X_{ii},Y_{ii})$, which is a nonnegative sum of negative definite kernels and is therefore itself negative definite.

definite kernels and is therefore itself negative definite.

Theorem 3.10 shows that $e^{-\beta \delta_S^2}$ is not a kernel for all $\beta > 0$, while Remark 3.11 mentions an extreme case for which $e^{-\beta \delta_S^2}$ is always a positive definte kernel. This prompts us to pose the following problem.

Open problem 1. Determine necessary and sufficient conditions on a set $\mathcal{X} \subset \mathbb{P}_n$, so that $e^{-\beta \delta_S^2(X,Y)}$ is a kernel function on $\mathcal{X} \times \mathcal{X}$ for all $\beta > 0$.

4. Connections with δ_R . This section returns to our original motivation: using S as an alternative to the Riemannian metric δ_R . In particular, in this section we show a sequence of results that highlight similarities between S and δ_R . Table 4.1 lists these to provide a quick summary. Thereafter, we develop the details.

Riemannian distance	Ref.	S-Divergence	Ref.
$\delta_R(X^*AX, X^*BX) = \delta_R(A, B)$	[10, Ch.6]	$\delta_S(X^*AX, X^*BX) = \delta_S(A, B)$	Prp.2.3
$\delta_R(A^{-1}, B^{-1}) = \delta_R(A, B)$	[10, Ch.6]	$\delta_S(A^{-1}, B^{-1}) = \delta_S(A, B)$	Prp.2.3
$\delta_R(A \otimes B, A \otimes C) = n\delta_R(B, C)$	E	$\delta_S^2(A \otimes B, A \otimes C) = n\delta_S^2(B, C)$	Prp.2.3
$\delta_R(A^t, B^t) \le t\delta_R(A, B)$	[10, Ex.6.5.4]	$\delta_S^2(A^t, B^t) \le t\delta_S^2(A, B)$	Th.4.5
$\delta_R(A^s, B^s) \le (s/u)\delta_R(A^u, B^u)$	Th.4.8	$\delta_S^2(A^s, B^s) \le (s/u)\delta_S^2(A^u, B^u)$	Th.4.8
$\delta_R(X,A)$ g-convex in X	[10, 6.1.11]	$\delta_S^2(X,Y)$ g-convex in X,Y	Th.4.4
$\delta_R(X^*AX, X^*BX) \le \delta_R(A, B)$	Cor. 4.18	$\delta_S(X^*AX, X^*BX) \le \delta_S(X, Y)$	Th.4.15
$\delta_R(A, A \sharp B) = \delta_R(B, A \sharp B)$	E	$\delta_S(A, A \sharp B) = \delta_S(B, A \sharp B)$	Th.4.1
$\delta_R(A, A\sharp_t B) = t\delta_R(A, B)$	[10, Th.6.1.6]	$\delta_S^2(A, A \sharp_t B) \le t \delta_S^2(A, B)$	Th.4.6
$\delta_R(A\sharp_t B, A\sharp_t C) \le t\delta_R(B, C)$	[10, Th.6.1.2]	$\delta_S^2(A\sharp_t B, A\sharp_t C) \le t\delta_S^2(B, C)$	Th.4.7
$\min_X \delta_R^2(X, A) + \delta_R^2(X, B)$	$[10, \S 6.2.8]$	$\min_X \delta_S^2(X, A) + \delta_S^2(X, B)$	Th.4.1
$\delta_R(A+X,A+Y) \le \delta_R(X,Y)$	[14]	$\delta_S^2(A+X,A+Y) \le \delta_S^2(X,Y)$	Th.4.10

Table 4.1

Similarities between δ_R and δ_S, δ_S^2 at a glance. All matrices are assumed to be in \mathbb{P}_n , except for X in Line 1, $X \in GL_n(\mathbb{C})$, and in Line 7, $X \in \mathbb{C}^{n \times k}$ $(k \leq n, \text{ full colrank})$. The scalars t, s, u satisfy $0 < t \leq 1, 1 \leq s \leq u < \infty$. An 'E' indicates an easily verifiable result.

4.1. Geometric mean. We begin by studying an object that connects δ_R and S most intimately: the matrix *geometric mean* (GM). For HPD matrices A and B, the GM is denoted by $A\sharp B$, and is given by the formula

$$A \sharp B := A^{1/2} (A^{-1/2} B A^{-1/2})^{1/2} A^{1/2}. \tag{4.1}$$

The GM (4.1) has numerous attractive properties—see for instance [1]—among which, the following variational characterization is very important [11]:

$$A\sharp B = \operatorname{argmin}_{X>0} \quad \delta_R^2(A, X) + \delta_R^2(B, X), \quad \text{and}$$

$$\delta_R(A, A\sharp B) = \delta_R(B, A\sharp B).$$
 (4.2)

Surprisingly, the GM enjoys a similar characterization even with δ_S^2 .

Theorem 4.1. Let A, B > 0. Then,

$$A\sharp B = \operatorname{argmin}_{X>0} \quad \left[h(X) := \delta_S^2(X, A) + \delta_S^2(X, B) \right]. \tag{4.3}$$

Moreover, $A \sharp B$ is equidistant from A and B, i.e., $\delta_S(A, A \sharp B) = \delta_S(B, A \sharp B)$.

Proof. If A = B, then clearly X = A minimizes h(X). Assume therefore, that $A \neq B$. Ignoring the constraint X > 0 for the moment, we see that any stationary point of h(X) must satisfy $\nabla h(X) = 0$. This condition translates into

$$\nabla h(X) = \left(\frac{X+A}{2}\right)^{-1} \frac{1}{2} + \left(\frac{X+B}{2}\right)^{-1} \frac{1}{2} - X^{-1} = 0,$$

$$\implies X^{-1} = (X+A)^{-1} + (X+B)^{-1}$$

$$\implies (X+A)X^{-1}(X+B) = 2X + A + B$$

$$\implies B = XA^{-1}X.$$
(4.4)

The last equation is a Riccati equation whose unique, positive definite solution is the geometric mean $X = A \sharp B$ (see [10, Prop 1.2.13]).

Next, we show that this stationary point is a local minimum, not a local maximum or saddle point. To that end, we show that the Hessian is positive definite at the stationary point $X = A \sharp B$. The Hessian of h(X) is given by

$$2\nabla^2 h(X) = X^{-1} \otimes X^{-1} - \left[(X+A)^{-1} \otimes (X+A)^{-1} + (X+B)^{-1} \otimes (X+B)^{-1} \right].$$

Writing $P = (X + A)^{-1}$, and $Q = (X + B)^{-1}$, upon using (4.4) we obtain

$$2\nabla^2 h(X) = (P+Q) \otimes (P+Q) - P \otimes P - Q \otimes Q$$

= $(P+Q) \otimes P + (P+Q) \otimes Q - P \otimes P - Q \otimes Q$
= $(Q \otimes P) + (P \otimes Q) > 0$.

Thus, $X = A \sharp B$ is a *strict* local minimum of (3.2). This local minimum is actually global as $\nabla h(X) = 0$ has a unique positive solution and h goes to $+\infty$ at the boundary. To prove the equidistance, recall that $A \sharp B = B \sharp A$; then observe that

$$\begin{split} S(A, A \sharp B) &= S(A, B \sharp A) = S(A, B^{1/2} (B^{-1/2} A B^{-1/2})^{1/2} B^{1/2}) \\ &= S(B^{-1/2} A B^{-1/2}, (B^{-1/2} A B^{-1/2})^{1/2}) \\ &= S(B^{1/2} (B^{-1/2} A B^{-1/2})^{1/2} B^{1/2}, B) \\ &= S(B \sharp A, B) = S(B, A \sharp B). \end{split}$$

4.2. Geodesic convexity. The above derivation concludes optimality from first principles. It was originally driven by the fact that δ_S is not geodesically convex [48]. However, we recently realized that the square δ_S^2 is actually geodesically convex. This realization leads to more insightful proof of uniqueness and optimality of the S-mean.

In fact even more is true: Theorem 4.4 shows that $\delta_S^2(X, Y)$ is not only geodesically convex, it is *jointly* geodesically convex. Before proving Theorem 4.4, we recall two useful results; the first immediately implies the second⁷.

THEOREM 4.2 ([36]). The GM of $A, B \in \mathbb{P}_n$ is given by the variational formula

$$A\sharp B = \max \big\{ X \in \mathbb{H}_n \mid \left[\begin{smallmatrix} A & X \\ X & B \end{smallmatrix} \right] \ge 0 \big\}.$$

Proposition 4.3 (Joint-concavity (see e.g. [36])). Let A, B, C, D > 0. Then,

$$(A\sharp B) + (C\sharp D) < (A+C)\sharp (B+D). \tag{4.5}$$

⁷It is a minor curiosity to note that [41, Thm. 2] proved a mixed-mean inequality for the matrix geometric and arithmetic means; Prop. 4.3 includes their result as a special case.

Proof. From one application of Thm. 4.2 we have

$$0 \preceq \begin{bmatrix} A & A \sharp B \\ A \sharp B & B \end{bmatrix} + \begin{bmatrix} C & C \sharp D \\ C \sharp D & D \end{bmatrix} = \begin{bmatrix} A + C & A \sharp B + C \sharp D \\ A \sharp B + C \sharp D & B + D \end{bmatrix}.$$

A second application of Thm. 4.2 then immediately yields (4.5).

THEOREM 4.4. The function $\delta_S^2(X,Y)$ is jointly g-convex for X,Y>0. Proof. Since δ_S^2 is continuous, it suffices to show that for $X_1,X_2,Y_1,Y_2>0$,

$$\delta_S^2(X_1 \sharp X_2, Y_1 \sharp Y_2) \le \frac{1}{2} \delta_S^2(X_1, Y_1) + \frac{1}{2} \delta_S^2(X_2, Y_2). \tag{4.6}$$

From Prop. 4.3 it follows that

$$X_1 \sharp X_2 + Y_1 \sharp Y_2 \le (X_1 + Y_1) \sharp (X_2 + Y_2).$$

Since log det is monotonic and determinant is multiplicative, this inequality implies

$$\begin{split} \log \det \left(\frac{X_1 \sharp X_2 + Y_1 \sharp Y_2}{2} \right) &\leq \log \det \left(\frac{(X_1 + Y_1) \sharp (X_2 + Y_2)}{2} \right) \\ &= \frac{1}{2} \log \det \left(\frac{X_1 + Y_1}{2} \right) + \frac{1}{2} \log \det \left(\frac{X_2 + Y_2}{2} \right). \end{split}$$

Combining this inequality with the identity

$$-\frac{1}{2}\log\det((X_1\sharp X_2)(Y_1\sharp Y_2)) = -\frac{1}{4}\log\det(X_1Y_1) - \frac{1}{4}\log\det(X_2Y_2) \tag{4.7}$$

we obtain inequality (4.6), establishing the joint g-convexity.

Since δ_S^2 is geodesically convex (to be precise, we define δ_S to be $+\infty$ whenever either of its arguments fails to be strictly positive), the objective function $h(X) = \sum_i w_i \delta_S^2(X, A_i)$ is also geodesically convex. A quick observation shows that $h(0) = h(\infty) = +\infty$, which suggests that h attains its minimum. Since it is strictly geodesically convex, the solution to $\nabla h(X) = 0$ is unique, and yields the desired minimum.

- **4.3. Basic contraction results.** In this section we show that δ_S and δ_R share several contraction properties. We will state properties either in terms of δ_S^2 or δ_S , depending on whichever appears more elegant.
 - **4.3.1. Power-contraction.** The metric δ_R satisfies (e.g., [10, Exercise 6.5.4])

$$\delta_R(A^t, B^t) \le t\delta_R(A, B), \quad \text{for} \quad A, B > 0 \text{ and } t \in [0, 1].$$
 (4.8)

Theorem 4.5 shows that S-Divergence satisfies the same relation.

THEOREM 4.5. Let A, B > 0, and let $t \in [0, 1]$. Then,

$$\delta_S^2(A^t, B^t) \le t\delta_S^2(A, B). \tag{4.9}$$

Moreover, if $t \geq 1$, then the inequality gets reversed.

Proof. Recall that for $t \in [0,1]$, the map $X \mapsto X^t$ is operator concave. Thus, $\frac{1}{2}(A^t + B^t) \leq \left(\frac{A+B}{2}\right)^t$; by monotonicity of the determinant it then follows that

$$\delta_S^2(A^t, B^t) = \log \frac{\det\left(\frac{1}{2}(A^t + B^t)\right)}{\det(A^t B^t)^{1/2}} \le \log \frac{\det\left(\frac{1}{2}(A + B)\right)^t}{\det(AB)^{t/2}} = t\delta_S^2(A, B).$$

The reverse inequality for $t \geq 1$, follows from (4.9) by considering $\delta_S^2(A^{1/t}, B^{1/t})$. \square

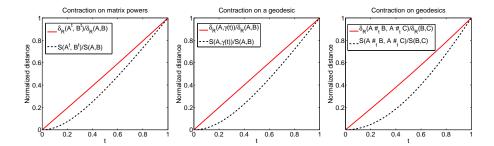


Fig. 4.1. Left to right: Illustration of Theorems 4.5, 4.6 and 4.7. As expected, the S-Divergence (denoted S in the plots) exhibits slightly stronger contraction than δ_R . Interestingly, the curves for δ_R are almost straight lines even for theorems 4.5 and 4.7, while those of S have a more complicated shape; empirically, for random A and B, the curves for S are fit fairly well using a cubic in t.

4.3.2. Contraction on geodesics. The curve

$$\gamma(t) := A^{1/2} (A^{-1/2} B A^{-1/2})^t A^{1/2}, \quad \text{for } t \in [0, 1], \tag{4.10}$$

parameterizes the *unique* geodesic between the positive matrices A and B on the manifold (\mathbb{P}_n, δ_R) [10, Thm. 6.1.6]. On this curve δ_R satisfies

$$\delta_R(A, \gamma(t)) = t\delta_R(A, B), \quad t \in [0, 1].$$

The S-Divergence satisfies a similar, albeit slightly weaker result.

THEOREM 4.6. Let A, B > 0, and $\gamma(t)$ be defined by (4.10). Then,

$$\delta_S^2(A, \gamma(t)) \le t \delta_S^2(A, B), \qquad 0 \le t \le 1. \tag{4.11}$$

Proof. The proof follows upon observing that

$$\begin{split} \delta_S^2(A,\gamma(t)) &= \delta_S^2(I,(A^{-1/2}BA^{-1/2})^t) \\ &\stackrel{(4.9)}{\leq} t \delta_S^2(I,A^{-1/2}BA^{-1/2}) = t \delta_S^2(A,B). \end{split}$$

The GM $A\sharp B$ is the midpoint $\gamma(1/2)$ on the curve (4.10); an arbitrary point on this geodesic is therefore, frequently written as

$$A\sharp_t B := A^{1/2} (A^{-1/2} B A^{-1/2})^t A^{1/2} \quad \text{for } t \in [0, 1]. \tag{4.12}$$

On this geodesics δ_R satisfies the following "cancellation" inequality [10, Thm. 6.1.12]:

$$\delta_R(A\sharp_t B, A\sharp_t C) \le t\delta_R(B, C)$$
 for $A, B, C > 0$, and $t \in [0, 1]$. (4.13)

We show that a similar inequality holds for S.

THEOREM 4.7. Let A, B, C > 0, and $t \in [0, 1]$. Then,

$$\delta_S^2(A\sharp_t B, A\sharp_t C) \le t\delta_S^2(B, C), \qquad t \in [0, 1]. \tag{4.14}$$

Proof. Prop. 2.3 and Theorem 4.5 help prove this claim as follows:

$$\begin{split} \delta_S^2(A\sharp_t B, A\sharp_t C) &= \delta_S^2(A^{1/2}(A^{-1/2}BA^{-1/2})^t A^{1/2}, A^{1/2}(A^{-1/2}CA^{-1/2})^t A^{1/2}) \\ &= \delta_S^2((A^{-1/2}BA^{-1/2})^t, (A^{-1/2}CA^{-1/2})^t) \\ &\overset{\text{Thm. 4.5}}{\leq} t \delta_S^2(A^{-1/2}BA^{-1/2}, A^{-1/2}CA^{-1/2}) = t \delta_S^2(B, C). \quad \Box \end{split}$$

4.3.3. A power-monotonicity property. Above we saw that δ_S^2 and δ_R show similar contractive behavior. Now we show that on matrix powers, they exhibit a similar monotonicity property (akin to a power-means inequality).

THEOREM 4.8. Let A, B > 0. Let scalars t and u satisfy $1 \le t \le u < \infty$. Then,

$$t^{-1}\delta_R(A^t, B^t) \le u^{-1}\delta_R(A^u, B^u) \tag{4.15}$$

$$t^{-1}\delta_S^2(A^t, B^t) \le u^{-1}\delta_S^2(A^u, B^u). \tag{4.16}$$

To our knowledge, even inequality (4.15) is new. Before proving Theorem 4.8 we first prove an auxiliary result (Prop. 4.9).

Let x and y be vectors in \mathbb{R}^n_+ . Denote by z^{\downarrow} the vector obtained by arranging the elements of z in decreasing order. We write,

$$x \prec_{w \log y}$$
, if $\prod_{j=1}^k x_j^{\downarrow} \le \prod_{j=1}^k y_j^{\downarrow}$, for $1 \le k \le n$; and (4.17)

$$x \prec_{\log} y$$
, if $x \prec_{w \log} y$ and $\prod_{j=1}^{n} x_{j}^{\downarrow} = \prod_{j=1}^{n} y_{j}^{\downarrow}$. (4.18)

Relation (4.17) is called *weak log-majorization*, while (4.18) is known as *log majorization* [9, Ch. 2]. Usual *weak majorization* is denoted as:

$$x \prec_w y$$
 if $\sum_{i=1}^k x_j^{\downarrow} \le \sum_{j=1}^k y_j^{\downarrow}$, for $1 \le k \le n$. (4.19)

We now state a simple "power-means" determinantal inequality (which also follows from a more general monotonicity theorem of [8] on power means).

Proposition 4.9. Let A, B > 0; let scalars t, u satisfy $1 \le t \le u < \infty$. Then,

$$\det^{1/t}\left(\frac{A^t + B^t}{2}\right) \le \det^{1/u}\left(\frac{A^u + B^u}{2}\right). \tag{4.20}$$

Proof. Let $P = A^{-1}$, and Q = B. To show (4.20), we may equivalently show that

$$\prod_{j=1}^{n} \left(\frac{1 + \lambda_j(P^t Q^t)}{2} \right)^{1/t} \le \prod_{j=1}^{n} \left(\frac{1 + \lambda_j(P^u Q^u)}{2} \right)^{1/u}. \tag{4.21}$$

Now recall the log-majorization [9, Theorem IX.2.9]:

$$\lambda^{1/t}(P^tQ^t) \prec_{\log} \lambda^{1/u}(P^uQ^u), \tag{4.22}$$

and apply to it the monotonic function $f(r) = \log(1 + r^u)$ to obtain the inequalities

$$\sum_{j=1}^{k} \log(1 + \lambda_j^{u/t}(P^t Q^t)) \le \sum_{j=1}^{k} \log(1 + \lambda_j(P^t Q^t)), \quad 1 \le k \le n.$$

Since log and $r \mapsto r^{1/u}$ are monotonic functions, these inequalities imply that

$$\prod\nolimits_{j = 1}^k {\left({\frac{{1 + \lambda _j^{u/t}(P^tQ^t)}}{2}} \right)^{1/u}} \le \quad \prod\nolimits_{j = 1}^k {\left({\frac{{1 + \lambda _j(P^uQ^u)}}{2}} \right)^{1/u}} \quad 1 \le k \le n.$$

But since $u \ge t$, the function $r \mapsto r^{u/t}$ is convex. Thus,

$$\prod_{j=1}^{k} \left(\frac{1 + \lambda_{j}^{u/t}(P^{t}Q^{t})}{2} \right)^{1/u} \ge \prod_{j=1}^{k} \left[\left(\frac{1 + \lambda_{j}(P^{t}Q^{t})}{2} \right)^{u/t} \right]^{1/u} \\
= \prod_{j=1}^{k} \left(\frac{1 + \lambda_{j}(P^{t}Q^{t})}{2} \right)^{1/t}. \quad \Box$$

Proof (Theorem 4.8).

Part (i): First observe that $\delta_R(X,Y) = \|\log E^{\downarrow}(XY^{-1})\|_F$. Thus, we need to show

$$\frac{1}{t} \|\log E^{\downarrow}(A^t B^{-t})\|_{\mathcal{F}} \le \frac{1}{u} \|\log E^{\downarrow}(A^u B^{-u})\|_{\mathcal{F}}.$$

Equivalently, for vectors of eigenvalues we may prove

$$\|\log \lambda^{1/t} (A^t B^{-t})\|_2 \le \|\log \lambda^{1/u} (A^u B^{-u})\|_2.$$
 (4.23)

The log-majorization (4.22) yields the majorization inequality

$$\log \lambda^{1/t} (A^t B^{-t}) \prec \log \lambda^{1/u} (A^u B^{-u}),$$

to which we apply the map $x \mapsto ||x||_2$ immediately obtaining (4.23). Notice, that we have in fact proved the more general result

$$\frac{1}{t} \|\log E^{\downarrow}(A^t B^{-t})\|_{\Phi} \leq \frac{1}{u} \|\log E^{\downarrow}(A^u B^{-u})\|_{\Phi},$$

where Φ is a symmetric gauge function (a permutation invariant absolute norm). Part (ii): To prove (4.16) we must show that

$$\frac{1}{t} \log \det((A^t + B^t)/2) - \frac{t}{2} \log \det(A^t B^t) \le \frac{1}{u} \log \det((A^u + B^u)/2) - \frac{u}{2} \log \det(A^u B^u).$$

But this inequality is immediate from Prop. 4.9 and the monotonicity of log. \Box

4.3.4. Contraction under translation. The last basic contraction result that we prove is an analogue of the following important property [14, Prop. 1.6]:

$$\delta_R(A+X,A+Y) \le \frac{\alpha}{\alpha+\beta}\delta_R(X,Y), \quad \text{for } A \ge 0, \text{ and } X,Y > 0,$$
 (4.24)

where $\alpha = \max\{\|X\|, \|Y\|\}$ and $\beta = \lambda_{\min}(A)$. This result plays a key role in deriving contractive maps for solving certain nonlinear matrix equations [39].

We show a similar result for the S-Divergence.

Theorem 4.10. Let X, Y > 0, and $A \ge 0$, then

$$g(A) := \delta_S^2(A + X, A + Y),$$
 (4.25)

is monotonically decreasing and convex in A.

Proof. We wish to show that if $A \leq B$, then $g(A) \geq g(B)$. Equivalently, we can show that the gradient $\nabla_A g(A) \leq 0$ [16, Section 3.6]; to that end, we compute

$$\nabla_A g(A) = \left(\frac{(A+X)+(A+Y)}{2}\right)^{-1} - \frac{1}{2}(A+X)^{-1} - \frac{1}{2}(A+Y)^{-1},$$

which is easily seen to be negative since $X\mapsto X^{-1}$ is operator convex.

To prove that g is convex, we look at its Hessian $\nabla^2 g(A)$. Using the shorthand $P = (A + X)^{-1}$ and $Q = (B + X)^{-1}$, this Hessian is seen to be

$$\nabla^2 g(A) = \frac{1}{2} (P \otimes P + Q \otimes Q) - \left(\frac{P^{-1} + Q^{-1}}{2} \right)^{-1} \otimes \left(\frac{P^{-1} + Q^{-1}}{2} \right)^{-1}.$$

Again using operator convexity of $X \mapsto X^{-1}$ we obtain

$$\nabla^2 g(A) \ge \frac{P \otimes P + Q \otimes Q}{2} - \frac{P + Q}{2} \otimes \frac{P + Q}{2}$$

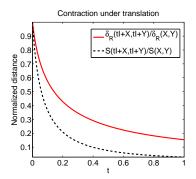


FIG. 4.2. Illustration of Thm. 4.10. The plot shows the amount of contraction displayed by δ_R and δ_S^2 , for a pair of matrices X and Y with eigenvalues in (0,1), when translated by tI $(t \in [0,1])$. We see that S is more contractive than δ_R ; more interestingly, the shape of the two curves is similar.

which is easily seen to be semidefinite because $P \geq Q$ and

$$P \otimes P + Q \otimes Q - P \otimes Q + Q \otimes P = (P - Q) \otimes (P - Q) \ge 0.$$

The following corollary is immediate (cf. (4.24)).

COROLLARY 4.11. Let X, Y > 0, $A \ge 0$, $\beta = \lambda_{\min}(A)$. Then,

$$\delta_S^2(A+X, A+Y) \le \delta_S^2(\beta I + X, \beta I + Y) \le \delta_S^2(X, Y).$$
 (4.26)

4.4. Contraction under compression. In this section we establish a powerful compression property of the S-divergence, which connects it intimately with the Hilbert and Thompson metrics. We begin by setting up a few key results.

PROPOSITION 4.12. Let $P \in \mathbb{C}^{n \times k}$ $(k \leq n)$ have full column rank. The function $f : \mathbb{P}_n \to \mathbb{R} \equiv X \mapsto \log \det(P^*XP) - \log \det(X)$ is operator decreasing.

Proof. It suffices to show that $\nabla f(X) \leq 0$. This amounts to establishing that

$$P(P^*XP)^{-1}P^* \le X^{-1} \Leftrightarrow \begin{bmatrix} X^{-1} & P \\ P^* & P^*XP \end{bmatrix} \ge 0.$$
 (4.27)

Since $\begin{bmatrix} X^{-1} & I \\ I & X \end{bmatrix} \ge 0$, the inequality (4.27) follows immediately upon realizing that

$$\begin{bmatrix} X^{-1} & P \\ P^* & P^*XP \end{bmatrix} = \begin{bmatrix} I & 0 \\ 0 & P^* \end{bmatrix} \begin{bmatrix} X^{-1} & I \\ I & X \end{bmatrix} \begin{bmatrix} I & 0 \\ 0 & P \end{bmatrix}. \quad \Box$$

COROLLARY 4.13. Let X, Y > 0. Let $A = \left(\frac{X+Y}{2}\right)$, $G = X \sharp Y$; and let $P \in \mathbb{C}^{n \times k}$ $(k \leq n)$ have full column rank. Then,

$$\frac{\det(P^*AP)}{\det(P^*GP)} \le \frac{\det(A)}{\det(G)}.$$
(4.28)

Proof. Since $A \geq G$, it follows from Prop. 4.12 that

$$\log \det(P^*AP) - \log \det(A) \le \log \det(P^*GP) - \log \det(G).$$

Rearranging, and using the fact that $P^*AP \ge P^*GP$, we obtain (4.28).

THEOREM 4.14 ([1, Thm. 3]). Let $\Pi : \mathbb{P}_n \to \mathbb{P}_k$ be a positive linear map. Then,

$$\Pi(A\sharp B) \le \Pi(A)\sharp \Pi(B) \quad \text{for } A, B \in \mathbb{P}_n.$$
 (4.29)

We are now ready to prove the main theorem of this section.

THEOREM 4.15. Let $P \in \mathbb{C}^{n \times k}$ $(k \leq n)$ have full column rank. Then,

$$\delta_S^2(P^*AP, P^*BP) \le \delta_S^2(A, B) \qquad \text{for } A, B \in \mathbb{P}_n. \tag{4.30}$$

Proof. Observe that (4.30) does not follow from the known inequality $f(U^*AU) \leq U^*f(A)U$ for operator convex f, because δ_S^2 is nonconvex. We need to show that

$$\log \frac{\det\left(\frac{P^*(A+B)P}{2}\right)}{\sqrt{\det(P^*AP)\det(P^*BP)}} \le \log \frac{\det\left(\frac{A+B}{2}\right)}{\sqrt{\det(AB)}}.$$
 (4.31)

From Prop. 4.14 it follows that $P^*(A\sharp B)P \leq (P^*AP)\sharp (P^*BP)$, which implies that

$$\frac{1}{\sqrt{\det(P^*AP)\det(P^*BP)}} = \frac{1}{\det[(P^*AP)\sharp(P^*BP)]} \leq \frac{1}{\det(P^*(A\sharp B)P)}.$$

Invoking Corollary 4.13 and taking logarithms we obtain (4.31).

Corollary 4.16. Let A, B, C, D > 0; let \circ denote the Hadamard product. Then,

$$\delta_S^2(A \circ B, C \circ D) \le \delta_S^2(A \otimes B, C \otimes D). \tag{4.32}$$

Proof. We know that $A \circ B$ is a principal submatrix of $A \otimes B$. In particular, there is a projection P such that $P^*(A \otimes B)P = A \circ B$. So, (4.32) reduces to showing that $\delta_S^2(P^*(A \otimes B)P, P^*(C \otimes D)P) \leq \delta_S^2(A \otimes B, C \otimes D)$, which follows from Thm. 4.15. \square

One may wonder if Theorem 4.15 holds more generally for all positive linear maps, not just congruence transforms. The answer turns out to be negative, as may be seen by considering $\Pi: X \mapsto X \oplus X$. Then, $\delta_S^2(\Pi(X), \Pi(Y)) = 2\delta_S^2(X, Y) \not\leq \delta_S^2(X, Y)$.

Next, one may ask whether a Theorem 4.15 extends to δ_R ? Corollary 4.18 shows that this compression does extend to δ_R , and actually follows from a more general theorem (Theorem 4.17); we believe that this basic theorem must exist in the literature, but provide our own proof for completeness.

THEOREM 4.17. Let $A, B \in \mathbb{P}_n$, and $P \in \mathbb{C}^{n \times k}$ $(k \leq n)$ have full colrank. Then,

$$\lambda_j^{\downarrow}(P^*AP, P^*BP) \le \lambda_j^{\downarrow}(A, B), \quad 1 \le j \le k. \tag{4.33}$$

Proof. Since B positive definite, the eigenvalue min-max theorem shows that

$$\lambda_j^{\downarrow}(A, B) = \min_{\dim V = j} \max_{x \in V} \frac{x^* A x}{x^* B x}.$$

From this variational representation it follows that

$$\lambda_{j}^{\downarrow}(A,B) = \min_{\dim V = j} \max_{w \in V} \frac{w^{*}Aw}{w^{*}Bw} \geq \min_{\dim V = j} \max_{w = Px, w \in V, x \neq 0} \frac{w^{*}Aw}{w^{*}Bw}$$
$$= \min_{\dim V = j} \max_{x \in V} \frac{x^{*}P^{*}APx}{x^{*}P^{*}BPx} = \lambda_{j}^{\downarrow}(P^{*}AP, P^{*}BP).$$

The second-to-last equality above holds since $\{Px|x \neq 0\}$ is a subspace of dimension j, due to P having full column rank.

COROLLARY 4.18. Let $P \in \mathbb{C}^{n \times k}$ $(k \leq n)$ have full column rank. Then,

$$\delta_{\Phi}(P^*AP, P^*BP) \le \delta_{\Phi}(A, B), \tag{4.34}$$

where Φ is any symmetric gauge function.

Proof. Recall that $\delta_{\Phi}(A, B) = \|\log E^{\downarrow}(A^{-1}B)\|_{\Phi}$. Thus, our task is to show that

$$\|\log E^{\downarrow}(P^*AP(P^*BP)^{-1})\|_{\Phi} \le \delta_{\Phi}(A, B).$$
 (4.35)

This result follows by realizing that $\lambda(A^{-1}B) = \lambda(A, B)$ and invoking Theorem 4.17.

4.5. Differences between δ_S and δ_R . So far we have highlighted similarities between δ_S and δ_R . It is worthwhile to highlight some differences too. Since we have implicitly already covered this ground, we summarize these differences in Table 4.2.

Riemannian metric	Ref.	S-Divergence	Ref.		
Eigenvalue computations needed	E	Cholesky decompositions suffice	E		
$e^{-\beta \delta_R^2(X,Y)}$ usually not a kernel	E	$e^{-\beta \delta_S^2(X,Y)}$ a kernel for many β	Th.3.10		
δ_R geodesically convex	[10, Th.6]	δ_S not geodesically convex	E		
(\mathbb{P}_n, δ_R) is a CAT(0)-space	[10, Ch.6]	(\mathbb{P}_n, δ_S) not a CAT(0)-space	E		
Computing means with δ_R^2 difficult	[13]	Computing means with δ_S^2 easier	Sec. 4.1		
Table 4.2					

Some differences between δ_R and δ_S at a glance. An 'E' indicates that it is easy to verify the claim or to find a counterexample.

4.6. Bi-Lipschitz-like comparison. We end our discussion of relations between δ_R and δ_S by showing how they directly compare with each other; here, our main result is the sandwiching inequality (4.36).

THEOREM 4.19. Let $A, B \in \mathbb{P}_n$. Then, we have the following bounds

$$8\delta_S^2(A, B) \le \delta_R^2(A, B) \le 2\delta_T(A, B) (\delta_S^2(A, B) + n \log 2).$$
 (4.36)

Proof. First we establish the upper bound. To that end, we first rewrite δ_R as

$$\delta_R(A, B) := \left(\sum_i \log^2 \lambda_i (AB^{-1})\right)^{1/2}.$$
 (4.37)

Since $\lambda_i(AB^{-1}) > 0$, we may write $\lambda_i(AB^{-1}) := e^{u_i}$ for some u_i , whereby

$$\delta_R(A, B) = ||u|| \text{ and } \delta_T(A, B) = ||u||_{\infty}.$$
 (4.38)

Using the same notation we also obtain

$$\delta_S^2(A, B) = \sum_{i} (\log(1 + e^{u_i}) - u_i/2 - \log 2). \tag{4.39}$$

To relate the quantities (4.38) and (4.39), it is helpful to consider the function

$$f(u) := \log(1 + e^u) - u/2 - \log 2.$$

If u < 0, then $\log(1 + e^u) \ge \log 1 = 0$ holds and -u/2 = |u|/2; while if $u \ge 0$, then $\log(1 + e^u) \ge \log e^u = u$ holds. For both cases, we have the inequality

$$f(u) \ge |u|/2 - \log 2. \tag{4.40}$$

Since $\delta_S^2(A,B) = \sum_i f(u_i)$, inequality (4.40) leads to the bound

$$\delta_S^2(A, B) \ge -n \log 2 + \frac{1}{2} \sum_i |u_i| = \frac{1}{2} ||u||_1 - n \log 2.$$
 (4.41)

From Hölder's inequality we know that $u^T u \leq ||u||_{\infty} ||u||_1$; so we immediately obtain

$$\delta_B^2(A, B) \le 2\delta_T(A, B)(\delta_S^2(A, B) + n \log 2).$$

To obtain the lower bound, consider the function

$$g(u,\sigma) := u^T u - \sigma(\log(1 + e^u) - u/2 - \log 2). \tag{4.42}$$

The first and second derivatives of q with respect to u are given by

$$g'(u,\sigma) = 2u - \frac{\sigma e^u}{1 + e^u} + \frac{\sigma}{2}, \qquad g''(u,\sigma) = 2 - \frac{\sigma e^u}{(1 + e^u)^2}.$$

Observe that for $u=0, \ g'(u,\sigma)=0$. To ensure that 0 is the minimizer of (4.42), we now determine the largest value of σ for which $g''\geq 0$. Write $z:=e^u$; we wish to ensure that $\sigma z/(1+z)^2\leq 2$. Since $z\geq 0$, the arithmetic-geometric inequality shows that $\frac{z}{(1+z)^2}=\frac{\sqrt{z}}{1+z}\frac{\sqrt{z}}{1+z}\leq \frac{1}{4}$. Thus, for $0\leq \sigma\leq 8$, the inequality $\sigma z/(1+z)^2\leq 2$ holds (or equivalently $g''(u,\sigma)\geq 0$). Hence, $0=g(0,\sigma)\leq g(u,\sigma)$, which implies that

$$\delta_R^2(A,B) - \sigma \delta_S^2(A,B) = \sum\nolimits_i g(u_i,\sigma) \ge 0, \quad \text{for } 0 \le \sigma \le 8.$$

5. S-Divergence-mean. We briefly mention the (nonconvex) problem of computing means for collection of input positive definite matrices. Similar conclusions (using different arguments) were previously obtained in [21]—our analysis provides a complementary view.

Given input matrices $A_1, \ldots, A_m \in \mathbb{P}_n$ and nonnegative weights $w_i \geq 0$ such that $\sum_{i=1}^m w_i = 1$, the *S-mean* problem is to compute

$$\min_{X>0} h(X) := \sum_{i=1}^{m} w_i \delta_S^2(X, A_i), \tag{5.1}$$

This problem was essentially studied in [24], and more thoroughly investigated by [21]. Both [21,24] considered the necessary optimality condition (ignoring X > 0 for now)

$$\nabla h(X) = 0 \quad \Leftrightarrow \quad X^{-1} = \sum_{i} w_i \left(\frac{X + A_i}{2}\right)^{-1}, \tag{5.2}$$

and both made a minor oversight by claiming the unique positive definite solution to (5.2) to be the global minimum of (5.1), whereas their proofs established only stationarity, neither global nor local optimality. This oversight is easily fixed.

Since δ_S^2 is strictly geodesically convex (Theorem 4.4), it follows that h(X) is also strictly geodesically convex. Thus, once existence of a minimizer has been established, its uniqueness is immediate—moreover, ensuring (5.2) is also sufficient. Existence is also easy, because if $X \to 0$ or $X \to \infty$, the objective $h(X) \to \infty$.

 $^{^{8}}$ We thank an anonymous referee for alerting us to the need of invoking the boundary behavior.

6. S-Divergence-median. Instead of minimizing a sum-of-squared distances, the geometric median problem seeks a solution to

$$\min_{X>0} \quad \phi(X) := \sum_{i=1}^{m} w_i \delta_S(X, A_i). \tag{6.1}$$

In some cases, geometric medians are more preferred than geometric means as they may be more robust [2, 19, 46]. The S-median (6.1) was recently also studied by [19], who used it for an application in diffusion tensor imaging.

To solve (6.1) we make the simplifying assumption that the median $\neq A_i$ for any $1 \le i \le m$ —in particular, for all $X \ne A_i$, $\phi(X)$ is differentiable. As before ignoring the constraint X > 0, we then obtain the first-order necessary condition

$$\nabla \phi(X) = \sum_{i=1}^{m} \frac{w_i}{\delta_S(X, A_i)} \left[\left(\frac{X + A_i}{2} \right)^{-1} - X^{-1} \right] = 0.$$
 (6.2)

For solving (6.2), [19] propose the iterating the following nonlinear map⁹

$$\mathcal{G}(X) = \sum_{i=1}^{m} \frac{w_i}{\delta_S(X, A_i)} \left[\sum_{i=1}^{m} \frac{w_i}{\delta_S(X, A_i)} \left(\frac{X + A_i}{2} \right)^{-1} \right]^{-1}.$$
 (6.3)

In [19] the authors claim the iteration $X_{k+1} = \mathcal{G}(X_k)$ to be a contraction under the Thompson metric, and use that claim to deduce existence, uniqueness, and construction of the S-median. Unfortunately, their contraction claim is erroneous. Indeed,

$$X = \begin{bmatrix} 10 & 3 \\ 3 & 9 \end{bmatrix}, \quad Y = \begin{bmatrix} 8 & -6 \\ -6 & 45 \end{bmatrix}, \quad A_1 = \begin{bmatrix} 5 & 5 \\ 5 & 10 \end{bmatrix}, \quad A_2 = \begin{bmatrix} 10 & 1 \\ 1 & 5 \end{bmatrix}, w_1 = w_2 = \frac{1}{2},$$

$$\implies \quad \delta_T(\mathcal{G}(X), \mathcal{G}(Y)) = 2.9314 > \delta_T(X, Y) = 1.8324,$$

which shows that $\mathcal{G}(X)$ is not a contraction under the Thompson metric δ_T .

Fortunately, the map (6.3) still leads to a valid fixed-point iteration, but with a different choice of metric. Specifically, instead of δ_T , we propose to use Hilbert's projective metric on \mathbb{P}_n which is given by [35, 40, see e.g.,]:

$$\delta_H(X,Y) := \log\left(\frac{\lambda_M(X,Y)}{\lambda_m(X,Y)}\right),$$
(6.4)

where λ_M (λ_m) denotes the largest (smallest) generalized eigenvalue of (X,Y).

To prove our main result (Theorem 6.2) for this section we need to first recall the following key properties of δ_H .

Proposition 6.1. The Hilbert projective metric δ_H satisfies the following:

- (i) $\delta_H(X^{-1}, Y^{-1}) = \delta_H(X, Y)$

- (ii) $\delta_H(\alpha X, \beta Y) = \delta_H(X, Y)$ for all $\alpha, \beta > 0$ and X, Y > 0. (iii) $\delta_H(\sum_{i=1}^m a_i X_i, \sum_{i=1}^m b_i Y_i) \leq \max_{1 \leq i \leq m} \delta_H(X_i, Y_i)$, for $a_i, b_i > 0$ and $X_i, Y_i > 0$. (iv) Let $A \geq 0$ and X, Y > 0; then, $\delta_H(A + X, A + Y) \leq \frac{\alpha}{\alpha + \beta} \delta_H(X, Y)$, where $\alpha = \max(\|X\|, \|Y\|)$ and $\beta = \lambda_{\min}(A)$.

Proof. Property (i) is obvious; (ii) is well-known [35]; (iii) follows the same argument as for δ_T in [38, Lemma 10.1(iv)]; and (iv) follows from [14, Prop. 1.6].

⁹There is a typo in [19]; the correct formula (6.2) is mentioned in [20, pg.19].

THEOREM 6.2. Let $A_i > 0$ $(1 \le i \le m)$, $w_i \ge 0$ with $\sum_{i=1}^m w_i = 1$. Let $\mathcal{G}: \mathbb{P}_n \to \mathbb{P}_n$ be the nonlinear map defined (6.3). Then, \mathcal{G} is nonexpansive in δ_H , i.e.,

$$\delta_H(\mathcal{G}(X), \mathcal{G}(Y)) \le \delta_H(X, Y), \qquad X, Y > 0,$$

Moreover, \mathcal{G} is contractive if not all A_i are equal (and $X \neq Y$).

Proof. The projective property (Prop. 6.1-(ii)) of δ_H proves crucial for analyzing (6.3). Indeed, write $\mathcal{G}(X) = \alpha(X)\mathcal{F}(X)$, where

$$\alpha(X) := \sum_{i=1}^{m} \frac{w_i}{\delta_S(X, A_i)} \quad \text{and} \quad \mathcal{F}(X) = \left[\sum_{i=1}^{m} \frac{w_i}{\delta_S(X, A_i)} \left(\frac{X + A_i}{2} \right)^{-1} \right]^{-1}.$$

Thus, we may perform the following calculations

$$\begin{split} \delta_{H}(\mathcal{G}(X),\mathcal{G}(Y)) &= \delta_{H}(\alpha(X)\mathcal{F}(X),\alpha(Y)\mathcal{F}(Y)) \\ &= \delta_{H}(\mathcal{F}(X),\mathcal{F}(Y)) \\ &\leq \delta_{H}(\sum_{i=1}^{m} \frac{w_{i}}{\delta_{S}(X,A_{i})} \left(\frac{X+A_{i}}{2}\right)^{-1}, \sum_{i=1}^{m} \frac{w_{i}}{\delta_{S}(X,A_{i})} \left(\frac{Y+A_{i}}{2}\right)^{-1}) \\ &\leq \max_{1 \leq i \leq m} \delta_{H}(X_{i},Y_{i}), \qquad X_{i} = X + A_{i}, Y_{i} = Y + A_{i} \\ &= \max_{1 \leq i \leq m} \delta_{H}(X+A_{i},Y+A_{i}) \\ &\leq \max_{1 \leq i \leq m} \gamma_{i} \delta_{H}(X,Y), \qquad \gamma_{i} < 1 \\ &= \gamma \delta_{H}(X,Y). \end{split}$$

where $\gamma_i := \text{and } \gamma := \max_{1 \leq i \leq m} \gamma_i$. The second inequality above uses Prop. 6.1-(ii),(iii), while the third one invokes Prop. 6.1-(iv). Clearly, if $X \neq Y$ and not all A_i are equal (in which case the median is just A_1), \mathcal{G} is a strict contraction.

COROLLARY 6.3. Starting with a suitable $X_0 > 0$, let $\{X_k\}_{k \geq 0}$ be the sequence generated by $X_{k+1} = \mathcal{G}(X_k)$. Assume that none of the A_i s is the median, and that $\delta_S(X_k, A_i) > 0$ for all k and i. Then, the sequence $\{X_k\}$ converges to a point X_* that is the unique positive definite solution to (6.2), and this point is the S-median.

Proof. Observe that $\phi(0) = \phi(X) = +\infty$; thus, since $\phi(X)$ is continuous on \mathbb{P}_n it must attain its minimum in the interior. Thus, (6.2) must have a positive definite solution. The metric space $(\{X \geq 0\}, \delta_H)$ is complete [35], and Theorem 6.2 shows that under our assumptions, \mathcal{G} is a strict contraction in δ_H . Therefore, if (6.3) has a solution, then from the fixed-point theorem of Edelstein [29], it follows that \mathcal{G} generates iterates which stay within a compact set and converge to the unique fixed point of \mathcal{G} . This fixed-point is positive definite by construction, and satisfies (6.2), whereby it is the desired S-median.

Figure 6.1 illustrates empirical behavior of the fixed-point (FP) iteration $X_{k+1} = \mathcal{G}(X_k)$ on three different collections of positive matrices. The plot compares the FP iteration against a manifold based conjugate gradient method by showing Frobenius norms of the gradients $\nabla \phi$ obtained as a function of running time. The FP iteration turns out to run remarkably faster than the manifold conjugate gradient method (taken from [15]). Both the compared methods are implemented in MATLAB and the experiments were run on a personal laptop with a quadcore Intel i7-3520M (2.90Ghz) processor under the Ubuntu 12.10 operating system.

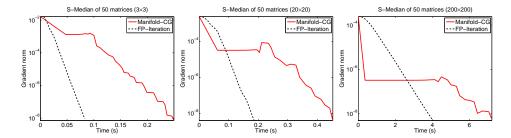


FIG. 6.1. Convergence comparison between fixed-point iteration using (6.3) and the Riemannian conjugate-gradient method from MANOPT [15]. The plots report the gradient-norm $\|\nabla \phi\|_F$ as a function of running time (secs) for collections of random (Wishart) matrices in \mathbb{P}_3 , \mathbb{P}_{20} , and \mathbb{P}_{200} .

7. Discussion and Future Work. In this paper we studied the S-Divergence (and its square-root) on positive definite matrices. We derived numerous results that uncovered qualitative similarities between the S-Divergence and the Riemannian distance on the manifold of Hermitian positive definite matrices. Notably, we showed that the square root of the S-Divergence actually defines a distance, albeit one that does not isometrically embed into any Hilbert space. As an application, we briefly discussed the problems of computing means and medians using the S-Divergence, and provided a fixed-point algorithm for computing medians of positive definite matrices.

Several directions of future work are open. We mention some below.

- Deriving refinements of the main inequalities presented in this paper.
- Studying properties of the metric space (\mathbb{P}^d, δ_S)
- Characterizing the subclass $\mathcal{X} \subset \mathbb{P}^d$ of positive matrices for which (\mathcal{X}, δ_S) admits an isometric Hilbert space embedding.
- Developing better algorithms to compute the S-mean and the S-median.
- Identifying more applications where δ_S^2 (or δ_S) can be useful.

We hope that our paper encourages other researchers to investigate new properties and applications of the S-Divergence.

Acknowledgments. I am grateful to Jeff Bilmes for hosting me at the EE Department at the University of Washington, during my unforeseen visit in July 2011. It was there where I first found the proof of Theorem 3.1.

REFERENCES

- [1] T. Ando, Concavity of certain maps on positive definite matrices and applications to hadamard products, Linear Algebra and its Applications, 26 (1979), pp. 203–241.
- [2] M. Arnaudon, F. Barbaresco, and Le Yang, Riemannian medians and means with applications to radar signal processing, IEEE Journal of Selected Topics in Signal Processing, 7 (2013), pp. 595–604.
- [3] V. Arsigny, P. Fillard, X. Pennec, and N. Ayache, Geometric means in a novel vector space structure on symmetric positive-definite matrices, SIAM J. Matrix Analysis and Applications, 29 (2008), p. 328.
- [4] A. BANERJEE, S. MERUGU, I. S. DHILLON, AND J. GHOSH, Clustering with Bregman Divergences, in SIAM International Conf. on Data Mining, Lake Buena Vista, Florida, April 2004, SIAM.
- [5] H. H. BAUSCHKE AND J. M. BORWEIN, Legendre functions and the method of random Bregman projections, Journal of Convex Analysis, 4 (1997), pp. 27–67.
- [6] A. Ben-Tal and A. Nemirovksii, Lectures on modern convex optimization: Analysis, algorithms, and engineering applications, SIAM, 2001.
- [7] C. Berg, J. P. R. Christensen, and P. Ressel, Harmonic analysis on semigroups: theory of positive definite and related functions, vol. 100 of GTM, Springer, 1984.

- [8] K. V. BHAGWAT AND R. SUBRAMANIAN, Inequalities between means of positive operators, Mathematical Proceedings of the Cambridge Philosophical Society, 83 (1978), pp. 393–401.
- [9] R. Bhatia, Matrix Analysis, Springer, 1997.
- [10] ——, Positive Definite Matrices, Princeton University Press, 2007.
- [11] R. Bhatia and J. A. R. Holbrook, *Riemannian geometry and matrix geometric means*, Linear Algebra Appl., 413 (2006), pp. 594–618.
- [12] A. BHATTACHARYYA, On a measure of divergence between two statistical populations defined by their probability distributions, Bull. Calcutta Math. Soc., 35 (1943), pp. 99–109.
- [13] D. A. BINI AND B. IANNAZZO, Computing the Karcher mean of symmetric positive definite matrices, Linear Algebra and its Applications, (2011). Available online.
- [14] P. BOUGEROL, Kalman Filtering with Random Coefficients and Contractions, SIAM J. Control Optim., 31 (1993), pp. 942–959.
- [15] N. BOUMAL, B. MISHRA, P.-A. ABSIL, AND R. SEPULCHRE, Manopt: a matlab toolbox for optimization on manifolds, arXiv Preprint 1308.5200, (2013).
- [16] S. BOYD AND L. VANDENBERGHE, Convex Optimization, Cambridge University Press, March 2004.
- [17] M. R. Bridson and A. Haeflinger, Metric Spaces of Non-Positive Curvature, Springer, 1999.
- [18] Y. CENSOR AND S. A. ZENIOS, Parallel Optimization: Theory, Algorithms, and Applications, Numerical Mathematics and Scientific Computation, Oxford University Press, 1997.
- [19] M. CHARFI, Z. CHEBBI, M. MOAKHER, AND B. C. VEMURI, Bhattacharyya median of symmetric positive-definite matrices and application to the denoising of diffusion-tensor fields, in IEEE 10th International Symposium on Biomedical Imaging (ISBI), 2013.
- [20] ——, Using the Bhattacharyya Mean for the Filtering and Clustering of Positive-Definite Matrices. http://www.see.asso.fr/file/4870/download/9637, August 2013.
- [21] Z. CHEBBI AND M. MOAHKER, Means of hermitian positive-definite matrices based on the log-determinant α-divergence function, Linear Algebra and its Applications, 436 (2012), pp. 1872–1889.
- [22] P. CHEN, Y. CHEN, AND M. RAO, Metrics defined by Bregman divergences: Part I, Communications on Mathematical Sciences, 6 (2008), pp. 9915–926.
- [23] ——, Metrics defined by Bregman divergences: Part II, Commun. Math. Sci., 6 (2008), pp. 927–948.
- [24] A. CHERIAN, S. SRA, A. BANERJEE, AND N. PAPANIKOLOPOULOS, Efficient Similarity Search for Covariance Matrices via the Jensen-Bregman LogDet Divergence, in International Conference on Computer Vision (ICCV), Nov. 2011, pp. 2399–2406.
- [25] ——, Jensen-Bregman LogDet Divergence with Application to Efficient Similarity Search for Covariance Matrices, IEEE Transactions on Pattern Analysis and Machine Intelligence (TPAMI), (2012).
- [26] T. M. COVER AND J. A. THOMAS, Elements of Information Theory, Wiley-Interscience, 1991.
- [27] M. CUTURI, K. FUKUMIZU, AND J. P. VERT, Semigroup kernels on measures, JMLR, 6 (2005), pp. 1169–1198.
- [28] I. S. DHILLON AND J. A. TROPP, Matrix Nearness Problems with Bregman Divergences, SIAM Journal on Matrix Analysis and Applications, 29 (2007), pp. 1120–1146.
- [29] M. EDELSTEIN, On Fixed and Periodic Points Under Contractive Mappings, Journal of the London Mathematical Society, s1-37 (1962), pp. 74-79.
- [30] J. FARAUT AND A. KORÁNYI, Analysis on Symmetric Cones, Clarendon Press, 1994.
- [31] M. HARANDI, C. SANDERSON, R. HARTLEY, AND B. LOVELL, Sparse Coding and Dictionary Learning for Symmetric Positive Definite Matrices: A Kernel Approach, in European Conference on Computer Vision (ECCV), 2012.
- [32] S. Helgason, Geometric Analysis on Symmetric Spaces, no. 39 in Mathematical Surveys and Monographs, AMS, second ed., 2008.
- [33] F. HIAI AND D. Petz, Riemannian metrics on positive definite matrices related to means, Linear Algebra and its Applications, 430 (2009), pp. 3105–3130.
- [34] B. Jeuris, R. Vandebril, and B. Vandereycken, A survey and comparison of contemporary algorithms for computing the matrix geometric mean, Electronic Transactions on Numerical Analysis, 39 (2012), pp. 379–402.
- [35] K. KOUFANY, Application of Hilbert's projective metric on symmetric cones, Acta Math. Sinica (Engl.), 22 (2006), pp. 1467–1472.
- [36] F. KUBO AND T. ANDO, Means of positive linear operators, Mathematische Annalen, 246 (1980), pp. 205–224.
- [37] B. Kulis, M. Sustik, and I. Dhillon, Low-Rank Kernel Learning with Bregman Matrix Divergences, Journal of Machine Learning Research, 10 (2009), pp. 341–376.
- [38] J. LAWSON AND Y. LIM, A general framework for extending means to higher orders, Colloq.

- Math., 113 (2008), pp. 191-221. (arXiv:math/0612293).
- [39] H. LEE AND Y. LIM, Invariant metrics, contractions and nonlinear matrix equations, Nonlinearity, 21 (2008), pp. 857–878.
- [40] B. LEMMENS AND R. NUSSBAUM, Nonlinear Perron-Frobenius Theory, Cambridge Univ. Press, 2012.
- [41] B. Mond and J.E. Pecčarić., A mixed arithmetic-mean-harmonic-mean matrix inequality, Linear Algebra and its Applications, 237 (1996), pp. 449–454.
- [42] R. J. Muirhead, Aspects of multivariate statistical theory, Wiley Interscience, 1982.
- [43] Yu. Nesterov and A. Nemirovskii, Interior-Point Polynomial Algorithms in Convex Programming, SIAM, 1987.
- [44] Yu. Nesterov and M. J. Todd, On the Riemannian geometry defined for self-concordant barriers and interior point methods, Found. Comput. Math., 2 (2002), pp. 333–361.
- [45] F. NIELSEN, Sided and symmetrized Bregman centroids, IEEE Transactions on Information Theory, 55 (2009).
- [46] F. Nielsen and R. Bhatia, eds., Matrix Information Geometry, Springer, 2013.
- [47] J. NOCEDAL AND S. J. WRIGHT, Numerical Optimization, Springer, 1999.
- [48] S. Sra, A new metric on the manifold of kernel matrices with application to matrix geometric means, in Advances in Neural Information Processing Systems (NIPS), Dec. 2012.
- [49] S. SRA, Positive definite matrices and the Symmetric Stein Divergence, arXiv: 1110.1773v1,v2, (2012).
- [50] C. STEIN, Inadmissibility of the usual estimator for the mean of a multivariate distribution, in Proc. Third Berkeley Symp. Math. Statist. Prob., vol. 1, 1956, pp. 197–206.
- [51] A. TERRAS, Harmonic Analysis on Symmetric Spaces and Applications, vol. II, Springer, 1988.
- [52] H. WOLKOWICZ, R. SAIGAL, AND L. VANDENBERGHE, eds., Handbook of Semidefinite Programming: Theory, Algorithms, and Applications, Kluwer Academic, 2000.