

Conic geometric optimisation on the manifold of positive definite matrices

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Abstract

We develop *geometric optimisation* on the manifold of hermitian positive definite (hpd) matrices. In particular, we consider optimising two types of cost functions: (i) geodesically convex (g-convex); and (ii) log-nonexpansive (LN). G-convex functions are nonconvex in the usual euclidean sense, but convex along the manifold and thus allow global optimisation. LN functions may fail to be even g-convex, but still remain globally optimisable due to their special structure. We develop theoretical tools to recognise and generate g-convex functions as well as cone theoretic fixed-point optimisation algorithms. We illustrate our techniques by applying them to maximum-likelihood parameter estimation for elliptically contoured distributions (a rich class that substantially generalises the multivariate normal distribution). We compare our fixed-point algorithms with sophisticated manifold optimisation methods and observe obtain notable speedups.

1 Introduction

Hermitian positive definite (hpd) matrices possess remarkably rich geometry that is a cornerstone of modern convex optimisation [39] and convex geometry [9]. In particular, hpd matrices form a convex cone, the strict interior of which is a differentiable Riemannian manifold which is also a prototypical CAT(0) space (i.e., a metric space of nonpositive curvature [12]). This rich structure enables “geometric optimisation” on the set of hpd matrices—enabling us to solve certain problems that may be nonconvex in the Euclidean sense but are convex in the manifold sense (see §2 or [53]), or failing that, still have enough geometry (see §4) so as to admit efficient optimisation.

This paper formally develops *conic geometric optimisation*¹ (GO) for hpd matrices. We present key results that help recognise geodesic convexity (g-convexity); we also present sufficient conditions that place even several non-g-convex functions within the grasp of GO.

Motivation

We begin by noting that the widely studied class of *geometric programs* ultimately reduces to the GO on 1×1 hpd matrices (i.e., positive scalars; see Remark 10). Geometric programming

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¹To our knowledge the name “geometric optimisation” has not been previously attached to g-convex and cone theoretic hpd matrix optimisation, though several scattered examples do exist. Our theorems provide a starting point for recognising and constructing numerous problems amenable to geometric optimisation.

has enjoyed great success across a spectrum of applications—see e.g., the survey of Boyd et al. [11]; we hope this paper helps GO gain wider exposure.

Perhaps the best known conic GO problem is computation of the Karcher (Fréchet) mean of a set of hpd matrices, a topic that has attracted great attention within matrix theory [7, 8, 26, 50], computer vision [16], radar imaging [42, Part II], medical imaging [17, 56]—we refer the reader to the recent book [42] for additional applications and references. Another GO problem arises as a subroutine in image search and matrix clustering [19].

GO problems also occur in several other areas: computer vision [18, 52], statistics (covariance shrinkage) [15], nonlinear matrix equations [32], Markov decision processes and the more broadly in the fascinating subject of nonlinear Perron-Frobenius theory [33].

As a concrete illustration of our ideas, we discuss the task of *maximum likelihood estimate* (mle) for *elliptically contoured distributions* (ECDs) [13, 22, 38]—see §5. We use ECDs to illustrate GO, not only because of their instructive value but also because of their importance in a variety of applications [43].

2 Geometric optimisation with geodesic convexity

Geodesic convexity (g-convexity) is a classical concept in geometry and analysis; it is used extensively in the study of Hadamard manifolds and metric spaces of nonpositive curvature [12, 44], i.e., metric spaces having a g-convex distance function. The concept of g-convexity has been previously explored in nonlinear optimisation [46], but its importance and applicability in statistical applications and optimisation has only recently gained more attention [53, 55]. It is worth remarking that geometric programming [11] ultimately relies on “geometric-mean” convexity [41], i.e., $f(x^\alpha y^{1-\alpha}) \leq [f(x)]^\alpha [f(y)]^{1-\alpha}$, a property that is nothing but logarithmic g-convexity for 1×1 hpd matrices (positive scalars).

To introduce g-convexity on $n \times n$ hpd matrices we first recall some key definitions—see [12, 44] for extensive details.

Definition 1 (g-convex sets). Let \mathcal{M} be a d -dimensional connected C^2 Riemannian manifold. A set $\mathcal{X} \subset \mathcal{M}$ is called *geodesically convex* if any two points of \mathcal{X} are joined by a geodesic lying in \mathcal{X} . That is, if $x, y \in \mathcal{X}$, then there exists a shortest path $\gamma : [0, 1] \rightarrow \mathcal{X}$ such that $\gamma(0) = x$ and $\gamma(1) = y$.

Definition 2 (g-convex functions). Let $\mathcal{X} \subset \mathcal{M}$ be a g-convex set. A function $\phi : \mathcal{X} \rightarrow \mathbb{R}$ is *geodesically convex*, if for any $x, y \in \mathcal{X}$ and a unit speed geodesic $\gamma : [0, 1] \rightarrow \mathcal{X}$ with $\gamma(0) = x$ and $\gamma(1) = y$, we have the inequality

$$\phi(\gamma(t)) \leq (1-t)\phi(\gamma(0)) + t\phi(\gamma(1)) = (1-t)\phi(x) + t\phi(y). \quad (1)$$

2.1 Recognising g-convexity

Unfortunately, unlike scalar g-convexity, recognising g-convexity for hpd matrices is not so easy. Indeed, for scalars, a function $f : \mathbb{R}_{++} \rightarrow \mathbb{R}$ is log-g-convex (and hence g-convex) if and only if $\log \circ f \circ \exp$ is convex. A similar characterisation does not seem to exist for hpd matrices, primarily due to the noncommutativity of matrix multiplication. We develop some theory below for helping recognise and construct g-convex functions.

To define g-convex functions on hpd matrices recall that \mathbb{P}_d is a differentiable Riemannian manifold where geodesics between points are available in closed form. Indeed, the tangent space to \mathbb{P}_d at any point can be identified with the set of Hermitian matrices, and the inner product on this space leads to a Riemannian metric on \mathbb{P}_d . At any point $A \in \mathbb{P}_d$, this metric

is given by the differential form $ds = \|A^{-1/2}dAA^{-1/2}\|_F$; for $A, B \in \mathbb{P}_d$ there is a unique geodesic path [6, Thm. 6.1.6]

$$\gamma(t) = A\#_t B := A^{1/2}(A^{-1/2}BA^{-1/2})^t A^{1/2}, \quad t \in [0, 1]. \quad (2)$$

The midpoint of this path, namely $A\#_{1/2}B$ is called the *matrix geometric mean*, which is an object of great interest [6, 7, 8, 26]—we drop the 1/2 and denote it simply by $A\#B$. Starting from the geodesic (2), many g-convex functions can be constructed by extending monotonic convex functions to matrices. To that end, first recall the fundamental operator inequality [2] (where \preceq denotes the Löwner partial order):

$$A\#_t B \preceq (1-t)A + tB. \quad (3)$$

Theorem 3 uses (3) to construct “tracial” g-convex functions.

Theorem 3. *Let $h : \mathbb{R}_+ \rightarrow \mathbb{R}$ be monotonically increasing and convex; let $\lambda : \mathbb{P}_n \rightarrow \mathbb{R}_+^n$ denote the eigenvalue map. Then, $\sum_{j=1}^k h(\lambda_j^\downarrow(\cdot))$ is g-convex for each $1 \leq k \leq n$.*

Proof. It suffices to establish midpoint convexity. Inequality (3) implies that

$$\lambda_j(A\#B) \leq \lambda_j\left(\frac{A+B}{2}\right), \quad \text{for } 1 \leq j \leq n.$$

Since h is monotonic, for $1 \leq k \leq n$ it follows that

$$\sum_{j=1}^k h(\lambda_j^\downarrow(A\#B)) \leq \sum_{j=1}^k h(\lambda_j^\downarrow\left(\frac{A+B}{2}\right)). \quad (4)$$

Lidskii’s theorem [5, Thm.III.4.1] yields the majorisation $\lambda^\downarrow\left(\frac{A+B}{2}\right) \prec \frac{\lambda^\downarrow(A) + \lambda^\downarrow(B)}{2}$, which combined with a celebrated result of Hardy et al. [24] and convexity of h yields

$$\sum_{j=1}^k h(\lambda_j^\downarrow\left(\frac{A+B}{2}\right)) \leq \sum_{j=1}^k h\left(\frac{\lambda_j^\downarrow(A) + \lambda_j^\downarrow(B)}{2}\right) \leq \frac{1}{2} \sum_{j=1}^k h(\lambda_j^\downarrow(A)) + \frac{1}{2} \sum_{j=1}^k h(\lambda_j^\downarrow(B)).$$

Now invoke inequality (4) to conclude that $\sum_{j=1}^k h(\lambda_j^\downarrow(\cdot))$ is g-convex. \square

Example 4. Theorem 3 shows that the following functions are g-convex: (i) $\phi(A) = \text{tr}(e^A)$; (ii) $\phi(A) = \text{tr}(A^\alpha)$ for $\alpha \geq 1$; (iii) $\lambda_1^\downarrow(e^A)$; (iv) $\lambda_1^\downarrow(A^\alpha)$ for $\alpha \geq 1$.

We now construct examples of g-convex functions different from those obtained via Theorem 3. Let us start with a motivating example.

Example 5. Let $z \in \mathbb{C}^d$. The function $\phi(A) := z^* A^{-1} z$ is g-convex. To prove this claim it suffices to verify midpoint convexity: $\phi(A\#B) \leq \frac{1}{2}\phi(A) + \frac{1}{2}\phi(B)$ for $A, B \in \mathbb{P}_d$. Since $(A\#B)^{-1} = A^{-1}\#B^{-1}$ and $A^{-1}\#B^{-1} \preceq \frac{A^{-1}+B^{-1}}{2}$ ([6, 4.16]), it follows that $\phi(A\#B) = z^*(A\#B)^{-1}z \leq \frac{1}{2}(z^*A^{-1}z + z^*B^{-1}z) = \frac{1}{2}(\phi(A) + \phi(B))$.

Below we substantially generalise this example; but first we must introduce some background.

Definition 6 (Positive linear map). A linear map Φ from Hilbert space \mathcal{H}_1 to a Hilbert space \mathcal{H}_2 is called *positive*, if for $0 \preceq A \in \mathcal{H}_1$, $\Phi(A) \succeq 0$. It is called *strictly positive* if $\Phi(A) \succ 0$ for $A \succ 0$; finally, it is called *unital* if $\Phi(I) = I$.

Lemma 7 (6, Ex.4.1.5). Define the parallel sum of hpd matrices A, B as

$$A : B := [A^{-1} + B^{-1}]^{-1}.$$

Then, for any positive linear map $\Pi : \mathbb{P}_d \rightarrow \mathbb{P}_k$, we have

$$\Phi(A : B) \preceq \Phi(A) : \Phi(B).$$

Building on Lemma 7, we are ready to state a key theorem that helps us recognise and construct g-convex functions (see Thm. 15, for instance). This result is by itself not new—e.g., it follows from the classic paper of Kubo and Ando [31]; due to its key importance we provide our own proof below for completeness.

Theorem 8. Let $\Phi : \mathbb{P}_d \rightarrow \mathbb{P}_k$ be a strictly positive linear map. Then,

$$\Phi(A \#_t B) \preceq \Phi(A) \#_t \Phi(B), \quad t \in [0, 1], \text{ for } A, B \in \mathbb{P}_d. \quad (5)$$

Proof. The key insight of the proof is to use the integral identity [3]:

$$\int_0^1 \frac{\lambda^{\alpha-1}(1-\lambda)^{\beta-1}}{[\lambda a^{-1} + (1-\lambda)b^{-1}]^{\alpha+\beta}} d\lambda = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha+\beta)} a^\alpha b^\beta$$

Using $\alpha = 1 - t$ and $\beta = t > 0$, for $C \succeq 0$ this yields the integral representation

$$C^t = \frac{\Gamma(1)}{\Gamma(t)\Gamma(1-t)} \int_0^1 \frac{[\lambda C^{-1} + (1-\lambda)I]^{-1}}{\lambda^t(1-\lambda)^{1-t}} d\lambda. \quad (6)$$

Consequently, since $A \#_t B = A^{1/2}(A^{-1/2}BA^{-1/2})^t A^{1/2}$, we may write it as

$$A \#_t B = \int_0^1 [(1-\lambda)A^{-1} + \lambda B^{-1}]^{-1} d\mu(\lambda), \quad (7)$$

for a suitable measure $d\mu(\lambda)$. Applying Φ to both sides of (7) we obtain

$$\begin{aligned} \Phi(A \#_t B) &= \int_0^1 \Phi([(1-\lambda)A^{-1} + \lambda B^{-1}]^{-1}) d\mu(\lambda) \\ &= \int_0^1 \Phi(\bar{A} : \bar{B}) d\mu(\lambda), \end{aligned}$$

where $\bar{A} = (1-\lambda)^{-1}A$ and $\bar{B} = \lambda^{-1}B$. From Lemma 7 and linearity of Φ it follows that

$$\begin{aligned} \int_0^1 \Phi(\bar{A} : \bar{B}) d\mu(\lambda) &\preceq \int_0^1 (\Phi(\bar{A}) : \Phi(\bar{B})) d\mu(\lambda) \\ &= \int_0^1 [(1-\lambda)\Phi(A)^{-1} + \lambda\Phi(B)^{-1}]^{-1} d\mu(\lambda) \\ &\stackrel{(7)}{=} \Phi(A) \#_t \Phi(B). \end{aligned} \quad \square$$

A corollary of Theorem 8 (that subsumes Example 5) follows.

Corollary 9. Let $A, B \in \mathbb{P}_d$, and let $X \in \mathbb{C}^{d \times k}$ have full column rank; then

$$\text{tr } X^*(A \#_t B)X \leq [\text{tr } X^*AX]^{1-t} [\text{tr } X^*BX]^t, \quad t \in [0, 1]. \quad (8)$$

Proof. Use the positive linear map $A \mapsto \text{tr } X^*AX$ in Theorem 8. \square

Remark 10. Corollary 9 actually proves a result stronger than g-convexity: it shows *log-g-convexity*, i.e., $\phi(X \# Y) \leq \sqrt{\phi(X)\phi(Y)}$, so that $\log \phi$ is g-convex. It is easy to verify that if ϕ_1, ϕ_2 are log-g-convex, then both $\phi_1\phi_2$ and $\phi_1 + \phi_2$ are log-g-convex.

Remark 11. More generally, if $h : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ is nondecreasing and log-convex, then the map $A \mapsto \sum_{i=1}^k \log h(\lambda_i(A))$ is g-convex. The proof is the same as of Theorem 3. For instance, if $h(x) = e^x$, we obtain the special case that $A \mapsto \log \operatorname{tr}(e^A)$ is g-convex, i.e.,

$$\log \sum_{i=1}^n e^{\lambda_i(A \# B)} \leq \log \sum_{i=1}^n e^{\frac{\lambda_i(A) + \lambda_i(B)}{2}} \leq \frac{1}{2} \log \sum_{i=1}^n e^{\lambda_i(A)} + \frac{1}{2} \log \sum_{i=1}^n e^{\lambda_i(B)}.$$

We mention now another corollary to Theorem 8; we note in passing that it subsumes a more complicated result of Gurvits and Samorodnitsky [23, Lem. 3.2].

Corollary 12. Let $A_i \in \mathbb{C}^{d \times k}$ with $k \leq d$ such that $\operatorname{rank}([A_i]_{i=1}^m) = k$; also let $B \succeq 0$. Then $\phi(X) := \log \det(B + \sum_i A_i^* X A_i)$ is g-convex on \mathbb{P}_d .

Proof. By our assumption on A_i and B , the map $\Phi = S \mapsto B + \sum_i A_i^* X A_i$ is strictly positive. Thm. 8 implies that $\Phi(X \# Y) = B + \sum_i A_i^*(X \# Y)A_i \preceq \Phi(X) \# \Phi(Y)$. This operator inequality is stronger than what we require. Indeed, since $\log \det$ is monotonic and determinants are multiplicative, from this inequality it follows that

$$\begin{aligned} \phi(S \# R) &= \log \det \Phi(S \# R) \leq \log \det(\Phi(S) \# \Phi(R)) \\ &\leq \frac{1}{2} \log \det \Phi(S) + \frac{1}{2} \log \det \Phi(R) = \frac{1}{2} \phi(S) + \frac{1}{2} \phi(R). \end{aligned}$$

Observe that one can extend the above result to $\phi(X) = \log \det(B + \int_0^\infty A_\lambda^* X A_\lambda d\mu(\lambda))$, where μ is some positive measure on $(0, \infty)$. \square

Remark 13. Corollary 12 may come as a surprise to some readers because $\log \det(X)$ is well-known to be concave (in the Euclidean sense), and yet $\log \det(B + A^* X A)$ turns out to be g-convex—moreover, $\log \det(X)$ is g-linear, i.e., both g-convex and g-concave.

Example 14. In [14, 19, 50] study a dissimilarity function (called the S-Divergence in [50]) to compare a pair of hpd matrices. Specifically, for $X, Y > 0$, this function is

$$S(X, Y) := \log \det \left(\frac{X+Y}{2} \right) - \frac{1}{2} \log \det(X) - \frac{1}{2} \log \det(Y). \quad (9)$$

This divergence proves useful in several applications [14, 19, 50], and very recently its joint g-convexity (in both variables) was discovered [51]. Corollary 12 along with Remark 13 on g-linearity of $\log \det(\cdot)$ yield g-convexity of $S(X, Y)$ in either X or Y .

We are now ready to state our next key g-convexity result. A similar result was obtained in [55]; our result is somewhat more general as it allows incorporation of positive linear maps. Moreover, our proof technique is completely different.

Theorem 15. Let $h : \mathbb{P}_k \rightarrow \mathbb{R}$ be nondecreasing (in Löwner order) and g-convex. Let $r \in \{\pm 1\}$, and let Φ be a positive linear map. Then, $\phi(S) = h(\Phi(S^r))$ is g-convex.

Proof. It suffices to prove midpoint geodesic convexity. Since $r \in \{\pm 1\}$, $(X \# Y)^r = X^r \# Y^r$. Thus, applying Theorem 8 to Φ and noting that h is nondecreasing it follows that

$$h(\Phi(X \# Y)^r) = h(\Phi(X^r \# Y^r)) \leq h(\Phi(X^r) \# \Phi(Y^r)). \quad (10)$$

By assumption h is g-convex, so the last inequality in (10) yields

$$h(\Phi(X^r) \# \Phi(Y^r)) \leq \frac{1}{2} h(\Phi(X^r)) + \frac{1}{2} h(\Phi(Y^r)) = \frac{1}{2} \phi(X) + \frac{1}{2} \phi(Y). \quad (11)$$

Notice that if h is strictly g-convex, then $\phi(S)$ is also strictly g-convex. \square

Example 16. Let $h = \log \det(X)$ and $\Phi(X) = B + \sum_i A_i^* X A_i$. Then, $\phi(X) = \log \det(B + \sum_i A_i^* X^r A_i)$ is g-convex. With $h(X) = \text{tr}(X^\alpha)$ for $\alpha \geq 1$, $\text{tr}(B + \sum_i A_i^* X^r A_i)^\alpha$ is g-convex.

Next, Theorem 17 presents a method for creating essentially logarithmic versions of our “tracial” g-convexity result Theorem 3.

Theorem 17. *If $f : \mathbb{R} \rightarrow \mathbb{R}$ is convex, for each $1 \leq k \leq n$, $\phi(\cdot) := \sum_{i=1}^k f(\log \lambda_i^\downarrow(\cdot))$ is g-convex. If $h : \mathbb{R} \rightarrow \mathbb{R}$ is nondecreasing and convex, $\phi(\cdot) = \sum_{i=1}^k h(|\log \lambda(\cdot)|)$ is g-convex.*

To prove Theorem 17 we will need the following majorisation.

Lemma 18. *Let \prec_{\log} denote the log-majorisation order, i.e., for $x, y \in \mathbb{R}_{++}^n$ ordered nonincreasingly, we say $x \prec_{\log} y$ if $\prod_{i=1}^{n-1} x_i \leq \prod_{i=1}^{n-1} y_i$ and $\prod_{i=1}^n x_i = \prod_{i=1}^n y_i$. Then, for $A, B \in \mathbb{P}_n$ and $t \in [0, 1]$, we have the log-majorisation between the eigenvalues:*

$$\lambda(A\#_t B) \prec_{\log} \lambda(A^{1-t} B^t) \prec_{\log} \lambda(A^{1-t}) \lambda(B^t).$$

Proof. The first majorisation follows from a recent result of Matharu and Aujla [36]. The second one follows easily from $\lambda_1(XY) \leq \sigma_1(XY) \leq \sigma_1(X)\sigma_1(Y)$, but this equals $\lambda_1(X)\lambda_1(Y)$ since X and Y are hpd. Apply this inequality to the antisymmetric (Grassmann) exterior product $\wedge^k(XY)$ to obtain $\lambda_1(\wedge^k(XY)) \leq \sigma_1(\wedge^k(XY))$; then set $X \leftarrow A^{1-t}$, $Y \leftarrow B^t$ and note that $\wedge^k(XY) = \wedge^k X \wedge^k Y$ and $\sigma_1(\wedge^k X) = \prod_{i=1}^k \sigma_i(X)$, which completes the proof. \square

Proof of Theorem 17. From Lemma 18 we have $\lambda(A\#_t B) \prec_{\log} \lambda(A^{1-t} B^t) \prec_{\log} \lambda(A^{1-t}) \lambda(B^t)$; or taking logarithms, this may be written as the equivalent majorisation inequality

$$\log \lambda(A\#_t B) \prec (1-t) \log \lambda(A) + t \log \lambda(B). \quad (12)$$

Using a result of [24] for a convex function f applied to a majorisation, from (12) we obtain

$$\begin{aligned} \phi(A\#_t B) &= \sum_{i=1}^k f(\log \lambda_i(A\#_t B)) \leq \sum_{i=1}^k f((1-t) \log \lambda_i(A) + t \log \lambda_i(B)) \\ &\leq (1-t) \sum_{i=1}^k f(\log \lambda_i(A)) + t \sum_{i=1}^k f(\log \lambda_i(B)) \\ &= (1-t)\phi(A) + t\phi(B). \end{aligned}$$

Applying the Ky-Fan norm $\sum_{i=1}^k \sigma_i(\cdot)$ —that is, the sum of top- k singular values—to (12), we obtain the weak-majorisation (see e.g., [5, Chapter II] for more on majorisation):

$$\sigma(\log A\#_t B) \prec_w \sigma[(1-t) \log \lambda(A) + t \log \lambda(B)] \prec_w (1-t)\sigma(\log A) + t\sigma(\log B). \quad (13)$$

Since h is monotone and convex, from (13) we obtain g-convexity of $\sum_{i=1}^k h(|\log \lambda_i(\cdot)|)$. \square

Corollary 19. *Let $\Phi : \mathbb{R}^n \rightarrow \mathbb{R}_+$ be a symmetric gauge function (i.e., Φ is a norm, invariant to permutation and sign changes). Also, let $X \in GL_n(\mathbb{C})$. Then, $\Phi(\sigma(\log(X^* A X)))$ is g-convex.*

Proof. Observe that $X^*(A\#B)X = (X^* A X)\#(X^* B X)$; now apply Theorem 17. \square

Example 20. Consider $\delta_R(A, X) := \|\log(X^{-1/2} A X^{-1/2})\|_F$ the Riemannian distance between $A, X \in \mathbb{P}_d$ [6, Ch. 6]. Since $\|\log \lambda(X^{-1/2} A X^{-1/2})\|_2 = \|\sigma(\log X^{-1/2} A X^{-1/2})\|_2$, it follows from Corollary 19 that $A \mapsto \delta_R(A, X)$ is g-convex (see also [6, Cor. 6.1.11]).

This immediately shows the computing the Fréchet (Karcher) mean and median of hpd matrices (also known as geometric mean and median of hpd matrices, respectively) are g-convex optimisation problems; formally, these problems are given by

$$\begin{aligned} \min_{X>0} \sum_{i=1}^m w_i \delta_R(X, A_i), & \quad (\text{Geometric Median}), \\ \min_{X>0} \sum_{i=1}^m w_i \delta_R^2(X, A_i), & \quad (\text{Geometric Mean}), \end{aligned}$$

where $\sum_i w_i = 1$, $w_i \geq 0$, and $A_i > 0$ for $1 \leq i \leq m$. The latter problem has received great interest in the literature [6, 7, 8, 26, 37, 42, 50], and its optimal solution is unique owing to the (strict) g-convexity of its objective. The former problem is less well-known but in some cases proves more favourable [4, 42]—again, despite the nonconvexity of the objective, its g-convexity ensures every local solution is global.

We conclude this section by using Lemma 18 to prove the following log-convexity analogue to Theorem 17 (*cf.* the scalar case studied in [40, Prop. 2.4]).

Theorem 21. *Let $f(x) = \sum_{j \geq 0} a_j x^j$ be real analytic with $a_j \geq 0$ for $j \geq 0$ and radius of convergence R . Then, $\phi(\cdot) = \prod_{i=1}^k f(\lambda_i(\cdot))$ is log-g-convex on matrices with spectrum in $(0, R)$.*

Proof. It suffices to verify that $\log \phi(A \# B) \leq \frac{1}{2} \log \phi(A) + \frac{1}{2} \log \phi(B)$. Since $f' \geq 0$, we have

$$\begin{aligned} \phi(A \# B) &= \prod_{i=1}^k f(\lambda_i(A \# B)) \leq \prod_{i=1}^k f(\lambda_i^{1/2}(A) \lambda_i^{1/2}(B)) \quad (\text{using Lemma 18}) \\ &\leq \prod_{i=1}^k \sqrt{f(\lambda_i(A))} \sqrt{f(\lambda_i(B))} \quad (\text{Cauchy-Schwarz on power-series of } f) \\ &= \sqrt{\phi(A)} \sqrt{\phi(B)}. \end{aligned}$$

Taking logarithms, we see that $\phi(\cdot)$ is log-g-convex (and hence also g-convex). \square

Example 22. Some examples of f that satisfy conditions of Theorem 21 are \exp , \sinh on $(0, \infty)$, $-\log(1-x)$ and $(1+x)/(1-x)$ on $(0, 1)$; see [40] for more examples.

2.2 Multivariable g-convexity

We describe now an extension of g-convexity to multiple matrices; a two-variable version was also partially explored in [53, 55], though under a different name. We begin our multivariable extension by recalling a few basic properties of the Kronecker product [35].

Lemma 23. *Let $A \in \mathbb{R}^{m \times n}$, $B \in \mathbb{R}^{p \times q}$. Then, $A \otimes B := [a_{ij} B] \in \mathbb{R}^{mp \times nq}$ satisfies:*

- (i) $(A \otimes B)^* = A^* \otimes B^*$
- (ii) $(A \otimes B)^{-1} = A^{-1} \otimes B^{-1}$
- (iii) *Assuming that the respective products exist,*

$$(AC \otimes BD) = (A \otimes B)(C \otimes D) \tag{14}$$

- (iv) $A \otimes (B \otimes C) = (A \otimes B) \otimes C$
- (v) *If $A = UD_1U^*$ and $B = VD_2V^*$ then $(A \otimes B) = (U \otimes V)(D_1 \otimes D_2)(U \otimes V)^*$.*
- (vi) *Let $A, B \succeq 0$, and $t \in \mathbb{R}$; then*

$$(A \otimes B)^t = A^t \otimes B^t. \tag{15}$$

- (vii) $f(A \otimes B) = (U \otimes V)(f(D_1) \otimes f(D_2))(U \otimes V)^*$
(viii) If $A \succeq B$ and $C \succeq D$, then $(A \otimes C) \succeq (B \otimes D)$.

Proof. Identities (i)–(iii) are classic; (v) follows easily from (i) and (iv), while (vi) and (vii) follow from (v); (viii) is an easy exercise. \square

We will need the following easy but key result on tensor products of geometric means.

Lemma 24. *Let $A, B \in \mathbb{P}_{d_1}$ and $C, D \in \mathbb{P}_{d_2}$. Then,*

$$(A\#B) \otimes (C\#D) = (A \otimes C)\#(B \otimes D). \quad (16)$$

Proof. Denote $\gamma(X, Y) := (X^{-1/2}YX^{-1/2})^{1/2}$. Observe that

$$\begin{aligned} \gamma(A, B) \otimes \gamma(C, D) &= (A^{-1/2}BA^{-1/2})^{1/2} \otimes (C^{-1/2}DC^{-1/2})^{1/2} \\ &= [(A^{-1/2}BA^{-1/2}) \otimes (C^{-1/2}DC^{-1/2})]^{1/2} \\ &= [(A \otimes C)^{-1/2}(B \otimes D)(A \otimes C)^{-1/2}]^{1/2} \\ &= \gamma(A \otimes C, B \otimes D), \end{aligned}$$

where the second equality follows from Lemma 23-(iii), while the third one from Lemma 23-(ii),(iii), and (vi). A similar manipulation then shows that

$$\begin{aligned} (A\#B) \otimes (C\#D) &= (A^{1/2}\gamma(A, B)A^{1/2}) \otimes (C^{1/2}\gamma(C, D)C^{1/2}), \\ &= (A^{1/2} \otimes C^{1/2})(\gamma(A, B) \otimes \gamma(C, D))(A^{1/2} \otimes C^{1/2}) \\ &= (A \otimes C)^{1/2}(\gamma(A, B) \otimes \gamma(C, D))(A \otimes C)^{1/2} \\ &= (A \otimes C)^{1/2}\gamma(A \otimes C, B \otimes D)(A \otimes C)^{1/2} \\ &= (A \otimes C)\#(B \otimes D), \end{aligned} \quad \square$$

Lemma 24 inductively extends to the multivariable case, so that

$$\bigotimes_{i=1}^m (A_i\#B_i) = \left(\bigotimes_{i=1}^m A_i\right) \# \left(\bigotimes_{i=1}^m B_i\right). \quad (17)$$

Using identity (17) we thus obtain the following multivariate analogue to Theorem 17.

Theorem 25. *Let h be an increasing convex function on $\mathbb{R}_+ \rightarrow \mathbb{R}$. Then, the map $\prod_{i=1}^m \text{tr} h(X_i)$ is jointly g -convex, i.e., $\text{tr} h(\bigotimes_{i=1}^m X_i)$ is g -convex in its variables.*

Proof. Let $(A_1, B_1), \dots, (A_m, B_m)$ be pairs of hpd matrices of arbitrary sizes (such that for each i , A_i, B_i are of the same size). Let j index the eigenvalues of the tensor product $\bigotimes_{i=1}^m (A_i\#B_i)$. Then, starting with identity (17) we obtain

$$\begin{aligned} \lambda_j [\bigotimes_{i=1}^m (A_i\#B_i)] &= \lambda_j [(\bigotimes_{i=1}^m A_i) \# (\bigotimes_{i=1}^m B_i)] \leq \frac{1}{2} \lambda_j [\bigotimes_{i=1}^m A_i + \bigotimes_{i=1}^m B_i] \\ \text{tr} h(\bigotimes_{i=1}^m (A_i\#B_i)) &= \sum_j h(\lambda_j [\bigotimes_{i=1}^m (A_i\#B_i)]) \leq \sum_j h\left(\frac{1}{2} \lambda_j [\bigotimes_{i=1}^m A_i + \bigotimes_{i=1}^m B_i]\right) \\ &\leq \frac{1}{2} \sum_j h(\lambda_j(\bigotimes_{i=1}^m A_i)) + \frac{1}{2} \sum_j h(\lambda_j(\bigotimes_{i=1}^m B_i)) \\ &= \frac{1}{2} \text{tr} h(\bigotimes_{i=1}^m A_i) + \frac{1}{2} \text{tr} h(\bigotimes_{i=1}^m B_i) \\ &= \frac{1}{2} \prod_{i=1}^m \text{tr} h(A_i) + \frac{1}{2} \prod_{i=1}^m \text{tr} h(B_i), \end{aligned}$$

which shows the desired multivariable g -convexity of the map $\text{tr} h(\bigotimes_{i=1}^m X_i)$. \square

Again, using (17) we obtain the following multivariate analogue to Theorem 8.

Theorem 26. *Let $(X_1, Y_1), \dots, (X_m, Y_m)$ be pairs of hpd matrices of arbitrary sizes (such that for each i , X_i, Y_i are of the same size). Let $\Phi_i : \mathcal{H}_i \rightarrow \mathcal{H}'_i$ be a positive linear map for each i , and Φ the positive multilinear map defined by $\Phi \equiv \otimes_{i=1}^m A_i \mapsto \otimes_{i=1}^m \Phi_i(A_i)$. Then,*

$$\Phi(\otimes_{i=1}^m (X_i \# Y_i)) \preceq \Phi(\otimes_i X_i) \# \Phi(\otimes_i Y_i). \quad (18)$$

Proof. Expanding the definition of Φ we have

$$\begin{aligned} \Phi(\otimes_i (X_i \# Y_i)) &= \otimes_i \Phi_i(X_i \# Y_i) \preceq \otimes_i [\Phi_i(X_i) \# \Phi_i(Y_i)] \\ &= [\otimes_i \Phi_i(X_i)] \# [\otimes_i \Phi_i(Y_i)] = \Phi(\otimes_i X_i) \# \Phi(\otimes_i Y_i). \end{aligned}$$

The operator inequality (18) follows upon invoking Theorem 8 and Lemma 23-(viii). \square

Building on Theorem 26, we also derive a generalisation to Theorem 15.

Theorem 27. *Let $h : \otimes_i \mathcal{H}'_i \rightarrow \mathbb{R}$ be nondecreasing (in Löwner order) and g -convex. Let $r_i \in \{\pm 1\}$ and let $\Phi : \otimes_i \mathcal{H}_i \rightarrow \otimes_i \mathcal{H}'_i$ be a strictly positive multilinear map. Then, $\phi(X_1, \dots, X_m) = (h \circ \Phi)(\otimes_i X_i^{r_i})$ is jointly g -convex (i.e., g -convex in X_1, \dots, X_m).*

Proof. Since ϕ is continuous, it suffices to establish midpoint g -convexity.

$$\begin{aligned} (h \circ \Phi)(\otimes_i (X_i \# Y_i)^{r_i}) &= (h \circ \Phi)(\otimes_i (X_i^{r_i} \# Y_i^{r_i})) \\ &\preceq h(\Phi(\otimes_i X_i^{r_i}) \# \Phi(\otimes_i Y_i^{r_i})) \\ &\preceq \frac{1}{2} ((h \circ \Phi)(\otimes_i X_i^{r_i}) + (h \circ \Phi)(\otimes_i Y_i^{r_i})) \\ &= \frac{1}{2} (\phi(X_1, \dots, X_m) + \phi(Y_1, \dots, Y_m)). \end{aligned}$$

Since h is nondecreasing, using Theorem 26 the first inequality follows. The second one follows as h is g -convex, which completes the proof. \square

Using identities (15) and (17) with Lemma 18 we obtain the following log-majorisations.

Proposition 28. *Let $(A_i, B_i)_{i=1}^m$ be pairs of hpd matrices of compatible sizes. Then,*

$$\begin{aligned} \lambda(\otimes_{i=1}^m A_i \#_t B_i) &\prec_{\log} \lambda([\otimes_{i=1}^m A_i]^{1-t} [\otimes_{i=1}^m B_i]^t), \quad t \in [0, 1] \\ \lambda([\otimes_{i=1}^m A_i]^{1-t} [\otimes_{i=1}^m B_i]^t) &\prec_{\log} \lambda[\otimes_{i=1}^m A_i^{1-t}] \lambda[\otimes_{i=1}^m B_i^t]. \end{aligned}$$

Proposition 28 allows us to derive the following multivariate analogue to Theorem 17.

Theorem 29. *If $f : \mathbb{R} \rightarrow \mathbb{R}$ is convex, then $\phi(\cdot) := \sum_{j=1}^k f(\log \lambda_j(\otimes_{i=1}^m X_i))$ is g -convex for $1 \leq k \leq n$. If $h : \mathbb{R} \rightarrow \mathbb{R}$ is nondecreasing and convex, then $\phi(\cdot) = \sum_{j=1}^k h(|\log \lambda_j(\otimes_{i=1}^m X_i)|)$ is g -convex for $1 \leq k \leq n$.*

Theorem 29 brings us to the end of our theoretical results on recognising and constructing g -convex functions. We are now ready to devote attention to optimisation algorithms. In particular, we first discuss manifold optimisation [1] techniques in §3. Then, in §4 we introduce a special class of functions that overlaps with g -convex functions, but not entirely, and admits simpler “conic fixed-point” algorithms.

3 Manifold optimisation for g-convex functions

Since \mathbb{P}_d is a smooth manifold, we can use optimisation techniques based on exploiting smooth manifold structure. In addition to common concepts such as tangent vectors and derivatives along manifolds, different optimisation methods need a subset of new definitions and explicit expressions for inner products, gradients, retractions, vector-transport and Hessians [1, 25].

Since \mathbb{P}_d can be viewed as a sub-manifold of the Euclidean space \mathbb{R}^{2d^2} , most of concepts of importance to our study can be defined by using the embedding structure of Euclidean space. The tangent space at any point is the space \mathbb{H}_d of $d \times d$ hermitian matrices. The derivative of a function on the manifold in any direction in the tangent space is simply the embedded Euclidean derivative in that direction.

For several optimisation algorithms, two different inner product formulations were tested in [26] for \mathbb{P}_d . The authors observed that the intrinsic inner product leads to the best convergence speed for the tested algorithms. We too observed that the intrinsic inner product yields more than a hundred times faster convergence for our algorithms compared to the induced inner product of Euclidean space. The *intrinsic inner product* of two tangent vectors at point X on the manifold is given by

$$g_X(\eta, \xi) = \text{tr}(\eta X^{-1} \xi X^{-1}), \quad \eta, \xi \in \mathbb{H}_d. \quad (19)$$

This intrinsic inner product leads to geodesics of the form (2). Now that we have set up an inner product tensor, we can define the gradient direction as the direction of the maximum change. The inner product between the gradient vector and a vector in the tangent space is equal to the gradient of the function in that direction. If $\text{grad}^H f(X) = \frac{1}{2}(\text{grad} f(X) + (\text{grad} f(X))^*)$ is the hermitian part of Euclidean gradient, then the gradient in intrinsic metric is given by:

$$\text{grad}^{\text{hpd}} f(X) = X \text{grad}^H f(X) X.$$

The simplest gradient descent approach, namely steepest-descent, also needs the notion of projection of a vector in the tangent space onto a point on the manifold. Such a projection is called *retraction*. If the manifold is Riemannian, a particular retraction is the exponential map, i.e., moving along a geodesic. If the inner product is the induced inner product of the manifold, then the retraction is normal retraction on the Euclidean space which is obtained by summing the point on the manifold and the vector on the tangent space. The intrinsic inner product of (19) of the Riemannian manifold leads to the following exponential map:

$$R_X^{\text{hpd}}(\xi) = X^{1/2} \exp(X^{-1/2} \xi X^{-1/2}) X^{1/2}, \quad \xi \in \mathbb{H}_d. \quad (20)$$

From a numerical perspective, our experiments revealed that the following compact representation of the retraction (20) gives the best computational speed:

$$R_X^{\text{hpd}}(\xi) = [X \exp(X^{-1} \xi)]^H, \quad \xi \in \mathbb{H}_d. \quad (21)$$

Definitions of the gradient and retraction suffice for implementing steepest descent on \mathbb{P}_d . For approaches such as conjugate gradients or quasi-newton methods, we need to relate the tangent vector at one point to the tangent vector at another point, i.e., we need to define *vector transport*. A special case of vector transport on a Riemannian manifold is parallel transport: for the induced Euclidean metric, parallel transport is simply the identity map. In order to compute the parallel transport one first needs to compute the *Levi-Civita connection*. This connection is a way to compute directional derivatives of vector fields. It is a map from the cartesian product of tangent bundles to the tangent bundle:

$$\nabla : TM \times TM \rightarrow TM,$$

where $T\mathcal{M}$ is the tangent bundle of manifold \mathcal{M} (i.e. the space of smooth vector fields on \mathcal{M}). It can be verified that for the intrinsic metric (19) the following connection satisfies all the needed properties (see e.g., [26]):

$$\nabla_{\zeta_X}^{\text{hpd}} \xi_X = D\xi(X)[\zeta_X] - \frac{1}{2}(\zeta_X X^{-1} \xi_X + \xi_X X^{-1} \zeta_X),$$

where $D\xi(X)$ denotes the classical Fréchet derivative of $\xi(X)$. ξ_X and ζ_X are vector fields on the manifold \mathbb{H}_d . Subindex X is used to discriminate a vector field from a tangent vector.

Consider $P(t)$, a vector field along the geodesic curve $\gamma(t)$. Parallel transport along a curve is given by the differential equation

$$D_t P(t) = \nabla_{\dot{\gamma}(t)} P(t) = 0, \quad \text{s.t. } P(0) = \eta.$$

For the intrinsic metric, the above equation becomes

$$\dot{P}(t) - \frac{1}{2}(\dot{\gamma}(t) X_t^{-1} P(t) + P(t) X_t^{-1} \dot{\gamma}(t)) = 0.$$

The geodesic passing through $\gamma(0) = X$ with $\dot{\gamma} = \xi$ is given by

$$\gamma(t) = X^{1/2} \exp(t X^{-1/2} \xi X^{-1/2}) X^{1/2}.$$

For $t = 1$ we get the retraction (20). It can be shown that along the geodesic curve the following equation gives the parallel transport:

$$P(t) = X^{1/2} \exp(t \frac{1}{2} X^{-1/2} \xi X^{-1/2}) X^{-1/2} \eta X^{-1/2} \exp(t \frac{1}{2} X^{-1/2} \xi X^{-1/2}) X^{1/2}.$$

Thus, parallel transport for the intrinsic inner product is given by

$$\mathcal{T}_{X,Y}^{\text{hpd}}(\eta) = X^{1/2} (X^{-1/2} Y X^{-1/2})^{1/2} X^{-1/2} \eta X^{-1/2} (X^{-1/2} Y X^{-1/2})^{1/2} X^{1/2}.$$

It is important to note that this parallel transport can be written in a compact form that is also computationally more advantageous, namely,

$$\mathcal{T}_{X,Y}^{\text{hpd}}(\eta) = E \eta E^*, \quad \text{where } E = (Y X^{-1})^{1/2}. \quad (22)$$

We are now ready to describe a quasi-newton method on \mathbb{P}_d . Different algorithms such as conjugate-gradient, BFGS, and trust-region methods for the Riemmanian manifold \mathbb{P}_d are explained in [26]. Here we only provide details for a limited memory version of Riemmanian BFGS (RBFGS). The RBFGS algorithm for general retraction and vector transport was originally explained in [45] and the proof of convergence appeared in [47], although for a slightly different version. It was proved that for g-convex functions and with line-search that satisfies Wolfe conditions, RBFGS algorithm has a (local) superlinear convergence rate. The RBFGS algorithm can be transformed into a limited-memory RBFGS (L-RBFGS) algorithm by unrolling the update step of the approximate Hessian computation as shown in Algorithm 1. As may be apparent from the algorithm, parallel transport and its inverse can be the computational bottlenecks. One possible speed-up is to store the matrix E and its inverse in (22).

4 Geometric optimisation for log-nonexpansive functions

Although manifold optimisation is powerful and widely applicable (see e.g., the excellent toolbox [10]), for a special class of geometric optimisation problems we may be able to circumvent its heavy machinery in favour of potentially much simpler algorithms.

Algorithm 1: L-RBFGS

Given: Riemannian manifold \mathcal{M} with Riemannian metric g ; vector transport \mathcal{T} on \mathcal{M} with associated retraction R ; initial value X_0 ; a smooth function f

Set initial $H_{\text{diag}} = 1/\sqrt{g_{X_0}(\text{grad}f(X_0), \text{grad}f(X_0))}$

for $k=0,1,\dots$ **do**

Obtain descent direction ξ_k by unrolling the RBFGS method

$\xi_k = \text{HESSMUL}(-\text{grad}f(X_k), k)$

Using a line-search to find α such that $f(R_{X_k}(\alpha\xi_k))$ is sufficiently smaller than $f(X_k)$

Calculate $X_{k+1} = R_{X_k}(\alpha\xi_k)$

Define $S_k = \mathcal{T}_{X_k, X_{k+1}}(\alpha\xi_k)$

Define $Y_k = \text{grad}f(X_{k+1}) - \mathcal{T}_{X_k, X_{k+1}}(\text{grad}f(X_k))$

Update $H_{\text{diag}} = g_{X_{k+1}}(S_k, Y_k)/g_{X_{k+1}}(Y_k, Y_k)$

Store $Y_k; S_k; g_{X_{k+1}}(S_k, Y_k); g_{X_{k+1}}(S_k, S_k)/g_{X_{k+1}}(S_k, Y_k); H_{\text{diag}}$

end for

return X_k

function $\text{HESSMUL}(P, k)$

if $k > 0$ **then**

$P_k = P - \frac{g_{X_{k+1}}(S_k, P_{k+1})}{g_{X_{k+1}}(Y_k, S_k)} Y_k$

$\hat{P} = \mathcal{T}_{X_k, X_{k+1}}^{-1} \text{HESSMUL}(\mathcal{T}_{X_k, X_{k+1}} P_k, k-1)$

return $\hat{P} - \frac{g_{X_{k+1}}(Y_k, \hat{P})}{g_{X_{k+1}}(Y_k, S_k)} S_k + \frac{g_{X_{k+1}}(S_k, S_k)}{g_{X_{k+1}}(Y_k, S_k)} P$

else

return $H_{\text{diag}} P$

end if

end function

This motivation underlies the material developed in this section, where ultimately our goal is to obtain fixed-point iterations by viewing \mathbb{P}_d as a convex cone instead of a Riemannian manifold. This viewpoint is grounded in nonlinear Perron-Frobenius theory [33], and it proves to be of practical value for our application in §5. Notably, for certain problems we can obtain globally optimal solutions even without g -convexity. We believe the general conic optimisation theory developed in this section may be of wider interest.

Consider for instance the following minimisation problem

$$\min_{S \succ 0} \Phi(S), \quad (23)$$

where Φ is a continuously differentiable real-valued function on \mathbb{P}_d . Since the constraint set $\{S \succ 0\}$ is an open subset of a Euclidean space, the first-order optimality condition for (23) is similar to that of unconstrained optimisation. A point S^* is a candidate local minimum of Φ only if its gradient at this point is zero, that is,

$$\nabla\Phi(S^*) = 0. \quad (24)$$

The nonlinear (matrix) equation (24) could be solved using numerical techniques such as Newton's method. But, such approaches can be much harder than original optimisation problem. We propose to exploit a fixed-point iteration that offers a simpler method for solving (24). *More importantly*, the fixed-point technique allows one to show that under

certain conditions the solution to (24) is unique, and therefore potentially a global minimum (essentially, if the global minimum is attained, then it must be this unique stationary point).

Assume therefore that (24) is rewritten as the fixed-point equation

$$S^* = \mathcal{G}(S^*). \quad (25)$$

Then, a fixed-point of the map $\mathcal{G} : \mathbb{P}_d \rightarrow \mathbb{P}_d$ is a potential solution (since it is a stationary point) to the minimisation problem (23). The natural question is how to find such a fixed-point, and starting with a feasible $S_0 \succ 0$, whether it suffices to perform the Picard iteration

$$S_{k+1} \leftarrow \mathcal{G}(S_k), \quad k = 0, 1, \dots \quad (26)$$

Iteration (26) is (usually) *not* a fixed-point iteration when cast in a normed vector space—the conic geometry of \mathbb{P}_d alluded to previously suggests that it might be better to analyse the iteration using a non-vectorial metric.

We provide below a class of sufficient conditions ensuring convergence of (26). Therein, the correct metric space in which to study convergence is neither the Euclidean (or Banach) space \mathbb{R}^n nor the Riemannian manifold \mathbb{P}_d with distance (51). Instead, a conic metric proves more suitable, namely, the Thompson part metric, an object of great interest in nonlinear Perron-Frobenius theory [32, 33].

Our sufficient conditions stem from the following key definition.

Definition 30 (Log-nonexpansive). Let $f : (0, \infty) \rightarrow (0, \infty)$. We say f is *q-log-nonexpansive* (LN) on a compact interval $I \subset (0, \infty)$ if there exists a constant $0 \leq q \leq 1$ such that

$$|\log f(t) - \log f(s)| \leq q |\log t - \log s|, \quad \forall s, t \in I. \quad (27)$$

If $q < 1$, we say f is *q-log-contractive*. If for every $s \neq t$ it holds that

$$|\log f(t) - \log f(s)| < |\log t - \log s|, \quad \forall s, t \quad s \neq t,$$

we say f is *log-contractive* (lc).

We use log-nonexpansive functions in a concrete optimisation task in Section 4.2. The proofs therein rely on core properties of the Thompson metric and contraction maps in the associated metric space—we cover requisite background in Section 4.1. The content of Section 4.1 is of independent interest as the theorems therein provide techniques for establishing contractivity (or nonexpansivity) of nonlinear maps from \mathbb{P}_d to \mathbb{P}_k .

4.1 Thompson metric and contractive maps

On \mathbb{P}_d , the *Thompson metric* is defined as (cf. δ_R which uses $\|\cdot\|_F$)

$$\delta_T(X, Y) := \|\log(Y^{-1/2}XY^{-1/2})\|, \quad (28)$$

where $\|\cdot\|$ is the usual operator norm (largest singular value), and ‘log’ is the matrix logarithm. Let us recall some core (known) properties of (28)—for details please see [32, 33, 34].

Proposition 31. *Unless noted otherwise, all matrices are assumed to be hpd.*

$$\delta_T(X^{-1}, Y^{-1}) = \delta_T(X, Y) \quad (29a)$$

$$\delta_T(B^*XB, B^*YB) = \delta_T(X, Y), \quad B \in GL_n(\mathbb{C}) \quad (29b)$$

$$\delta_T(X^t, Y^t) \leq |t| \delta_T(X, Y), \quad \text{for } t \in [-1, 1] \quad (29c)$$

$$\delta_T\left(\sum_i w_i X_i, \sum_i w_i Y_i\right) \leq \max_{1 \leq i \leq m} \delta_T(X_i, Y_i), \quad w_i \geq 0, w \neq 0 \quad (29d)$$

$$\delta_T(X + A, Y + A) \leq \frac{\alpha}{\alpha + \beta} \delta_T(X, Y), \quad A \succeq 0, \quad (29e)$$

where $\alpha = \max \{\|X\|, \|Y\|\}$ and $\beta = \lambda_{\min}(A)$.

We prove now a powerful refinement to (29b), which shows contraction under “compression.”

Theorem 32. *Let $X \in \mathbb{C}^{d \times p}$, where $p \leq d$ have full column rank. Let $A, B \in \mathbb{P}_d$. Then,*

$$\delta_T(X^*AX, X^*BX) \leq \delta_T(A, B). \quad (30)$$

First, we need a lemma that proves contraction for a special case.

Lemma 33. *Let $U \in \mathbb{C}^{d \times p}$ satisfy $U^*U = I$. Let $A, B \in \mathbb{P}_d$. Then,*

$$\delta_T(U^*AU, U^*BU) \leq \delta_T(A, B). \quad (31)$$

Proof. Let $A_U = U^*AU$ and $B_U = U^*BU$ denote the compressions of A and B , respectively. The largest generalised eigenvalue of the pencil (A, B) is given by

$$\lambda_1(A, B) := \lambda_1(A^{-1}B) = \max_{x \neq 0} \frac{x^*Bx}{x^*Ax}. \quad (32)$$

Starting with (32) we have the following argument:

$$\begin{aligned} \lambda_1(A^{-1}B) &= \lambda_1(A^{-1/2}BA^{-1/2}) = \max_{x \neq 0} \frac{x^*A^{-1/2}BA^{-1/2}x}{x^*x} \\ &= \max_{w \neq 0} \frac{w^*Bw}{(A^{1/2}w)^*(A^{1/2}w)} = \max_{w \neq 0} \frac{w^*Bw}{w^*Aw} \\ &\geq \max_{w=U_p, p \neq 0} \frac{w^*Bw}{w^*Aw} = \max_{p \neq 0} \frac{p^*U^*BU p}{p^*U^*AU p} \\ &= \max_{p \neq 0} \frac{p^*B_C p}{p^*A_C p} = \lambda_1(A_C^{-1}B_C) = \lambda_1(A_C^{-1/2}B A_C^{-1/2}). \end{aligned}$$

Similarly, we can show that $\lambda_1(B^{-1}A) = \lambda_1(B^{-1/2}AB^{-1/2}) \geq \lambda_1(B_C^{-1/2}A_C B_C^{-1/2})$. Since A, B and the compressions A_C, B_C are all positive, we may conclude

$$\max \{ \log \lambda_1(A_C^{-1}B_C), \log \lambda_1(B_C^{-1}A_C) \} \leq \max \{ \log \lambda_1(A^{-1}B), \log \lambda_1(B^{-1}A) \}, \quad (33)$$

which is nothing but the desired claim $\delta_T(U^*AU, U^*BU) \leq \delta_T(A, B)$. \square

Proof. (Theorem 32). Write X using its full-SVD $X = U\Sigma V^*$. Then,

$$\begin{aligned} \delta_T(X^*AX, X^*TBX) &= \delta_T(V\Sigma U^*AU\Sigma V^*, V\Sigma U^*BU\Sigma V^*) \\ &= \delta_T(\Sigma_+ U_p^*AU_p \Sigma_+, \Sigma_+ U_p^*BU_p \Sigma_+) \\ &= \delta_T(U_p^*AU_p, U_p^*BU_p) \\ &\leq \delta_T(A, B). \end{aligned}$$

where the final inequality follows from Lemma 33. \square

Theorem 32 can be extended to encompass more general “compression” maps, namely to those defined by operator monotone functions, a class that enjoys great importance in matrix theory—see e.g., [5, Ch. V] and [6].

Theorem 34. Let f be an operator monotone (i.e., if $X \preceq Y$, then $f(X) \preceq f(Y)$) function on $(0, \infty)$ such that $f(0) \geq 0$. Then,

$$\delta_T(f(X), f(Y)) \leq \delta_T(X, Y), \quad X, Y \in \mathbb{P}_d. \quad (34)$$

Proof. First, we show that if f is operator monotone with $f(0) \geq 0$, then $\delta_T(f(A), f(B)) \leq \delta_T(A, B)$ for $A, B \in \mathbb{P}_k$. It is known that f admits the integral representation [5, (V.53)]

$$f(t) = \gamma + \beta t + \int_0^\infty \frac{\lambda t}{\lambda + t} d\mu(\lambda), \quad (35)$$

where $\gamma = f(0)$, $\beta \geq 0$, and $d\mu(t)$ is a nonnegative measure. Using representation (35) we get

$$f(A) = \gamma I + \beta A + \int_0^\infty (\lambda A)(\lambda I + A)^{-1} d\mu(\lambda) =: \gamma I + \beta A + M(A).$$

Similarly, we obtain $f(B) = \gamma I + \beta B + M(B)$. Thus, we see that

$$\begin{aligned} \delta_T(M(A), M(B)) &= \delta_T\left(\int \lambda A(\lambda I + A)^{-1} d\mu(t), \int \lambda A(\lambda I + A)^{-1} d\mu(t)\right) \\ &\leq \max_\lambda \delta_T(\lambda A(\lambda I + A)^{-1}, \lambda B(\lambda I + B)^{-1}) \\ &\leq \max_\lambda \delta_T((\lambda A^{-1} + I)^{-1}, (\lambda B^{-1} + I)^{-1}) \\ &= \max_\lambda \delta_T(I + \lambda A^{-1}, I + \lambda B^{-1}) \\ &\leq \max_\lambda \frac{\bar{\alpha}}{\bar{\alpha} + 1} \delta_T(\lambda A^{-1}, \lambda B^{-1}), \quad \bar{\alpha} := \max\{\|A^{-1}\|, \|B^{-1}\|\}, \\ &= \frac{\bar{\alpha}}{\bar{\alpha} + 1} \delta_T(A, B) < \delta_T(A, B). \end{aligned}$$

This contraction between $M(A)$ and $M(B)$ then helps prove

$$\begin{aligned} \delta_T(f(A), f(B)) &= \delta_T(\gamma I + \beta A + M(A), \gamma I + \beta B + M(B)) \\ &\leq \frac{\alpha}{\alpha + \gamma} \delta_T(\beta A + M(A), \beta B + M(B)), \quad \alpha := \max\|\beta A + M(A)\|, \|\beta B + M(B)\| \\ &\leq \frac{\alpha}{\alpha + \gamma} \max\{\delta_T(\beta A, \beta B), \delta_T(M(A), M(B))\} \\ &\leq \frac{\alpha}{\alpha + \gamma} \delta_T(A, B). \end{aligned}$$

Moreover, for $A \neq B$ the inequality is strict if $f(0) > 0$. □

Example 35. Let $X \in \mathbb{C}^{d \times k}$, and let $f = t^r$ on $t \in (0, \infty)$ where $r \in (0, 1)$. Then,

$$\begin{aligned} \delta_T((X^* A X)^r, (X^* B X)^r) &\leq \delta_T(A, B), \quad \forall A, B \in \mathbb{P}_d, \\ \delta_T(X^* A^r X, X^* B^r X) &\leq \delta_T(A, B), \quad \forall A, B \in \mathbb{P}_d. \end{aligned}$$

Theorem 32 and Theorem 34 together also yield the following useful contraction result.

Corollary 36. Let $\Phi : \mathbb{P}_d \rightarrow \mathbb{P}_k$ ($k \leq d$), and $\Psi : \mathbb{P}_k \rightarrow \mathbb{P}_r$ ($r \leq k$) be completely positive (see e.g., [6, Ch. 3]) maps. Then,

$$\delta_T(f(\Phi(X)), f(\Phi(Y))) \leq \delta_T(X, Y), \quad X, Y \in \mathbb{P}_d, \quad (36)$$

$$\delta_T(\Psi(f(X)), \Psi(f(Y))) \leq \delta_T(X, Y), \quad X, Y \in \mathbb{P}_k. \quad (37)$$

Proof. We prove (36); the proof of (37) is similar, hence omitted. From Theorem 34 it follows that $\delta_T(f(\Phi(X)), f(\Phi(Y))) \leq \delta_T(\Phi(X), \Phi(Y))$. Since Φ is completely positive, it follows from a result of Choi [20] and Kraus [30] that there exist matrices $V_j \in \mathbb{C}^{d \times k}$, $1 \leq j \leq dk$, such that

$$\Phi(X) = \sum_{i=1}^{nk} V_j^* X V_j \quad X \in \mathbb{P}_d.$$

Theorem 32 and property (29d) imply that $\delta_T(\Phi(X), \Phi(Y)) \leq \delta_T(X, Y)$, which proves (36). \square

Thompson log-nonexpansive maps. Let \mathcal{G} be a map from $\mathcal{X} \subseteq \mathbb{P}_d \rightarrow \mathcal{X}$. Analogous to (27), we say \mathcal{G} is (Thompson) *log-nonexpansive* if

$$\delta_T(\mathcal{G}(X), \mathcal{G}(Y)) \leq \delta_T(X, Y), \quad \forall X, Y \in \mathcal{X};$$

the maps is called *log-contractive* if the inequality is strict. We present now a key result that justifies our nomenclature and the analogy to (27): it shows that the sum of a log-contractive map and a log-nonexpansive map is log-contractive. This behaviour is a striking feature of the nonpositive curvature of \mathbb{P}_d ; such a result does *not* hold in normed vector spaces.

Theorem 37. *Let \mathcal{G} be a log-nonexpansive map and \mathcal{F} be a log-contractive one. Then, their sum $\mathcal{G} + \mathcal{F}$ is log-contractive.*

Proof. We start by writing Thompson metric in an alternative form [33]:

$$\delta_T(A, B) = \max\{\log W(A/B), \log W(B/A)\}, \quad (38)$$

where $W(A/B) := \inf\{\lambda > 0, A \preceq \lambda B\}$. Let $\lambda = \exp(\delta_T(X, Y))$; then it follows that $X \preceq \lambda Y$. Since \mathcal{G} is nonexpansive in δ_T , using (38) it further follows that

$$\mathcal{G}(X) \preceq \lambda \mathcal{G}(Y),$$

and \mathcal{F} is log-contractive map, we obtain the inequality

$$\mathcal{F}(X) \prec \lambda^t \mathcal{F}(Y), \quad \text{where } t \leq 1.$$

Write $\mathcal{H} := \mathcal{G} + \mathcal{F}$; then, we have the following inequalities:

$$\begin{aligned} \mathcal{H}(X) &\prec \lambda \mathcal{H}(Y) + (\lambda^t - \lambda) \mathcal{F}(Y) \\ \mathcal{H}(Y)^{-1/2} \mathcal{H}(X) \mathcal{H}(Y)^{-1/2} &\prec \lambda I + (\lambda^t - \lambda) \mathcal{H}(Y)^{-1/2} \mathcal{F}(Y) \mathcal{H}(Y)^{-1/2} \\ \mathcal{H}(Y)^{-1/2} \mathcal{H}(X) \mathcal{H}(Y)^{-1/2} &\prec \lambda I + (\lambda^t - \lambda) \lambda_{\min}(\mathcal{H}(Y)^{-1/2} \mathcal{F}(Y) \mathcal{H}(Y)^{-1/2}) I, \end{aligned}$$

Since $\lambda_{\max}(\mathcal{H}(Y)^{-1/2} \mathcal{H}(X) \mathcal{H}(Y)^{-1/2}) > \lambda_{\max}(\mathcal{H}(X)^{-1/2} \mathcal{H}(Y) \mathcal{H}(X)^{-1/2})$, using (38) we have

$$\delta_T(\mathcal{H}(X), \mathcal{H}(Y)) < \delta_T(X, Y) + \log(1 + \lambda_{\min}(\mathcal{H}(Y)^{-1/2} \mathcal{F}(Y) \mathcal{H}(Y)^{-1/2}) [\lambda^{t-1} - 1]). \quad (39)$$

We also have the following eigenvalue inequality

$$\lambda_{\min}(\mathcal{H}(Y)^{-1/2} \mathcal{F}(Y) \mathcal{H}(Y)^{-1/2}) \leq \frac{\lambda_{\min}(\mathcal{F}(Y))}{\lambda_{\max}(\mathcal{G}(Y)) + \lambda_{\min}(\mathcal{F}(Y))}. \quad (40)$$

Combining inequalities (39) and (40) we see that

$$\delta_T(\mathcal{H}(X), \mathcal{H}(Y)) < \delta_T(X, Y) + \log\left(1 + \frac{\lambda_{\min}(\mathcal{F}(Y))}{\lambda_{\max}(\mathcal{G}(Y)) + \lambda_{\min}(\mathcal{F}(Y))} [\exp(\delta_T(X, Y))^{t-1} - 1]\right). \quad (41)$$

Similarly, we also have $\lambda_{\max}(\mathcal{H}(Y)^{-1/2}\mathcal{H}(X)\mathcal{H}(Y)^{-1/2}) < \lambda_{\max}(\mathcal{H}(X)^{-1/2}\mathcal{H}(Y)\mathcal{H}(X)^{-1/2})$, so that we also obtain the bound (notice we now have $\mathcal{F}(X)$ instead of $\mathcal{F}(Y)$)

$$\delta_T(\mathcal{H}(X), \mathcal{H}(Y)) < \delta_T(X, Y) + \log\left(1 + \frac{\lambda_{\min}(\mathcal{F}(X))}{\lambda_{\max}(\mathcal{G}(X)) + \lambda_{\min}(\mathcal{F}(X))}\right) [\exp(\delta_T(X, Y))^{t-1} - 1]. \quad (42)$$

Combining (41) and (42) into a single inequality, we get

$$\delta_T(\mathcal{H}(X), \mathcal{H}(Y)) < \delta_T(X, Y) + \log\left(1 + \frac{\lambda_{\min}(\mathcal{F}(X), \mathcal{F}(Y))}{\lambda_{\max}(\mathcal{G}(X), \mathcal{G}(Y)) + \lambda_{\min}(\mathcal{F}(X), \mathcal{F}(Y))}\right) [\exp(\delta_T(X, Y))^{t-1} - 1].$$

Since the second term is ≤ 0 , the inequality is strict, which proves \mathcal{H} is log-contractive. \square

Using log-contractivity we may finally state our main convergence result for this section.

Theorem 38. *If \mathcal{G} is log-contractive and equation (25) has a solution, then this solution is unique and iteration (26) converges to it.*

Proof. If (45) has a solution, then from a theorem of Edelstein [21], it follows that the log-contractive map \mathcal{G} yields iterates that stay within a compact set and converge to a unique fixed point of \mathcal{G} . This fixed-point is positive definite by construction (starting from a positive definite matrix, none of the operations in (45) violates positivity). Thus, the unique solution is positive definite. \square

4.2 Example of log-nonexpansive optimisation

To illustrate how to exploit log-nonexpansive functions for optimisation, let us consider the following minimisation problem

$$\min_{S \succ 0} \Phi(S) := \frac{1}{2}n \log \det(S) - \sum_i \log \varphi(x_i^T S^{-1} x_i), \quad (43)$$

which arises in maximum-likelihood estimation of ECDs (see Section 5 for further examples and details) and also M-estimation of the scatter matrix [28].

The first-order necessary optimality condition for (43) stipulates that a candidate solution $S \succ 0$ must satisfy

$$\frac{\partial \Phi(S)}{\partial S} = 0 \iff \frac{1}{2}nS^{-1} + \sum_{i=1}^n \frac{\varphi'(x_i^T S^{-1} x_i)}{\varphi(x_i^T S^{-1} x_i)} S^{-1} x_i x_i^T S^{-1} = 0. \quad (44)$$

Defining $h \equiv -\varphi'/\varphi$, (44) may be rewritten more compactly in matrix notation as the equation

$$S = \frac{2}{n} \sum_{i=1}^n x_i h(x_i^T S^{-1} x_i) x_i^T = \frac{2}{n} X D_S X^T, \quad (45)$$

where $D_S := \text{Diag}(h(x_i^T S^{-1} x_i))$, and $X = [x_1, \dots, x_m]$. We then solve the nonlinear equation (45) via a fixed-point iteration. Introducing the nonlinear map $\mathcal{G} : \mathbb{P}_d \rightarrow \mathbb{P}_d$ that maps S to the right hand side of (45), we use fixed-point iteration (26) to find the solution. In order to show that the Picard iteration converges (to the unique fixed-point), it is enough to show that \mathcal{G} is log-contractive (see Theorem 38). The following proposition gives sufficient condition on h , under which the map is log-contractive.

Proposition 39. *Let h be log-nonexpansive. Then, the map \mathcal{G} in (26) is log-nonexpansive. Moreover, if h is log-contractive, then \mathcal{G} is log-contractive.*

Proof. Let $S, R \succ 0$ be arbitrary. Then, we have the following chain of inequalities

$$\begin{aligned} \delta_T(\mathcal{G}(S), \mathcal{G}(R)) &= \delta_T\left(\frac{2}{n}Xh(D_S)X^T, \frac{2}{n}Xh(D_R)X^T\right) \\ &\leq \delta_T(h(D_S), h(D_R)) \leq \max_{1 \leq i \leq n} \delta_T(h(x_i^T S^{-1}x_i), h(x_i^T R^{-1}x_i)) \\ &\leq \max_{1 \leq i \leq n} \delta_T(x_i^T S^{-1}x_i, x_i^T R^{-1}x_i) \leq \delta_T(S^{-1}, R^{-1}) = \delta_T(S, R). \end{aligned}$$

The first inequality follows from (29b) and Theorem 32; the second inequality follows since $h(D_S)$ and $h(D_R)$ are diagonal; the third follows from (29d); the fourth from another application of Theorem 32, while the final equality is via (29a). This proves log-nonexpansivity (i.e., nonexpansivity in δ_T). If in addition h is log-contractive and $S \neq R$, then the second inequality above is strict, that is,

$$\delta_T(\mathcal{G}(S), \mathcal{G}(R)) < \delta_T(S, R) \quad \forall S, R \quad \text{and} \quad S \neq R. \quad \square$$

If h is merely log-nonexpansive (not log-contractive), it is still possible to show uniqueness of (45) up to a constant. Our proof depends on the compression property of δ_T proved in Theorem 32.

Theorem 40. *Let the data $\mathcal{X} = \{x_1, \dots, x_n\}$ span the whole space. If h is LN, and $S_1 \neq S_2$ are solutions to equation (45), then iteration (26) converges to a solution, and $S_1 \propto S_2$.*

Proof. Without loss of generality assume that $S_1 = I$. Let $S_2 \neq cI$. Theorem 32 implies that

$$\begin{aligned} &\delta_T(x_i h(x_i^T S_2^{-1} x_i) x_i^T, x_i h(x_i^T S_1^{-1} x_i) x_i) \\ &\leq \delta_T(h(x_i^T S_2^{-1} x_i), h(x_i^T x_i)) \leq \delta_T(x_i^T S_2^{-1} x_i, x_i^T x_i) = \left| \log \frac{x_i^T S_2^{-1} x_i}{x_i^T x_i} \right|. \end{aligned}$$

As per assumption, the data span the whole space. Since $S_2 \neq cI$, we can find x_1 such that

$$\left| \log \frac{x_1^T S_2^{-1} x_1}{x_1^T x_1} \right| < \delta_T(S_2, I).$$

Therefore, we obtain the following inequality for point x_1 :

$$\delta_T(x_1 h(x_1^T S_2^{-1} x_1) x_1^T, x_1 h(x_1^T S_1^{-1} x_1) x_1) < \delta_T(S_2, S_1). \quad (46)$$

Using Proposition 39 and invoking Theorem 37, it then follows that

$$\delta_T(\mathcal{G}(S_2), \mathcal{G}(S_1)) < \delta_T(S_2, S_1).$$

But this means that S_2 cannot be a solution to (45), a contradiction. Therefore, $S_2 \propto S_1$. \square

Computational efficiency. So far we did not address computational efficacy of the fixed-point algorithm. The rate of convergence depends heavily on the contraction factor, and as we will see in the experiments, without further care one obtains poor contraction factors that can lead to a very slow convergence. We briefly discuss below a useful speedup technique that seems to have a dramatic impact on the empirical convergence speed (see Figure 2).

At the fixed point S^* we have $\mathcal{G}(S^*) = S^*$, or equivalently for a new map \mathcal{M} we have

$$\mathcal{M}(S^*) := S^{*-1/2} \mathcal{G}(S^*) S^{*-1/2} = I.$$

Therefore, one way to analyse the convergence behaviour is to assess how fast $\mathcal{M}(S_k)$ converges to identity. Using the theory developed beforehand, it is easy to show that

$$\delta_T(\mathcal{M}(S_{k+1}), I) \leq \eta \delta_T(\mathcal{M}(S_k), I),$$

where η is the contraction factor between S_k and S_{k+1} , so that

$$\delta_T(\mathcal{G}(S_{k+1}), \mathcal{G}(S_k)) < \eta \delta_T(S_{k+1}, S_k).$$

To increase the convergence speed we may replace S_{k+1} by its scaled version $\alpha_k S_{k+1}$ such that

$$\delta_T(\mathcal{M}(\alpha_k S_{k+1}), I) \leq \delta_T(\mathcal{M}(S_{k+1}), I).$$

One can do a line search to find a good α_k . Clearly, the sequence $S_{k+1} = \alpha_k \mathcal{G}(S_k)$ converges at a faster pace. We will see in the experimental result section that scaling with α_k has a remarkable effect on the convergence speed. An intuitive reasoning why this happens is that the additional scaling factor can resolve the problematic cases where the contraction factor become small. These problematic cases are those where both the smallest and the largest eigenvalues of $\mathcal{M}(S_k)$ become smaller (or larger) than one, whereby the contraction factor (for \mathcal{G}) becomes small, which may lead to a very slow convergence. The scaling factor, however, makes the smallest eigenvalues of $\mathcal{M}(S_k)$ always smaller and its largest eigenvalue larger than one. One way to avoid line search is to choose α_k such that $\text{trace}(\mathcal{M}(S_{k+1})) = d$ —though with a small caveat: empirically this simple choice of α_k works very well, but our convergence proof does not hold anymore. Extending our convergence theory to incorporate this specific choice of scaling α_k is a part of our future work.

5 Application to Elliptically Contoured Distributions

In this section we present details for a concrete application of conic geometric optimisation: mle for ECDs [13, 22, 38]. We use ECDs as a platform for illustrating geometric optimisation because ECDs are widely important (see e.g., the survey [43]), and are instructive in illustrating our theory.

First, some basics. If an ECD has density on \mathbb{R}^d , it assumes the form²

$$\forall x \in \mathbb{R}^d, \quad \mathcal{E}_\varphi(x; S) \propto \det(S)^{-1/2} \varphi(x^T S^{-1} x), \quad (47)$$

where $S \in \mathbb{P}_d$ is the scatter matrix and $\varphi : \mathbb{R} \rightarrow \mathbb{R}_{++}$ is the *density generating function* (dgf). If the ECD has finite covariance, then the scatter matrix is proportional to the covariance matrix [13].

Example 41. Let $\varphi(t) = e^{-t/2}$; then, (47) reduces to the multivariate Gaussian density. For

$$\varphi(t) = t^{\alpha-d/2} \exp(-(t/b)^\beta), \quad (48)$$

where $\alpha, b, \beta > 0$ are fixed, density (47) yields the rich class called *Kotz-type distributions* that have powerful modelling abilities [27, §3.2]; they include as special cases multivariate power exponentials, elliptical gamma, multivariate W-distributions, for instance. Other examples include multivariate student-t, multivariate logistic, and Weibull dgfs (see §5.2).

²For simplicity we describe only mean zero families; the extension to the general case is easy.

5.1 Maximum likelihood parameter estimation

Let (x_1, \dots, x_n) be i.i.d. samples from an ECD $\mathcal{E}_\varphi(S)$. Ignoring constants, the log-likelihood is

$$\mathcal{L}(x_1, \dots, x_n; S) = -\frac{1}{2}n \log \det S + \sum_{i=1}^n \log \varphi(x_i^T S^{-1} x_i). \quad (49)$$

To compute a mle we equivalently consider the minimisation problem (43), which we restate here for convenience

$$\min_{S \succ 0} \Phi(S) := \frac{1}{2}n \log \det(S) - \sum_i \log \varphi(x_i^T S^{-1} x_i). \quad (50)$$

Unfortunately, (50) is in general very difficult: Φ may be nonconvex and may have multiple local minima (observe that $\log \det(S)$ is concave in S and we are minimising). Since statistical estimation relies on having access to globally optimal estimates, it is important to be able to solve (50) globally. These difficulties notwithstanding, using our theory we identify a rich class of ECDs for which we can solve (50) globally. Some examples are already known [28, 43, 55], but our techniques yield results strictly more general: they subsume previous examples while advancing the broader idea of geometric optimisation over hpd matrices.

Building on §2 and §4, we divide our study into the following three classes of dgfs:

- (i) **Geodesically convex (g-convex)**: This class contains functions for which the negative log-likelihood $\Phi(S)$ is g-convex. Some members of this class have been previously studied (though sometimes without recognising or directly exploiting g-convexity);
- (ii) **Log-Nonexpansive (LN)**: This is a new class introduced in this paper. It exploits the “non-positive curvature” property of the hpd manifold. To our knowledge, this class of ECDs was beyond the grasp of previous methods [28, 53, 55]. The iterative algorithm for finding the global minimum of the objective is similar to that of the class LC.
- (iii) **Log-Convex (LC)**: We cover this class for completeness; it covers the case of log-convex φ , but leads to nonconvex Φ (due to the $-\log \varphi$ term). However, the structure of the problem is such that one can derive an efficient algorithm for finding a local minimum of the objective function.

As illustrated in Figure 1, these three classes can overlap. When a function is in the overlap between classes LC and g-convex, one can be sure that the iterative algorithm derived for the class LN will converge to a unique minimum.

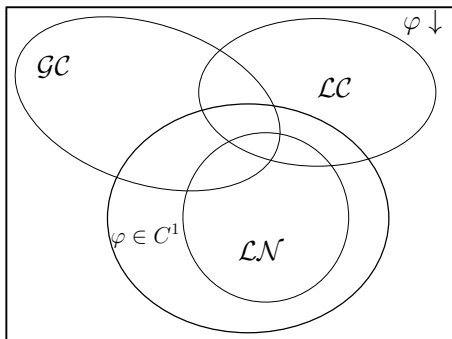


Figure 1: Overview of dgf functions classes for nonincreasing φ .

5.2 MLE for distributions in class g-convex

If the log-likelihood is strictly g-convex then (50) cannot have multiple solutions. Moreover, for any local optimisation method that ensures a local solution to (50), g-convexity ensures that this solution is globally optimal.

First we state a corollary of Theorem 15 that helps recognise g-convexity of ECDs. We remark that a result equivalent to Corollary 42 was also recently discovered in [55]. Theorem 15 is more general and uses a completely different argument founded on matrix-theoretic results.

Corollary 42. *If $h : \mathbb{R}_{++} \rightarrow \mathbb{R}$ is nondecreasing and g-convex (i.e., $h(x^{1-\lambda}y^\lambda) \leq (1-\lambda)h(x) + \lambda h(y)$), then for $r \in \{\pm 1\}$, $\phi : \mathbb{P}_d \rightarrow \mathbb{R} : S \mapsto \sum_i h(x_i^T S^r x_i) \pm \log \det(S)$ is g-convex.*

Proof. Immediate from Theorem 15 upon noting that $x_i^T S^r x_i$ is a positive linear map. \square

For reference, we summarise several examples of g-convex ECDs in Corollary 43 below.

Corollary 43. *The negative log-likelihood (50) is g-convex for the following distributions: (i) Kotz with $\alpha \leq \frac{d}{2}$ (its special cases include Gaussian, multivariate power exponential, multivariate W-distribution with shape parameter smaller than one, elliptical gamma with shape parameter $\nu \leq \frac{d}{2}$); (ii) Multivariate-t; (iii) Multivariate Pearson type II with positive shape parameter; (iv) Elliptical multivariate logistic distribution.*³

Even though g-convexity ensures that every local solution will be globally optimal, we must first ensure that there exists a solution at all, that is, *does (50) have a solution?* Answering this question is nontrivial even in special cases [28, 55]. We provide below a fairly general result that helps establish existence.

Theorem 44. *Let $\Phi(S)$ satisfy the following: (i) $-\log \varphi(t)$ is lower semi-continuous (lsc) for $t > 0$, and (ii) $\Phi(S) \rightarrow \infty$ as $\|S\| \rightarrow \infty$ or $\|S^{-1}\| \rightarrow \infty$, then $\Phi(S)$ attains its minimum.*

Proof. Consider the metric space (\mathbb{P}_d, d_R) , where d_R is the Riemannian distance,

$$d_R(A, B) = \|\log(A^{-1/2}BA^{-1/2})\|_F \quad A, B \in \mathbb{P}_d. \quad (51)$$

If $\Phi(S) \rightarrow \infty$ as $\|S\| \rightarrow \infty$ or as $\|S^{-1}\| \rightarrow \infty$, then $\Phi(S)$ has bounded lower-level sets in (\mathbb{P}_d, d_R) . It is a well-known result in variational analysis that an lsc function which has bounded lower-level sets in a metric space attains its minimum [48]. Since $-\log \varphi(t)$ is lsc and $\log \det(S^{-1})$ is continuous, $\Phi(S)$ is lsc on (\mathbb{P}_d, d_R) . Therefore it attains its minimum. \square

A key consequence of this theorem is its utility in showing existence of solutions to (50) for a variety of different ECDs. We show an example application to Kotz-type distributions [27, 29] below. For these distributions, the function $\Phi(S)$ assumes the form

$$K(S) = \frac{n}{2} \log \det(S) + \left(\frac{d}{2} - \alpha\right) \sum_{i=1}^n \log x_i^T S^{-1} x_i + \sum_{i=1}^n \left(\frac{x_i^T S^{-1} x_i}{b}\right)^\beta. \quad (52)$$

Lemma 45 shows that $K(S) \rightarrow \infty$ whenever $\|S^{-1}\| \rightarrow \infty$ or $\|S\| \rightarrow \infty$.

³The dgfs of different distributions are brought here for the reader's convenience. Multivariate power exponential: $\phi(t) = \exp(-t^\nu/b)$, $\nu > 0$; Multivariate W-distribution: $\phi(t) = t^{\nu-1} \exp(-t^\nu/b)$, $\nu > 0$; Elliptical gamma: $\phi(t) = t^{\nu-d/2} \exp(-t/b)$, $\nu > 0$; Multivariate t: $\phi(t) = (1+t/\nu)^{-(\nu+d)/2}$, $\nu > 0$; Multivariate Pearson type II: $\phi(t) = (1-t)^\nu$, $\nu > -1, 0 \leq t \leq 1$; Elliptical multivariate logistic: $\phi(t) = \exp(-\sqrt{t})/(1+\exp(-\sqrt{t}))^2$.

Lemma 45. *Let the data $\mathcal{X} = \{x_1, \dots, x_n\}$ span the whole space and for $\alpha < \frac{d}{2}$ satisfy*

$$\frac{|\mathcal{X} \cap L|}{|\mathcal{X}|} < \frac{d_L}{d - 2\alpha}, \quad (53)$$

where L is an arbitrary subspace with dimension $d_L < d$ and $|\mathcal{X} \cap L|$ is the number of datapoints that lie in the subspace L . If $\|S^{-1}\| \rightarrow \infty$ or $\|S\| \rightarrow \infty$, then $K(S) \rightarrow \infty$.

Proof. If $\|S^{-1}\| \rightarrow \infty$ and since the data span the whole space, it is possible to find a datum x_1 such that $t_1 = x_1^T S^{-1} x_1 \rightarrow \infty$. Since

$$\lim_{t \rightarrow \infty} c_1 \log(t) + t^{c_2} + c_3 \rightarrow \infty$$

for constants c_1, c_3 and $c_2 > 0$, it follows that $K(S) \rightarrow \infty$ whenever $\|S^{-1}\| \rightarrow \infty$.

If $\|S\| \rightarrow \infty$ and $\|S^{-1}\|$ is bounded, then the third term in expression of $K(S)$ is bounded. Assume that d_L is the number of eigenvalues of S that go to ∞ and $|\mathcal{X} \cap L|$ is the number of data that lie in the subspace span by these eigenvalues. Then in the limit when eigenvalues of S go to ∞ , $K(S)$ converges to the following limit

$$\lim_{\lambda \rightarrow \infty} \frac{n}{2} d_L \log \lambda + \left(\frac{d}{2} - \alpha\right) |\mathcal{X} \cap L| \log \lambda^{-1} + c$$

Apparently if $\frac{n}{2} d_L + \left(\frac{d}{2} - \alpha\right) |\mathcal{X} \cap L| > 0$, then $K(S) \rightarrow \infty$ and the proof is complete. \square

It is important to note that overlap condition (53) can be fulfilled easily by assuming that the number of data points is larger than their dimensionality and that they are noisy. Using Lemma 45 with Theorem 44 we obtain the following key result for Kotz-type distributions.

Theorem 46 (Existence of mle). *If the data samples satisfy condition (53), then the negative log-likelihood of Kotz-type distribution has a minimiser (i.e., there exists an mle).*

5.2.1 Optimisation algorithm

Once existence is ensured, one may use any local optimisation method to minimise (50) to obtain the desired mle. For members of the class g-convex that do not lie in class LN or class LC, we recommend invoking the manifold optimisation techniques summarised in §3.

5.3 MLE for distributions in class LN

For negative log-likelihoods (50) in class LN, we can circumvent the heavy machinery of manifold optimisation, and obtain simple fixed-point algorithms by appealing to the contraction results developed in §4. We note that some members of class g-convex may also turn out to lie in class LN, so the discussion below also applies to them.

As an illustrative example of these results, consider the problem of finding the minimum of negative log-likelihood solution of Kotz-type distribution (52). If the corresponding nonlinear equation (45) with corresponding $h(\cdot) = \left(\frac{d}{2} - \alpha\right)(\cdot)^{-1} + \frac{\beta}{b\beta}(\cdot)^{\beta-1}$ has a positive definite solution, then it is a candidate mle; if it is unique, then it is the desired solution to (52).

But how should we solve (45)? This is where the theory developed in §4 comes into play. Convergence of the iteration (26) as applied to (45) can be obtained from Theorem 40. But in the Kotz case we can actually show a stronger result that helps ensure better geometric convergence rates for the fixed-point iteration.

Lemma 47. *If $c > 0$ and $-1 < b < 1$, the function $g(x) = x + cx^b$ is log-contractive.*

Proof. Without loss of generality assume $t = ks$ with $k \geq 1$. Assume that $g(t) \geq g(s)$:

$$\begin{aligned}
\log g(t) &= \log(t + ct^b) \\
&= \log(ks + ck^b s^b) \\
&= \log(k(s + cs^b) + ck^b s^b - cks^b) \\
&= \log k(s + cs^b) \left(1 + \frac{ck^b s^b - cks^b}{k(s + cs^b)}\right) \\
&= \log k + \log g(s) + \log \left(1 + \frac{cs^b(k^{b-1} - 1)}{(s + cs^b)}\right) \\
|\log g(t) - \log g(s)| &= |\log t - \log s| + \log \left(1 + \frac{cs^b(k^{b-1} - 1)}{(s + cs^b)}\right)
\end{aligned}$$

Since the second term is negative, therefore g is log-contractive. Consider the other case $g(t) \geq g(s)$, that could happen only when $b \leq 0$.

$$\begin{aligned}
\log g(s) &= \log(s + cs^b) \\
&= \log(t/k + ck^{|b|}t^b) \\
&= \log(k(t + ct^b) + ck^{|b|}t^b + t/k - kt - ckt^b) \\
&= \log k(t + ct^b) \left(1 + \frac{ck^{|b|}t^b + t/k - kt - ckt^b}{k(t + ct^b)}\right) \\
&= \log k + \log g(t) + \log \left(1 + \frac{t(k^{-2} - 1) + ct^b(k^{|b|-1} - 1)}{(t + ct^b)}\right) \\
|\log g(t) - \log g(s)| &= |\log t - \log s| + \log \left(1 + \frac{t(\frac{1}{k^2} - 1) + ct^b(k^{|b|-1} - 1)}{(t + ct^b)}\right).
\end{aligned}$$

In this case, the second term is also negative. Therefore h is log-contractive. \square

Assume $b = 1 - \beta$, $c = \frac{b^\beta(d/2 - \alpha)}{\beta}$ and knowing that $h(\cdot) = g((\frac{d}{2} - \alpha)(\cdot)^{-1})$ has the same contraction factor as $g(\cdot)$, Lemma 47 implies that h in the iteration (45) for the Kotz-type distributions with $0 < \beta < 2$ and $\alpha < \frac{d}{2}$ is log-contractive. Based on Theorem 46, $K(S)$ has at least one minimum. Thus using Theorem 38, we have the following main convergence result.

Theorem 48. *If the data samples satisfy condition (53), then the Iteration (45) for Kotz-type distributions with $0 < \beta < 2$ and $\alpha < \frac{d}{2}$ converges to a unique fixed point.*

5.4 MLE for distributions in class LC

For completeness, we briefly mention class LC here, which is perhaps one of the most studied classes of ECDs, at least from an algorithmic point-of-view [28]. Therefore, we only discuss it summarily, presenting our new results.

For the class LC, we assume that the dgf φ is log-convex. Without assumptions that are typically made in the literature, it can be that neither the GC nor the LN analysis applies to class LC. However, the optimisation problem still has structure that allows simple and efficient algorithms. Specifically, here the objective function $\Phi(S)$ can be written as a difference of two convex functions by introducing the variable $P = S^{-1}$, wherewith we have $\Phi(P) = -an \log \det(P) - \sum_i \log \varphi(x_i^T P x_i)$.

To this representation of Φ we may now apply the CCCP procedure [54] to search for a locally optimal point. The method operates as follows

$$P^{k+1} \leftarrow \underset{P \succ 0}{\operatorname{argmin}} \quad -\frac{n}{2} \log \det(P) + \operatorname{tr} \left(P \sum_i h(x_i^T P^k x_i) x_i x_i^T \right),$$

which yields the update

$$P^{k+1} = \left(\frac{2}{n} \sum_i h(x_i^T P^k x_i) x_i x_i^T \right)^{-1}. \quad (54)$$

By this construction, we see that the sequence $\{\Phi(P^k)\}$ is monotonically decreasing. Furthermore, since we assumed h to be nonnegative, therefore the iteration stays within positive semidefinite cone. If the cost function goes to infinity whenever the covariance matrix is singular, then using Theorem 44 we can conclude that iteration converges to a positive definite matrix. Thus, we can state the following key result for class LC.

Theorem 49 (Convergence). *Assume that $\Phi(P)$ goes to infinity whenever P reaches the boundary of \mathbb{P}^d , i.e. $\|P\| \rightarrow \infty \vee \|P^{-1}\| \rightarrow \infty \implies \Phi(P) \rightarrow \infty$. Furthermore if $-\log \varphi$ is concave and h is non-negative, then each step of the iterative algorithm given in (54) decreases the cost function and furthermore it converges to a positive definite solution.*

A similar theorem but under more strict conditions was established in Kent and Tyler [28]. Knowing that the iterative algorithm in (54) is the same as (45) and using Theorem 49 with the existence result of Theorem 46 and uniqueness result of Corollary 43, we can state the following theorem for Kotz-type distributions (*cf.* Theorem 48).

Theorem 50. *If the data samples satisfy condition (53), then the Iteration (45) for Kotz-type distributions with $\beta > 1$ and $\alpha < \frac{d}{2}$ converges to a unique fixed point.*

Theorem 50 and Theorem 48 together show that the iteration (45) for Kotz-type distributions with $\alpha < \frac{d}{2}$ and regardless of the value of β always converges to the unique mle estimate whenever it exists.

6 Numerical results

We briefly illustrate the numerical performance of our fixed-point iteration. The key message here is that our fixed-point iterations solve nonconvex problems that are further complicated by a positive definiteness constraint. But by construction the fixed-point iterations satisfy the constraint, so no extra eigenvalue computation is needed, which can provide substantial computational savings. In contrast, a general nonlinear solver must perform constrained optimisation, which may be unduly expensive.

We show two simple experiments (Figs. 2 and 3) to demonstrate scalability of the fixed-point iteration with increasing dimensionality of the input matrix and for varying β parameter of the Kotz distribution which influences convergence rate of our fixed-point iteration. For all simulations, we sampled 10,000 datapoints from the Kotz-type distribution with given α and β parameters and a random covariance matrix.

We note that the problems are nonconvex with an open set as a constraint—this precludes direct application of semidefinite programming or approaches such as gradient-projection (projection requires closed sets). We also tried interior-point methods but we did not include them in the comparisons because of their extremely slow convergence speed on this problem. So we choose to show the result of (Riemannian) manifold optimisation techniques [1].

We compare our fixed-point iteration against four different manifold optimisation methods: (i) steepest descent (SD); (ii) conjugate gradients (CG); (iii) trust-region (TR); and (iv) LBFGS, which implements Algorithm 1. All methods are implemented in MATLAB (including the fixed-point iteration); for manifold optimisation we extend the excellent MANOPT toolbox [10] to support the hpd manifold⁴ as well as Algorithm 1.

From Figure 2 we see that the basic fixed-point algorithm (FP) does not perform better than SD, the most basic manifold optimisation method. Moreover, even when FP performs better than CG, TR, or LBFGS (Figure 3), it seems to closely follow the performance of SD. However, the scaling idea introduced in §4.2 leads to a fixed-point method (FP2) that outperforms all other methods, both with increasing dimensionality as well as varying β .

These results are merely to indicate that the fixed-point approach can be competitive. A more thorough experimental study to assess our algorithms remains to be undertaken.

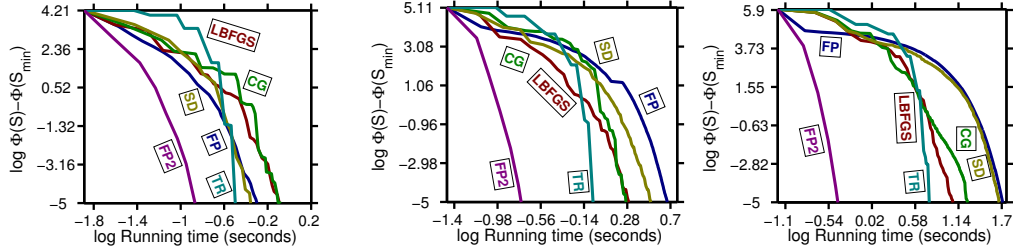


Figure 2: Running times comparison of the fixed-point iterations compared with four different manifold optimization techniques to maximise a Kotz-likelihood with $\beta = 0.5$ and $\alpha = 2$ (see text for details). FP denoted normal fixed-point iteration and FP2 is the fixed-point iteration with scaling factor. Manifold optimization methods are steepest descent (SD), conjugate gradient (CG), limited-memory RBFGS (LBFGS) and trust-region (TR). The plots show (from left to right), running times for estimating $S \in \mathbb{P}_d$, for $d \in \{4, 16, 64\}$.

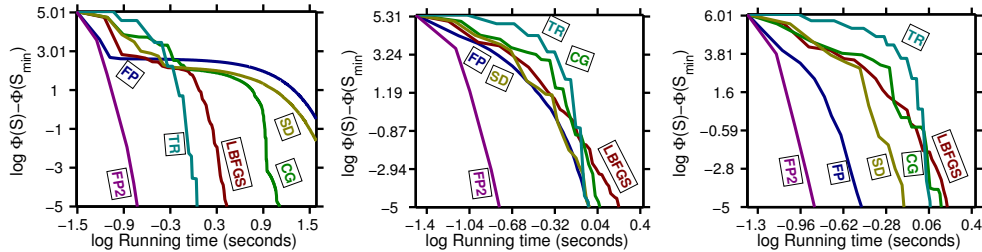


Figure 3: In the Kotz-type distribution, when β gets close to zero or 2, the contraction factor becomes smaller which can impact the convergence rate. This figure shows running time variance for Kotz-type distributions with fixed $d = 16$, and $\alpha = 2$, for different values of $\beta \in \{0.1, 1, 1.7\}$.

7 Conclusion

We studied geometric optimisation for minimising certain nonconvex functions over the set of positive definite matrices. We showed key results that help recognise geodesic convexity;

⁴The newest version of the MANOPT toolbox ships with an implementation of the hpd manifold, but we use our own implementation as it includes some utilities specific to LBFGS.

we also introduced a new class of log-nonexpansive functions which contains functions that need not be geodesically convex, but can still be optimised efficiently. Key to our ideas was a construction of fixed-point iterations in a suitable metric space on positive definite matrices.

Additionally, we developed and applied our results in the context of maximum likelihood estimation for elliptically contoured distributions, covering instances substantially beyond the state-of-the-art. We believe that the general geometric optimisation techniques that we developed in this paper will prove to be of wider use and interest beyond our motivating examples and applications. Moreover, developing a more extensive geometric optimisation numerical package is an ongoing project.

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