ENTROPIC COVARIANCE MODELS

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In covariance matrix estimation, one of the challenges lies in finding a suitable model and an efficient estimation method. Two commonly used modelling approaches in the literature involve imposing linear restrictions on the covariance matrix or its inverse. Another approach considers linear restrictions on the matrix logarithm of the covariance matrix. In this paper, we present a general framework for linear restrictions on different transformations of the covariance matrix, including the mentioned examples. Our proposed estimation method solves a convex problem and yields an M-estimator, allowing for relatively straightforward asymptotic and finite sample analysis. After developing the general theory, we focus on modelling correlation matrices and on sparsity. Our geometric insights allow to extend various recent results in covariance matrix modelling. This includes providing unrestricted parametrizations of the space of correlation matrices, which is alternative to a recent result utilizing the matrix logarithm.

1. Introduction. Estimating the covariance matrix is a fundamental problem in many fields, including multivariate statistics, spatial statistics, finance, and machine learning. The literature offers a wide range of models that have been considered for this purpose; e.g. Anderson (1970); Jennrich and Schluchter (1986); Boik (2002); Pourahmadi (2013). One popular approach involves exploiting linear restrictions on factors in a decomposition of Σ or its transformation Pourahmadi (2011). For instance, in linear structural equation models, specific entries of the matrix L in the LDL decomposition $\Sigma^{-1} = LDL^{\top}$ are set to zero.

Since modelling via the LDL decomposition heavily relies on the variable ordering in the system, as an alternative, linear restrictions can be directly imposed on the covariance matrix Σ or some transformation of it; e.g. Anderson (1970); Dempster (1972); Sturmfels and Uhler (2010). This approach has gained attention due to the prevalence of such structures in multiple applications. Examples include Toeplitz matrices or block-Toeplitz matrices in time series and spatial statistics Anderson (1978), linear structures encoded by trees in Brownian motion tree models Zwiernik, Uhler and Richards (2017), and other types of symmetries Szatrowski (2004). Gaussian graphical models, which enforce sparsity on the inverse of Σ , and their colored versions have also been widely used in multivariate statistics and machine learning Dempster (1972); Lauritzen (1996); Højsgaard and Lauritzen (2008). These models are popular due to their interpretability, as the entries of Σ and its inverse correspond to correlations or partial correlations.

Another type of restriction considered in the literature involves linear constraints on the matrix logarithm of the covariance matrix Leonard and Hsu (1992); Chiu, Leonard and Tsui (1996); Battey (2017). While the interpretation of such constraints is generally less clear, these models have gained popularity because modelling the matrix logarithm $\log(\Sigma)$ does not require handling the positivity constraints. When Σ is diagonal, these models can be viewed as extensions of classical log-linear models for heterogeneous variances. The matrix logarithm of the covariance matrix has found applications in stochastic volatility models, medical imaging, spatial statistics, and quantum geometry Kawakatsu (2006);

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Ishihara, Omori and Asai (2016); Asai and So (2015); Bauer and Vorkink (2011); Zhu et al. (2009); LeSage and Pace (2007); Pavlov, Sturmfels and Telen (2022).

Notably, the fact that the matrix logarithm of a covariance matrix is an unrestricted symmetric matrix has important theoretical implications. For instance, in recent work Archakov and Hansen (2021) have shown that the logarithm of the correlation matrix has properties similar to Fisher's Z-transformation. Having an unrestricted parametrization of correlation matrices is considered a major breakthrough in temporal modelling of correlation matrices, which is critical in the GARCH approach. Leveraging similar ideas, we provide an unrestricted parameterization of Gaussian graphical models and various other covariance models, which may be of independent interest. In this context, we propose to study the mapping $\Sigma \mapsto \Sigma - \Sigma^{-1}$ as a more tractable alternative to the matrix logarithm.

Main goals of this paper: The research on the matrix logarithm has motivated the exploration of linear restrictions on more general functions of the covariance matrix. In this statistical context, functions such as the matrix logarithm are treated as link functions, analogous to generalized linear models (GLMs) Pourahmadi (2011); Zou et al. (2017); Lin, Müller and Park (2023). Our paper contributes to the development of a GLM methodology and a data-based framework for modelling covariance matrices, building on the work initiated by Anderson, Pourahmadi, and others. The main goals of this paper are twofold:

- (i) To propose a general framework for modelling covariance matrices that allows for efficient estimation procedures based on convex optimization.
- (ii) To enhance the understanding of the geometry of covariance matrices and show how convexity simplifies the statistical analysis.

We now briefly describe how these goals are approached.

Entropic covariance models (informal): Our general insight is similar to the construction of generalized exponential families and matrix nearness problems Grünwald and Dawid (2004); Dhillon and Tropp (2008), albeit applied to covariance matrices in a broader sense than previously explored. The key idea is to utilize the gradient mapping $\nabla F(\Sigma)$ of a general strictly convex and differentiable function defined on the positive definite cone. This mapping induces a one-to-one transformation of covariance matrices, and we impose affine (or general convex) restrictions on the result of this transformation. Affine constraints can arise from regression of the covariance matrix (or its transformation) on auxiliary information Zou et al. (2017); Lin, Müller and Park (2023), specific symmetry patterns Szatrowski (2004), or sparsity Dempster (1972); Hastie, Tibshirani and Wainwright (2015).

For a concrete example, consider the set of 3×3 covariance matrices Σ such that $L = \log(\Sigma)$ satisfies $L_{13} = 0$. This example appears later in Section 6.2. Models with zero restrictions on $\log \Sigma$ have been recently studied in Rybak and Battey (2021); Pavlov (2023). Here the main problem is that simple constraints in L translate to complicated constraint in Σ , which may potentially complicate the estimation process. This is one of the problems we fully address in this article.

Estimation under linear constraints: Estimating models under linear restrictions on the inverse covariance matrix is relatively straightforward. Let $\mathbf{X} \in \mathbb{R}^{n \times m}$ be the data matrix with independent rows coming from a mean zero distribution with covariance Σ . A natural approach is to optimize the Gaussian log-likelihood, which, up to additive constants, is given by

(1)
$$\ell(K) = \frac{n}{2} \log \det(K) - \frac{n}{2} \operatorname{tr}(S_n K), \qquad S_n = \frac{1}{n} \mathbf{X}^{\top} \mathbf{X},$$

where $K = \Sigma^{-1}$ satisfies the given constraints Anderson (1970); Sturmfels and Uhler (2010); Barratt and Boyd (2022). This optimization problem is convex since $\ell(K)$ is a strictly concave function of K, and the constraints are linear in K. However, in the case of linear constraints on Σ , a canonical estimation approach is less obvious, and the Gaussian

log-likelihood becomes multimodal Zwiernik, Uhler and Richards (2017). This has motivated research on alternative estimation methods Anderson (1973); Christensen (1989); Sturmfels, Timme and Zwiernik (2019); Améndola and Zwiernik (2021). One natural approach is to replace the maximum likelihood estimator (MLE) with the least squares estimator, which minimizes $\|\Sigma - S_n\|_F^2$ over all Σ in the given linear subspace.

In this paper, by utilizing the Bregman divergence Bregman (1967), we generalize both the least squares approach for estimating under linear restrictions on Σ and the problem of minimizing $\ell(K)$ for restrictions that are linear in K. Bregman matrix divergences have been used for matrix estimation and matrix approximation problems; e.g. Dhillon and Tropp (2008); Ravikumar, Wainwright and Lafferty (2010); Cai and Zhou (2012); Llorens-Terrazas and Brownlees (2022). However, in these papers, Bregman divergence was used to analyze existing covariance models. Here, it is studied in the context of new models and to provide more insight in covariance matrix geometry.

For every entropic model the resulting loss function is strictly convex, and its Hessian does not depend on the data. This is similar to the negative log-likelihood function in exponential families, making the theoretical analysis of this estimator rather straightforward following the elegant work of Niemiro (1992). In particular, we show that our proposed estimator, which we call the Bregman estimator, is consistent and asymptotically normal.

Geometry of entropic models: One of the contributions of this paper is providing new insights into the geometry of various covariance models that explain and sometimes greatly generalize existing results. One example is a far reaching generalization of Theorem 1 in Archakov and Hansen (2021), which provides an unrestricted parametrization for correlation matrices; see Section 5.2. Another class of insights is related with the Jordan algebras of symmetric matrices, which we discuss in Section 6.4. These results explain why for certain entropic models the maximum likelihood estimator is available in closed form; e.g. LeSage and Pace (2007). We expect these results will greatly improve our understanding of the linear models on the matrix logarithm of Σ and other entropic models.

The article is organized as follows. Section 2 provides a brief overview of the necessary background in convex analysis and introduces the main definitions and running examples. Our proposed estimation method is presented in Section 3, where we also demonstrate the convexity of the underlying optimization problem. Section 4 presents basic statistical analyses of the resulting estimator. Section 5 investigates the geometry of entropic models in connection with convex analysis and mixed parametrization. In Section 6, we present various general results that contribute to our understanding of this model class. Specifically, Section 6.1 proposes simple numerical algorithms, and Section 6.2 focuses on sparsity patterns. Section 6.3 provides some motivation for modelling under linear restrictions on higher powers of Σ^{-1} . Finally, Section 6.4 provides insights into a particular type of linear constraints that define Jordan algebras.

- **2. Preliminaries and definitions.** Let \mathbb{S}^m denote the real vector space of symmetric $m \times m$ matrices, and let \mathbb{S}^m_+ and $\overline{\mathbb{S}}^m_+$ represent the subsets of matrices that are positive definite and positive semidefinite, respectively. We equip \mathbb{S}^m with the standard inner product $\langle A,B\rangle=\operatorname{tr}(AB)$ and the induced Frobenius norm $\|A\|_F=\sqrt{\langle A,A\rangle}$.
- 2.1. Convex functions on \mathbb{S}^m . By $\operatorname{Conv}(\mathbb{S}^m)$ denote the set of convex functions $F: \mathbb{S}^m \to \mathbb{R} \cup \{+\infty\}$ that are not identically equal to $+\infty$ (these are called sometimes proper convex functions). The domain of $F \in \operatorname{Conv}(\mathbb{S}^m)$ is the nonempty set $\operatorname{dom}(F) = \{A \in \mathbb{S}^m : F(A) < +\infty\}$. By $\operatorname{Conv}(\mathbb{S}^m)$ denote the class of all functions in $\operatorname{Conv}(\mathbb{S}^m)$ that are lower semicontinuous on \mathbb{S}^m these are also known as closed convex functions. Recall that F

is lower semicontinuous if the lower level-set $\{A: F(A) \leq t\}$ is closed for all $t \in \mathbb{R}$. Because convex functions are always continuous in the interior of their domain, this involves conditions on how F behaves on the boundary of $\operatorname{dom} F^1$.

Reserve a special notation \mathcal{E}^m for functions $F: \mathbb{S}^m \to \mathbb{R} \cup \{+\infty\}$ such that:

- (i) $F \in C\overline{\text{onv}}(\mathbb{S}^m)$,
- (ii) $\mathbb{S}_{+}^{m} \subseteq \text{dom}(F) \subseteq \overline{\mathbb{S}}_{+}^{m}$ or equivalently $\text{int}(\text{dom}(F)) = \mathbb{S}_{+}^{m}$, (iii) F is strictly convex and continuously differentiable on \mathbb{S}_{+}^{m} .

In this paper we only consider functions on \mathbb{S}^m that belong to the class \mathcal{E}^m

REMARK 2.1. If F satisfies only (i) and (iii), we replace F(A) with

$$F(A) + i_{\overline{\mathbb{S}}_{+}^{m}}(A), \quad \text{where} \quad i_{\overline{\mathbb{S}}_{+}^{m}}(A) = \begin{cases} 0 & \text{if } A \in \overline{\mathbb{S}}_{+}^{m}, \\ +\infty & \text{otherwise.} \end{cases}$$

Because $\overline{\mathbb{S}}_+^m$ is closed and convex, $\mathbf{i}_{\overline{\mathbb{S}}_+^m} \in \overline{\mathrm{Conv}}(\mathbb{S}^m)$, and so also $F(A) + \mathbf{i}_{\overline{\mathbb{S}}_+^m}(A) \in \overline{\mathrm{Conv}}(\mathbb{S}^m)$. Moreover, the interior of the domain of $F(A) + i_{\overline{\mathbb{S}}_{\perp}^m}(A)$ is \mathbb{S}_{+}^m . For brevity we often include the indicator function only implicitly.

A special subclass of functions in \mathcal{E}^m are functions that satisfy in addition:

(iv) $\|\nabla F(\Sigma_k)\| \to \infty$ for any sequence (Σ_k) in \mathbb{S}^n_+ that converges to the boundary of \mathbb{S}^m_+ .

If $F \in \mathcal{E}^m$ satisfies (iv), we say that F is essentially smooth.

In our running examples below we define the function $F(\Sigma)$ for $\Sigma \in \mathbb{S}_+^m$, The function is then extended by lower semicontinuity to the boundary of $\overline{\mathbb{S}}_+^m$, and it is equal to $+\infty$ for all other points. The following are our running examples:

(A)
$$F_A(\Sigma) = -\log \det \Sigma$$
 (B) $F_B(\Sigma) = \frac{1}{2} \operatorname{tr}(\Sigma^2)$

(C)
$$F_C(\Sigma) = -\operatorname{tr}(\Sigma - \Sigma \log \Sigma)$$
 (D) $F_D(\Sigma) = \operatorname{tr}(\Sigma^{-1})$

and the details on the lower semicontinuous extension are provided in Appendix A.2. The function $-F_A$ is called the Gaussian entropy. The function $2F_B$ is the squared Frobenius norm of Σ . The function $-F_C$ is the von Neumann entropy. Both (B) and (D) can be easily generalized:

(B')
$$F_{B,p}(\Sigma) = \frac{1}{n} \operatorname{tr}(\Sigma^p)$$
 for $p \ge 1$ (D') $F_{D,p}(\Sigma) = \frac{1}{n} \operatorname{tr}(\Sigma^{-p})$ for $p \ge 0$.

Note that $pF_{B,p}$ is the p-Schatten norm of Σ raised to power p, $F_{B,p}(\Sigma) = \frac{1}{n} \|\Sigma\|_p^p$, where denoting by $\lambda_1, \ldots, \lambda_m$ the eigenvalues of $\Sigma \in \mathbb{S}_+^m$ we have

(2)
$$\|\Sigma\|_p = \sqrt[p]{\lambda_1^p + \ldots + \lambda_m^p}.$$

Although we try to keep our theory as general as possible, we note that all our running examples are spectral functions of the form $F(\Sigma) = \operatorname{tr}(\phi(\Sigma))$ where $\phi: \mathbb{R} \to \mathbb{R}$ and the notation $\phi(\Sigma)$ means the corresponding matrix function; see, e.g., Higham (2008). We call such functions spectral sums.

We will later show that examples (A), (C), and (D) are also essentially smooth. In example (C) this is quite surprising because the function itself extends to $\overline{\mathbb{S}}_{+}^{m}$ (see Appendix A.2).

¹We refer to Rockafellar (1970); Hiriart-Urruty and Lemaréchal (2012) as good references for convex analysis. Chapter 5 of Barndorff-Nielsen (1978) provides a good exposition of the most statistically-relevant results from Rockafellar (1970). Our discussion of Bregman divergences is closely related to Bauschke and Borwein (1997)

2.2. Entropic covariance models. We are now ready to describe our set-up. The main object in our analysis is the gradient ∇F of F. We start with the following well-known fact.

LEMMA 2.2. If $F \in \mathcal{E}^m$, then $\nabla F : \mathbb{S}^m_+ \to \mathbb{S}^m$ defines a one-to-one function on \mathbb{S}^m_+ .

PROOF. Fix $A \in \mathbb{S}^m$ and note that the function $\langle A, \Sigma \rangle - F(\Sigma)$ is strictly concave and continuously differentiable on \mathbb{S}^m_+ . Thus, if its maximum in \mathbb{S}^m_+ exists, it must be a stationary point and so it must satisfy $\nabla F(\Sigma) = A$. By convexity it must be the unique such point. This shows that for each $A \in \mathbb{S}^m$ there exists at most one point $\Sigma \in \mathbb{S}^m_+$ such that $\nabla F(\Sigma) = A$. \square

Our modelling technique is to apply the transformation $\nabla F(\Sigma)$ and impose restrictions on it. It is useful to denote

$$\mathbb{L}_{+}^{m} := \nabla F(\mathbb{S}_{+}^{m}).$$

Lemma 2.2 motivates the following definition.

DEFINITION 2.3 (Linear Entropic Covariance Model). Fix an affine subspace $\mathcal{L} \subseteq \mathbb{S}^m$. The corresponding linear entropic model is

$$M_F(\mathcal{L}) := \{ \Sigma \in \mathbb{S}_+^m : \nabla F(\Sigma) \in \mathcal{L} \} = \mathcal{L} \cap \mathbb{L}_+^m.$$

In the definition we implicitly assumed that $M_F(\mathcal{L})$ is non-empty. This is a recurrent assumption of this paper.

ASSUMPTION 1: The mapping $F \in \mathcal{E}^m$ and the subspace $\mathcal{L} \subseteq \mathbb{S}^m$ satisfy $\mathcal{L} \cap \mathbb{L}_+^m \neq \emptyset$.

Some interesting examples of the function F are given by popular matrix entropy functions like the negative Gaussian entropy (A) and the negative von Neumann entropy (C) (hence the name). For now, F is relevant for us only through the mapping $\nabla F(\Sigma)$, which defines a suitable reparametrization of the covariance matrix. In the following examples, we refer to Proposition A.3 for a simple technique to compute $\nabla F(\Sigma) = \nabla \operatorname{tr}(\phi(\Sigma))$ by computing the derivative of ϕ . The functions $\phi_A, \phi_B, \phi_C, \phi_D$ were defined in (30)-(33).

EXAMPLE 2.4 (A). If x > 0 then $\phi_A'(x) = -\frac{1}{x}$ and so $\nabla F_A(\Sigma) = -\Sigma^{-1}$ by Proposition A.3. The model $M_{F_A}(\mathcal{L})$ is described by all $\Sigma \in \mathbb{S}_+^m$ such that $-\Sigma^{-1} \in \mathcal{L}$. Here $\mathbb{L}_+^m = -\mathbb{S}_+^m$ and we use the notation \mathcal{L}_+^{-1} to refer to this model. Models of this form are classically known in statistics Dempster (1972); Anderson (1973); see also the introduction for a more comprehensive literature overview.

Although linear restrictions on the inverse covariance matrix have many applications, there are important areas (e.g. signal processing) where it is more natural to impose linear symmetry restrictions directly on the covariance matrix. This leads to our second example.

EXAMPLE 2.5 (B). If x>0 then $\phi_B'(x)=x$ and so $\nabla F_B(\Sigma)=\Sigma$. The corresponding entropic model is given by all $\Sigma\in\mathbb{S}_+^m$ such that $\Sigma\in\mathcal{L}$. Here $\mathbb{L}_+^m=\mathbb{S}_+^m$ and we denote this model by \mathcal{L}_+ . This imposes linear restrictions on the covariance matrix as discussed in the introduction. This example can be generalized to the p-th Schatten norm of $\Sigma\in\mathbb{S}_+^m$, $\nabla F_{B,p}(\Sigma)=\Sigma^{p-1}$, which allows us to model linear restrictions on an arbitrary positive power of Σ .

$F(\Sigma)$	$\nabla F(\Sigma)$	$F^*(L)$	$D_F(S,L)$
$-\log\det(\Sigma)$	$-\Sigma^{-1}$	$-m - \log \det(-L)$	$-\log\det((-L)S) + \operatorname{tr}((-L)S - I_m)$
$\tfrac{1}{2}\ \Sigma\ _F^2$	Σ	$\frac{1}{2}\operatorname{tr}(L^2)$	$\frac{1}{2}\ L-S\ _F^2$
$\operatorname{tr}(\Sigma^{-1})$	$-\Sigma^{-2}$	$-2\operatorname{tr}(\sqrt{-L})$	$\operatorname{tr}(S^{-1}) - 2\operatorname{tr}(\sqrt{-L}) + \operatorname{tr}((-L)S)$
$-\operatorname{tr}(\Sigma - \Sigma \log(\Sigma))$	$\log(\Sigma)$	$\operatorname{tr}(e^L)$	$-\operatorname{tr}(S - S\log(S)) + \operatorname{tr}(e^{L}) - \operatorname{tr}(LS)$
$\frac{1}{p} \ \Sigma\ _p^p, p \geqslant 1$	Σ^{p-1}	$\frac{1}{q}\ L\ _q^q, \ q = \frac{p}{p-1}$	$\frac{1}{p} \ S\ _p^p + \frac{1}{q} \ L\ _q^q - \text{tr}(LS)$
$\frac{1}{p} \ \Sigma^{-1} \ _p^p, p > 0$	$-\Sigma^{-p-1}$	$-\frac{1}{q}\ -L\ _q^q, \ q=\frac{p}{p+1}$	$\frac{1}{p} \ S^{-1}\ _p^p - \frac{1}{q} \ - L\ _q^q + \operatorname{tr}((-L)S)$

TABLE 1

Our running examples with the corresponding gradients, conjugate functions, and the Bregman divergence.

This setting is however completely general and, as we argue below, it is a natural framework to discuss the generalized models for covariance matrices Pourahmadi (2000); Zou et al. (2017); Lin, Müller and Park (2023). Example (C) again links to a model well studied in the literature.

EXAMPLE 2.6 (C). If x>0 then $\phi'_C(x)=\log(x)$ and so $\nabla F_C(\Sigma)=\log(\Sigma)$. The model is given by all Σ such that $\log(\Sigma)\in\mathcal{L}$. This imposes linear restrictions on the matrix logarithm of the covariance matrix. Denote this model by $e^{\mathcal{L}}$. One of the reasons, why this model is useful is because every matrix $L\in\mathbb{S}^m$ is a matrix logarithm of some $\Sigma\in\mathbb{S}^m_+$. In other words, $\mathbb{L}^m_+=\mathbb{S}^m$. In the introduction we provide an extensive literature overview for this model. Some further theoretical justification will be given in Section 5.

We discuss one more example whose relevance will be explained later.

EXAMPLE 2.7 (D). If x>0 then $\phi_D'(x)=-\frac{1}{x}$ and so $\nabla F_D(\Sigma)=-\Sigma^{-2}$. The model is given by all $\Sigma\in\mathbb{S}_+^m$ such that $\Sigma^{-2}\in\mathcal{L}$. Denote this model by \mathcal{L}_+^{-2} . This example has a straightforward generalization: $\nabla F_{D,p}(\Sigma)=-\Sigma^{-p-1}$ for any $p\geqslant 0$, which allows to impose linear restrictions on powers of Σ^{-1} . In Section 6.3 we motivate such zero restrictions.

All our examples are summarized in Table 1. The gradient is given in the second column and the other columns will be discussed in detail later.

2.3. Dual construction of $M_F(\mathcal{L})$. We note the following dual construction. Suppose $\pi: \mathbb{S}^m \to \mathbb{R}^d$, for some $d \ge 1$ is an affine. In the spirit of (generalized) exponential families Barndorff-Nielsen (1978); Grünwald and Dawid (2004), we refer to π as a sufficient statistics. Given $b \in \mathbb{R}^d$, consider the optimization problem

(4) minimize
$$F(\Sigma) - \langle A_0, \Sigma \rangle$$
 subject to $\pi(\Sigma) = b$,

where $A_0 \in \mathbb{S}^m$ is a fixed matrix. If $F \in \mathcal{E}^m$ then this problem has at most one optimal solution in \mathbb{S}^m_+ . Since the set $\mathbb{S}^m_+ \cap \{\Sigma : \pi(\Sigma) = b\}$ is relatively open (in the affine subspace $\{\Sigma : \pi(\Sigma) = b\}$), this optimal point $\hat{\Sigma}$, if exists, must satisfy the regular first order conditions: we must have that $\pi(\hat{\Sigma}) = b$ and, for every $U \in \mathbb{S}^m$ such that $\pi(U) = 0$, it must hold that $\langle \nabla F(\hat{\Sigma}) - A_0, U \rangle = 0$, that is, the directional derivatives in all permitted directions must be zero. In other words,

(5)
$$\nabla F(\Sigma) - A_0 \in \ker(\pi)^{\perp} =: \mathcal{L}_0.$$

Note that this equation and the affine space $\mathcal{L} := A_0 + \mathcal{L}_0$ do not depend on the vector b and so the condition $\nabla F(\Sigma) \in \mathcal{L}$ describes all such potential optimizers.

PROPOSITION 2.8. A point $\widehat{\Sigma} \in \mathbb{S}_{+}^{m}$ solves (4) for some $b \in \mathbb{R}^{d}$ if and only if $\nabla F(\widehat{\Sigma}) \in \mathcal{L}$.

PROOF. The right direction was argued above. If $\nabla F(\widehat{\Sigma}) \in \mathcal{L}$ then take $b := \pi(\widehat{\Sigma})$. Now $\widehat{\Sigma}$ clearly is an optimum of (4) for this b.

For example, if \mathcal{L} is given by zero restrictions on some coordinates, we get an explicit link to positive definite completion problems.

EXAMPLE 2.9 (Positive definite completion). Fix a graph G on m nodes and edge set E. We allow G to have self-loops that is edges from i to i. Let $\pi:\mathbb{S}^m\to\mathbb{R}^{|E|}$ be given by $\pi(\Sigma)=((\Sigma_{ij})_{ij\in E})$. In this case $\ker(\pi)$ is the set of symmetric matrices with zeros on the entries corresponding to the edges of G. Thus, \mathcal{L}_0 is the set of symmetric matrices with zero entries for all non-edges of G: $\mathcal{L}_0=\{L\in\mathbb{S}^m:\ L_{ij}=0\ \text{if}\ ij\notin E\}$. Given $S\in\mathbb{S}^m_+$, the solution to (5) with $b:=\pi(S)$ and $A_0=0$ is the unique matrix $\widehat{\Sigma}$ that agrees with S on all the entries $ij\in E$ and such that $\widehat{L}=\nabla F(\widehat{\Sigma})$ is zero on the complementary entries.

3. The Bregman estimator. Consider data X_1, \ldots, X_n from a centered distribution with a covariance matrix Σ_0 in an entropic model $M_F(\mathcal{L})$. Throughout the paper we make the following assumption.

ASSUMPTION 2: $\Sigma_0 \in \mathbb{S}_+^m$ and $\nabla F(\Sigma_0) \in \mathcal{L}$.

We can estimate the covariance matrix using the Gaussian log-likelihood (1). In the case of non-Gaussian data, this log-likelihood is considered as one of the suitable loss functions. This gives an asymptotically statistically optimal procedure as long as all fourth order cumulants of the underlying distribution vanish Browne (1974). For the model \mathcal{L}_{+}^{-1} in Example 2.4 this approach is canonical not only because it leads to an efficient estimator but also because it requires solving a convex optimization problem. Indeed, the Gaussian log-likelihood in (1) is a strictly concave function in $K = \Sigma^{-1}$.

The problem for the general entropic model $M_F(\mathcal{L})$ is that optimizing the Gaussian log-likelihood may be quite complicated since the linear constraints in $L = \nabla F(\Sigma)$ translate into non-linear constraints in K. This observation has motivated a lot of research on the estimation of linear covariance models \mathcal{L}_+ . One valid solution is to use the dual MLE, which provides an efficient alternative to the MLE Christensen (1989); Kauermann (1996); Lauritzen and Zwiernik (2022); Améndola and Zwiernik (2021). Alternatively, the least squares estimator or generalized least squares estimator has also been used Browne (1974).

3.1. Definition of the Bregman estimator. In this section, we propose an estimation procedure for linear entropic models, which offers a natural alternative to the MLE. It generalizes the use of Gaussian likelihood for linear concentration models \mathcal{L}_+^{-1} and the least squares estimation for linear covariance models \mathcal{L}_+ . An important ingredient of our statistical analysis is the Bregman divergence:

(6)
$$D_F(S,\Sigma) = F(S) - F(\Sigma) - \langle \nabla F(\Sigma), S - \Sigma \rangle.$$

Note that one of the characterizations of strict convexity for differentiable functions over \mathbb{S}^m_+ assures that $D_F(S,\Sigma) \geqslant 0$ for all $S \in \mathbb{S}^m_+$ with equality if and only if $S = \Sigma$.

Let S_n be the sample covariance matrix defined in (1). Our proposed estimator is obtained by minimizing the Bregman divergence $D_F(S_n, \Sigma)$ over the entropic model $M_F(\mathcal{L})$.

DEFINITION 3.1. The Bregman estimator $\widehat{\Sigma}$ (if exists) is the global minimizer of $D_F(S_n, \Sigma)$ subject to $\nabla F(\Sigma) \in \mathcal{L} \cap \mathbb{L}_+^m$.

Note that this is different than the regular Bregman projection, for which the minimization is with respect to the first argument; Bauschke and Borwein (1997); Dhillon and Tropp (2008); Llorens-Terrazas and Brownlees (2022).

There are two crucial aspects regarding the underlying optimization problem that we will formally state later in this section. Firstly, in Theorem 3.7, we demonstrate that $D_F(S_n, \Sigma)$ is a strictly convex function of $\nabla F(\Sigma) \in \mathbb{L}_+^m$. Secondly, in Theorem 3.13, we establish that if $F \in \mathcal{E}^m$ is essentially smooth, then the optimum always exists whenever $S_n \in \mathbb{S}_+^m$. In such cases, there is no explicit need to impose the restriction $\nabla F(\Sigma) \in \mathbb{L}_+^m$ as first-order optimization methods will naturally remain within \mathbb{S}_+^m . Before formally proving these assertions, we will examine some examples.

EXAMPLE 3.2 (A). In the Gaussian entropy example we have

$$D_{F_A}(S_n, \Sigma) = -\log \det(S_n \Sigma^{-1}) + \operatorname{tr}(S_n \Sigma^{-1} - I_m),$$

which is just the standard Kullback-Leibler divergence between two mean zero Gaussian distributions, with covariances S_n and Σ respectively. Here a potential issue arises when S_n is not positive definite. The standard approach is to drop the $F_A(S_n)$ term, which anyway does not depend on Σ , and work with the Gaussian log-likelihood directly.

EXAMPLE 3.3 (B). In the Frobenius norm example we have

$$D_{F_B}(S_n, \Sigma) = F_B(S_n) - F_B(\Sigma) - \langle \Sigma, S_n - \Sigma \rangle = \frac{1}{2} \|\Sigma - S_n\|_F^2.$$

Thus, minimizing $D_{F_B}(S_n, \Sigma)$ over $\Sigma \in \mathcal{L}_+$ simply gives the orthogonal projection of S_n on \mathcal{L} if this projection is positive definite. Note that in this example F_B is not essentially smooth.

The next example proposes a new way of estimating parameters in models that are linear in $\log(\Sigma)$. This provides an alternative to the maximum likelihood estimation considered in Chiu, Leonard and Tsui (1996).

EXAMPLE 3.4 (C). In the von Neumann case we have

$$D_{F_C}(S_n, \Sigma) = -\operatorname{tr}(S_n - S_n \log(S_n)) + \operatorname{tr}(\Sigma - \Sigma \log(\Sigma)) - \langle \log(\Sigma), S_n - \Sigma \rangle$$

= -\text{tr}(S_n - S_n \log(S_n)) + \text{tr}(\Sigma - S_n \log(\Sigma)).

The next example provides some curious connections to empirical score matching loss.

EXAMPLE 3.5 (D). In our last example given by $F_D(\Sigma) = \operatorname{tr}(\Sigma^{-1})$, we have

$$D_{F_D}(S_n, \Sigma) = \operatorname{tr}(S_n^{-1}) - \operatorname{tr}(\Sigma^{-1}) + \langle \Sigma^{-2}, S_n - \Sigma \rangle$$

= $\operatorname{tr}(S_n^{-1}) - 2\operatorname{tr}(\Sigma^{-1} - \Sigma^{-1}S_n\Sigma^{-1}).$

Note that this function is convex in Σ^{-1} and it corresponds to the empirical score matching loss of Lin, Drton and Shojaie (2016).

3.2. Convexity of the underlying optimization problem. We next analyze $D_F(S_n, \Sigma)$ as a function of $L = \nabla F(\Sigma)$. The conjugate of $F(\Sigma)$ is

(7)
$$F^*(L) := \sup_{\Sigma \in \mathbb{S}^m} \{ \langle \Sigma, L \rangle - F(\Sigma) \}.$$

The third column of Table 1 contains the convex conjugates for our leading examples. Note that we use notation $||L||_q$ introduced in (2) also if q < 1, in which case this is formally not a norm. Explicit calculations for spectral functions could be done by utilizing Theorem 2.3 in Lewis (1996a). For the special case of spectral sums we use Lemma A.5.

Understanding the domain of F^* in general may be complicated but showing that it contains $\mathbb{L}_+^m = \nabla F(\mathbb{S}_+^m)$, as in the examples above, is straightforward. In the next proposition we collect several known results.

PROPOSITION 3.6. If $F \in \mathcal{E}^m$ then (a) $F^* \in \overline{\operatorname{Conv}}(\mathbb{S}^m)$, (b) F^* is continuously differentiable on int $\operatorname{dom}(F^*)$, (c) $\mathbb{L}_+^m \subseteq \operatorname{dom}(F^*)$, and (d) F^* is strictly convex on each convex subset of \mathbb{L}_+^m .

PROOF. Statements (a), (b), and (d) follow from Theorem E.1.1.2, Theorem E.4.1.1, and Theorem E.4.1.2 in Hiriart-Urruty and Lemaréchal (2001). To prove (c), note that if $S \in \mathbb{S}_+^m$ and $L = \nabla F(S)$ then $\langle \Sigma, L \rangle - F(\Sigma)$ is strictly concave and well-defined over \mathbb{S}_+^m . Since S is a stationary point it must be the optimum.

To illustrate Proposition 3.6 and how it is subtle, consider the situation in (34). We have $dom(F_B^*) = \mathbb{S}^m$ (as calculated in Appendix A.3) and the function is continuously differentiable everywhere (part (b)), however it is *not* strictly convex everywhere. Since in this case $\mathbb{L}_+^m = \mathbb{S}_+^m$, we confirm that F^* is strictly convex on this smaller subset (part (d)).

Directly by definition $F(\Sigma) + F^*(L) - \langle L, \Sigma \rangle \ge 0$ for all $\Sigma, L \in \mathbb{S}^m$. However, for any $\Sigma \in \mathbb{S}^m_+$ and $L \in \mathbb{L}^m_+$ we also have the following equivalence; see Corollary E.1.4.4 in Hiriart-Urruty and Lemaréchal (2001)

(8)
$$F(\Sigma) + F^*(L) - \langle L, \Sigma \rangle = 0 \iff L = \nabla F(\Sigma) \iff \Sigma = \nabla F^*(L).$$

In particular, the second equivalence shows that ∇F and ∇F^* are inverses of each other. In other words, $L = \nabla F(\Sigma)$ if and only if $\Sigma = \nabla F^*(L)$.

THEOREM 3.7. If $F \in \mathcal{E}^m$ then the function $D_F(S, \nabla F^*(L))$ takes the form

$$(9) D_F(S, \nabla F^*(L)) = F(S) + F^*(L) - \langle L, S \rangle.$$

In particular, $D_F(S, \nabla F^*(L))$ is differentiable both in $S \in \mathbb{S}_+^m$ and in $L \in \operatorname{int}(\mathbb{L}_+^m)$ and it is strictly convex in S on \mathbb{S}_+^m and in L on every convex subset of \mathbb{L}_+^m .

PROOF. First note that by the first equivalence in (8) we get $F^*(\nabla F(\Sigma)) = \langle \nabla F(\Sigma), \Sigma \rangle - F(\Sigma)$. Thus,

$$D_F(S,\Sigma) = F(S) - F(\Sigma) + \langle \nabla F(\Sigma), \Sigma - S \rangle = F(S) + F^*(\nabla F(\Sigma)) - \langle \nabla F(\Sigma), S \rangle.$$

Expressing this in $L = \nabla F(\Sigma)$ we get (9), which is strictly convex and differentiable in $L \in \mathbb{L}_+^m$ by Proposition 3.6.

REMARK 3.8. Slightly abusing notation, from now on, we will write $D_F(S, L)$ to refer to $D_F(S, \nabla F^*(L))$. This notation is also used in the last column of Table 1, where the corresponding Bregman divergences computed above are expressed in terms of L.

We mention an important observation that follows from the fact that $F^{**} = F$ if $F \in \mathcal{E}^m$.

LEMMA 3.9. If
$$F \in \mathcal{E}^m$$
 then $D_F(S, L) = D_{F^*}(L, S)$.

In analogy to the log-likelihood function, we equivalently solve

(10) maximize
$$\mathscr{J}_n(L) := -F^*(L) + \langle L, S_n \rangle$$
 subject to $L \in \mathcal{L} \cap \mathbb{L}_+^m$.

We easily see that the gradient of g_n is well defined on \mathbb{L}_+^m and

$$\nabla_{\mathscr{J}n}(L) = -\nabla F^*(L) + S_n.$$

The KKT conditions are easy to obtain.

THEOREM 3.10. Suppose that \mathbb{L}^m_+ is open. The optimum in (10), if exists, is uniquely given by the pair $(\hat{\Sigma}, \hat{L}) \in \mathbb{S}^m_+ \times \mathbb{L}^m_+$ with $\hat{L} = \nabla F(\hat{\Sigma})$ satisfying

(11)
$$\hat{L} \in \mathcal{L} \quad and \quad \hat{\Sigma} - S_n \in \mathcal{L}^{\perp}.$$

PROOF. First note that $\nabla F^*(L) = \Sigma$ by (8). Since \mathbb{L}_+^m is open, $\mathcal{L} \cap \mathbb{L}_+^m$ is relatively open, and so $\widehat{L} \in \mathcal{L} \cap \mathbb{L}_+^m$ is optimal if and only if the gradient is orthogonal to \mathcal{L} .

PROPOSITION 3.11. Let $A_0 \in \mathcal{L}$. The dual problem to (10) is

(12) minimize
$$F(\Sigma) - \langle A_0, \Sigma \rangle$$
 subject to $\Sigma - S_n \in \mathcal{L}^{\perp}$.

PROOF. This is a convex problem over a relatively open set $\mathcal{L}^{\perp} \cap \mathbb{S}_{+}^{m}$. The optimum, if exists, must be a stationary point: $\widehat{\Sigma} - S_n \in \mathcal{L}^{\perp}$ and $\nabla F(\widehat{\Sigma}) - A_0 \in (\mathcal{L}^{\perp})^{\perp}$. Note that \mathcal{L}^{\perp} is the linear space orthogonal to the affine space \mathcal{L} and so $(\mathcal{L}^{\perp})^{\perp}$ is the linear space parallel to \mathcal{L} . Since $A_0 \in \mathcal{L}$ we recover the condition $\widehat{L} = \nabla F(\widehat{\Sigma}) \in \mathcal{L}$. This is exactly the same as (11), which proves that the problem in (12) is equivalent to the problem in (10).

Another important consequence of this characterization is the following well-known version of the Pythagorean theorem. We provide proof for completeness.

PROPOSITION 3.12. Fix an affine subspace $\mathcal{L} \subset \mathbb{S}^m$ and suppose that $\widehat{\Sigma}$ is the minimizer of $D_F(S,L)$ for $L \in \mathcal{L}$ and let $\widehat{L} = \nabla F(\widehat{\Sigma}) \in \mathcal{L}$. Then for every $L \in \mathcal{L}$

$$D_F(S, L) = D_F(S, \widehat{L}) + D_F(\widehat{\Sigma}, L).$$

PROOF. Writing down both sides in terms of F and F^* and using the fact that $F(\widehat{\Sigma}) + F^*(\widehat{L}) = \langle \widehat{\Sigma}, \widehat{L} \rangle$ by (8), we see that it is enough to show that $\langle \widehat{L} - L, \widehat{\Sigma} - S \rangle = 0$ but this follows from the fact that $\widehat{\Sigma} - S \in \mathcal{L}^{\perp}$.

3.3. The advantageous essentially smooth case. We now explain the significance of essentially smooth functions in our analysis. It is worth noting that for spectral sums $F(\Sigma) = \operatorname{tr}(\phi(\Sigma))$, essential smoothness corresponds to a similar condition on ϕ : $\lim_{x\to 0^+} |\phi'(x)| = +\infty$. We observe that F_A , F_C , and F_D are essentially smooth, whereas F_B is not. This distinction has a crucial implication for optimizing the Bregman divergence.

In convex analysis, when $F \in \mathcal{E}^m$ is essentially smooth, the pair (F, \mathbb{S}_+^m) is referred to as being of Legendre type. This falls under a broader definition, which we will not provide here (see page 258 in Rockafellar (1970)), and all the relevant findings in Rockafellar (1970) are expressed in this terminology.

THEOREM 3.13. If $F \in \mathcal{E}^m$ is essentially smooth then $\operatorname{int}(\operatorname{dom}(F^*)) = \mathbb{L}_+^m$. In particular \mathbb{L}_+^m is open. Moreover, if $S_n \in \mathbb{S}_+^m$ and $\operatorname{dom}(F^*) = \mathbb{L}_+^m$, then the optimum of $\mathscr{J}_n(L)$ over $L \in \mathcal{L} \cap \mathbb{L}_+^m$ exists.

PROOF. The first statement follows from Theorem 26.5 in Rockafellar (1970) and the fact that (F, \mathbb{S}_+^m) is of Legendre type. Now, if $S \in \mathbb{S}_+^m$ then the unrestricted optimum of $\mathscr{J}_n(L)$ over \mathbb{L}_+^m is $\widehat{L} = \nabla F(S)$. The fact that $\mathscr{J}_n(L)$ is uniquely optimized over \mathbb{L}_+^m implies that every level-set $\{L \in \mathbb{S}^m : \mathscr{J}_n(L) \geq t\}$ is convex and compact (c.f. Proposition B.3.2.4 in Hiriart-Urruty and Lemaréchal (2001)). As $\mathrm{dom}(F^*) = \mathbb{L}_+^m$ is open, all these level sets are contained in \mathbb{L}_+^m . Since $\mathcal{L} \cap \mathbb{L}_+^m \neq \emptyset$, eventually, one of these level sets will have a nonempty intersection with \mathcal{L} and this intersection will contain the constrained optimum. \square

Recall that examples (A), (C), and (D) are all essentially smooth. By calculations in Appendix A.3 we have that $\operatorname{dom}(F_A^*) = \operatorname{dom}(F_D^*) = -\mathbb{S}_+^m$ and $\operatorname{dom}(F_C^*) = \mathbb{S}^m$ are all open and so Theorem 3.13 will apply in these cases. For a quick illustration why essential smoothness is necessary consider the following example.

EXAMPLE 3.14. Let m=3 and consider the function F_B in (31) with $\nabla F_B(\Sigma) = \Sigma$. Suppose \mathcal{L} is given by a single equation $L_{13}=0$. Consider two matrices

$$S_n = \begin{bmatrix} 1 & \frac{2}{3} & \frac{2}{3} \\ \frac{2}{3} & 1 & \frac{2}{3} \\ \frac{2}{3} & \frac{2}{3} & 1 \end{bmatrix} \quad \text{and} \quad \widehat{\Sigma} = \begin{bmatrix} 1 & \frac{2}{3} & 0 \\ \frac{2}{3} & 1 & \frac{2}{3} \\ 0 & \frac{2}{3} & 1 \end{bmatrix}.$$

Note that S_n is positive definite, $\widehat{L} = \widehat{\Sigma} \in \mathcal{L}$, $\widehat{\Sigma} - S_n \in \mathcal{L}^{\perp}$. However, $\widehat{\Sigma}$ is not positive definite and so it cannot be a solution to (10). This does not contradict Theorem 3.13 because F_B is not essentially smooth.

REMARK 3.15. If $S \notin \mathbb{S}_+^m$ the optimum in Theorem 3.13 may still exist. When this happens is however a much more sophisticated question, which depends on F, S, and \mathcal{L} . In the case of Gaussian graphical models this has been extensively studied Buhl (1993); Uhler (2012); Gross and Sullivant (2018); Blekherman and Sinn (2019); Bernstein, Blekherman and Sinn (2020); Bernstein et al. (2021). Our paper suggest that a similar question could be studied for examples (C) and (D) and other examples introduced later.

We discuss how to numerically solve problems (10) and (12) in Section 6.1.

4. Basic statistical analysis. In this section we use explicitly the parametrization of the affine space \mathcal{L} defining the entropic model:

$$L(\theta) = A_0 + \sum_{i=1}^{d} \theta_i A_i \qquad \theta = (\theta_1, \dots, \theta_d) \in \mathbb{R}^d,$$

where A_0, A_1, \ldots, A_d are fixed matrices that may depend on external information. We assume that this parametrization is one-to-one, or, in other words, $\dim(\mathcal{L}) = d$. In this way, we can work directly with the parameter vector θ rather than the affine subspace $\mathcal{L} \subseteq \mathbb{S}^m$. To keep the notation compact, we write $\mathscr{J}_n(\theta)$ for $\mathscr{J}_n(L(\theta))$.

4.1. Consistency and asymptotic Gaussianity. Consider a random sample X_1, \ldots, X_n from a zero mean distribution with positive definite covariance matrix $\Sigma_0 = \nabla F^*(L_0)$ with $L_0 = L(\theta_0)$ for some $\theta_0 \in \mathbb{R}^d$. The estimator obtained by solving (10) is a convex M-estimator and the standard asymptotic theory, as presented in Haberman (1989); Niemiro (1992), can be applied. Indeed, define $m : \mathbb{R}^d \times \mathbb{R}^m \to \mathbb{R} \cup \{+\infty\}$ by

$$m(\theta, x) = F^*(L(\theta)) - x^{\mathsf{T}}L(\theta)x$$

then maximizing $y_n(\theta)$ is equivalent to minimizing the strictly convex function

(13)
$$M_n(\theta) = \frac{1}{n} \sum_{i=1}^n m(\theta, X_i) = F^*(L(\theta)) - \langle L(\theta), S_n \rangle = -\mathscr{J}_n(\theta).$$

The corresponding minimizer $\hat{\theta}_n$ is still called the Bregman estimator for $M_F(\mathcal{L})$ although now the estimator depends on the choice of basis A_0, A_1, \ldots, A_d .

Note that $\mathbb{E}S_n = \Sigma_0$ and the function

(14)
$$M(\theta) := \mathbb{E}M_n(\theta) = F^*(L(\theta)) - \operatorname{tr}(L(\theta)\Sigma_0)$$

is strictly convex in the interior of its domain. We have

$$dom(M) = \{\theta \in \mathbb{R}^d : L(\theta) \in dom(F^*)\} \supseteq \{\theta : L(\theta) \in \mathbb{L}_+^m\} =: \Theta_+$$

and we assume $\theta_0 \in \Theta_+$. Note that if \mathbb{L}_+^m is open, so is Θ_+ . Theorem 1 in Niemiro (1992) immediately gives the following result.

PROPOSITION 4.1. Suppose $F \in \mathcal{E}^m$ and $\mathbb{E}(S_n) = \Sigma_0 \in \mathbb{S}_+^m$. The Bregman estimator $\hat{\theta}_n$ in $M_F(\mathcal{L})$ is a consistent estimator of θ_0 , where θ_0 is the unique point such that $\nabla F^*(L(\theta_0)) = \Sigma_0$.

The main reason, why such nice results exist follows from the fundamental property of convex functions that pointwise convergence implies uniform convergence; see also Theorem II.1 in Andersen and Gill (1982).

If we assume existence of higher order moments, we obtain a stronger conclusion. Let

(15)
$$h(\theta, x) = \nabla_{\theta} m(\theta, x) = [\langle \Sigma(\theta) - xx^{\top}, A_i \rangle]_{i=1}^{d}.$$

PROPOSITION 4.2. If the distribution of X has finite moments up to order 2r (equiv. $\mathbb{E}\|h(\theta,X)\|^r < \infty$) for some $r \ge 1$ then for every $\epsilon > 0$

$$\mathbb{P}(\sup_{k \ge n} \|\widehat{\theta}_k - \theta_0\| > \epsilon) = o(n^{1-r}), \quad n \to \infty.$$

The proof follows immediately from Theorem 2 in Niemiro (1992).

We now turn to proving asymptotic Gaussianity. Denoting $S = \mathbb{V}(X_1 X_1^\top)$ to be the covariance of $X_1 X_1^\top$ we get

(16)
$$\mathbb{V}(S_n) = \frac{1}{n^2} \sum_{i=1}^n \mathbb{V}(X_i X_i^\top) = \frac{1}{n} \mathcal{S}.$$

Note that S is a covariance of a matrix valued random variable. Similarly as in the standard vector-valued case, S is a positive semidefinite and self-adjoint linear map from \mathbb{S}^m to \mathbb{S}^m so that for all $A, B \in \mathbb{S}^m$ we have

$$\langle A, SA \rangle \geqslant 0$$
 and $\langle A, SB \rangle = \langle SA, B \rangle$.

The notation SA denotes the action of the linear mapping $S: \mathbb{S}^m \to \mathbb{S}^m$ on A; see, for example, Section 2 and Appendix A in Lauritzen (2023).

A corollary from Theorem 3.10 is that the Hessian $\nabla^2 M_n(\theta)$ of $M_n(\theta)$ does not depend on the data and it is equal to the Hessian of $M(\theta)$. We use the notation

(17)
$$\mathcal{I}(\theta) = \nabla^2 M_n(\theta) = \nabla^2 M(\theta) \in \mathbb{S}^d,$$

which is the counterpart of the Fisher information matrix in exponential families. Since $M(\theta)$ is strictly concave in Θ_+ , for every fixed θ , $\mathcal{I}(\theta)$ is a positive definite matrix. We write \mathcal{I}_0 for $\mathcal{I}(\theta_0)$.

THEOREM 4.3. Denote by $\widehat{\theta}_n$ the Bregman estimator obtained under data S_n generated from a mean zero distribution with positive definite covariance $\mathbb{E}S_n = \Sigma_0 = \nabla F^*(L(\theta_0))$ and such that $\mathbb{V}(S_n) = \frac{1}{n}\mathcal{S}$ (the fourth order moments are assumed finite). Then

$$\sqrt{n}(\widehat{\theta}_n - \theta_0) \stackrel{d}{\longrightarrow} N_m(0, \mathcal{I}_0^{-1}\Omega \mathcal{I}_0^{-1}),$$

where $\Omega_{ij} = \langle A_i, SA_j \rangle$ for all i, j = 1, ..., m.

PROOF. By Theorem 4 in Niemiro (1992)

$$\sqrt{n}(\widehat{\theta}_n - \theta_0) = -\mathcal{I}_0^{-1} \sqrt{n} \nabla M_n(\theta_0) + o_P(1).$$

It is then enough to show that $\sqrt{n}\nabla M_n(\theta_0) \stackrel{d}{\to} N_m(0,\Omega)$. We have $\nabla M_n(\theta_0) = \frac{1}{n}\sum_i h(\theta_0,X_i)$, where the function $h(\theta,x)$ was defined in (15). We have

$$\mathbb{E}h(\theta_0, X) = [\langle \Sigma_0 - \mathbb{E}XX^\top, A_i \rangle]_{i=1}^d = 0$$

and since the fourth moments exist, the central limit theorem gives that $\sqrt{n}\nabla M_n(\theta_0)$ converges in distribution to $N(0,\Omega)$.

4.2. Finite sample bounds. Obtaining finite sample bounds is also rather straightforward but we need to be more careful about the existence of the estimator. In this section, we always assume that the solution to (10) exists; see Theorem 3.13 for some sufficient conditions.

Denote $g(\omega) = \mathbb{E}(M_n(\theta_0 + \omega) - M_n(\theta_0))$ so that, by (14),

$$g(\omega) = F^*(L(\theta_0 + \omega)) - F^*(L_0) - \text{tr}(\Sigma_0(L(\theta_0 + \omega) - L_0)).$$

This function is strictly convex in the interior of its domain, nonnegative, and g(0) = 0. Since Σ_0 is positive definite, 0 lies in the interior of the domain of g at least whenever \mathbb{L}_+^m is open. Define $\Delta^{(n)} \in \mathbb{R}^d$ as

(18)
$$\Delta_i^{(n)} = \langle S_n - \Sigma_0, A_i \rangle \quad \text{for } i = 1, \dots, d.$$

LEMMA 4.4. If $\hat{\theta}_n$ is the Bregman estimator based on the sample covariance matrix S_n from the true distribution corresponding to parameter θ_0 then for every $n \ge 1$ and for every $\epsilon > 0$

$$\mathbb{P}(\|\widehat{\theta}_n - \theta_0\| \leqslant \epsilon) = \mathbb{P}(\Delta^{(n)} \in \nabla g(\epsilon \mathbb{B}_2)),$$

where $\mathbb{B}_2 = \{x \in \mathbb{R}^d : ||x|| \le 1\}$. It also holds that $\nabla g(0) = 0$.

PROOF. Recall the definition of $M_n(\theta)$ in (13). We have

$$M_n(\theta_0 + \omega) - M_n(\theta_0) = g(\omega) - \operatorname{tr}((S_n - \Sigma_0)(L(\theta_0 + \omega) - L_0)).$$

and $\operatorname{tr}((S_n - \Sigma_0)(L(\theta_0 + \omega) - L_0)) = \langle \omega, \Delta^{(n)} \rangle$, which gives

$$M_n(\theta_0 + \omega) - M_n(\theta_0) = g(\omega) - \langle \omega, \Delta^{(n)} \rangle.$$

By the definition of the convex conjugate, the optimal value of $M_n(\theta_0 + \omega) - M_n(\theta_0)$, if exists, is obtained for $\hat{\omega} = \hat{\theta}_n - \theta_0 = \nabla g^*(\Delta^{(n)})$. Note that $\nabla g^*(0) = 0$ simply by the fact that 0 is the global minimizer of g. We get

$$\mathbb{P}(\|\widehat{\theta}_n - \theta_0\| \leqslant \epsilon) = \mathbb{P}(\nabla g^*(\Delta^{(n)}) \in \epsilon \mathbb{B}_2) = \mathbb{P}(\Delta^{(n)} \in \nabla g(\epsilon \mathbb{B}_2)),$$

where we used the fact that ∇g and ∇g^* are inverses of each other. Now the claim easily follows.

Define for $\epsilon > 0$:

$$\kappa_{\infty}(\epsilon) := \inf_{\|\omega\|=1} \|\nabla g(\epsilon\omega)\|_{\infty} > 0.$$

Since ∇g is continuous and $\nabla g(\omega) = 0$ if and only if $\omega = 0$, it is clear that $\kappa_{\infty}(\epsilon)$ is bounded away from zero for any $\epsilon > 0$. In fact, we have the following basic lemma.

LEMMA 4.5. If g is strongly convex in $\epsilon \mathbb{B}_2$ with modulus c then $\kappa_{\infty}(\epsilon) > \frac{c}{2\sqrt{d}}$ for every $\epsilon > 0$.

PROOF. By definition of strong convexity in $\epsilon \mathbb{B}_2$, for all $\omega \in \mathbb{B}_2$

$$g(0) \geqslant g(\epsilon \omega) + \langle \nabla g(\epsilon \omega), -\epsilon \omega \rangle + \frac{c}{2} \epsilon \|\omega\|^2.$$

Using the fact that $\|\omega\|=1$, g(0)=0, and $g\geqslant 0$ we get that for every $\epsilon>0$

(19)
$$\langle \nabla g(\epsilon \omega), \omega \rangle \geqslant \frac{1}{\epsilon} g(\epsilon \omega) + \frac{c}{2} > \frac{c}{2}.$$

Note that $\|x\|_{\infty} = \sup_{y \in \mathbb{B}_1} \langle x, y \rangle$ (\mathbb{B}_1 is the ℓ_1 -ball) and so $\langle \nabla g(\epsilon \omega), \frac{\omega}{\|\omega\|_1} \rangle \leqslant \|\nabla g(\epsilon \omega)\|_{\infty}$. Thus, dividing (19) by $\|\omega\|_1$ we get that

$$\|\nabla g(\epsilon\omega)\|_{\infty} > \frac{c}{2\|\omega\|_{1}} \leqslant \frac{c}{2\sqrt{d}},$$

where the last inequality follows from the fact that $\|\omega\|_1 \leqslant \sqrt{d} \|\omega\|$

From the definition of $\kappa_{\infty}(\epsilon)$, it directly follows that:

(20)
$$\mathbb{P}(\Delta^{(n)} \in \nabla g(\epsilon \mathbb{B}_2)) \geqslant \mathbb{P}(\|\Delta^{(n)}\|_{\infty} \leqslant \kappa_{\infty}(\epsilon)).$$

If the distribution of the sample has a bounded support, finite sample bounds for $\|\Delta^{(n)}\|_{\infty}$ can be easily obtained using maximal inequalities for sub-Gaussian random variables. However, this strategy is not applicable in the Gaussian case. The following method is an alternative approach that has the potential for extension to other situations.

THEOREM 4.6. Fix $F \in \mathcal{E}^m$, an affine subspace \mathcal{L} , and the corresponding entropic model $M_F(\mathcal{L})$. Suppose X_1, \ldots, X_n is a random sample from $N(0, \Sigma_0)$ with $\nabla F(\Sigma_0) \in \mathcal{L}$. If $\hat{\theta}_n$ is the corresponding Bregman estimator of the true parameter θ_0 then

$$\mathbb{P}(\|\widehat{\theta}_n - \theta_0\| > \epsilon) \leqslant \begin{cases} 2d \exp\{-\frac{\kappa_{\infty}^2(\epsilon)n}{8\beta^2}\} & \text{if } 0 \leqslant \kappa_{\infty}(\epsilon) \leqslant \frac{\beta^2}{\gamma}, \\ 2d \exp\{-\frac{\kappa_{\infty}(\epsilon)n}{4\gamma}\} & \text{if } \kappa_{\infty}(\epsilon) > \frac{\beta^2}{\gamma}. \end{cases}$$

where $\beta = \max_{k=1,...,d} \|A_k\|_F$, $\gamma = \max_{k=1,...,d} \|A_k\|$ (Frobenius and spectral norms).

PROOF. By Lemma 4.4, equation (20), and the union bound, we get

(21)
$$\mathbb{P}(\|\widehat{\theta}_n - \theta_0\| > \epsilon) \leq \mathbb{P}(\|\Delta^{(n)}\|_{\infty} > \kappa_{\infty}(\epsilon)) \leq \sum_{k=1}^{d} \mathbb{P}(|\Delta_k^{(n)}| > \kappa_{\infty}(\epsilon)).$$

We will bound each term on the right of (21). Given Σ_0 and $A_1, \ldots, A_d \in \mathbb{S}^m$ denote the eigenvalues of $\sqrt{\Sigma_0} A_k \sqrt{\Sigma_0}$ by

$$\lambda_{jk} = \lambda_j(\sqrt{\Sigma_0}A_k\sqrt{\Sigma_0}) \in \mathbb{R}.$$

If $X \sim N(0, \Sigma_0)$ then $X^\top A_k X = \sum_{j=1}^m \lambda_{jk} Z_j^2$, where $Z \sim N_m(0, I_m)$. Thus, for every X_i in our sample we have

$$\Delta_k^{(n)} = \frac{1}{n} \sum_{i=1}^n (X_i^\top A_k X_i - \operatorname{tr}(\Sigma_0 A_k)) = \frac{1}{n} \sum_{i=1}^n \sum_{j=1}^m \lambda_{jk} (Z_{ij}^2 - 1),$$

where $Z_{ij} \sim N(0,1)$ are all independent of each other. Since each Z_{ij}^2-1 is a sub-exponential random variable with parameters $(\nu,\alpha)=(2,4)$ (e.g. Example 2.8 in Wainwright (2019)) then $\Delta_k^{(n)}$ is sub-exponential with parameters (ν_*,α_*) with

$$\nu_* = \sqrt{\sum_{i=1}^n \sum_{j=1}^m 4\frac{1}{n}\lambda_{jk}^2} = \frac{2}{\sqrt{n}}\sqrt{\sum_{j=1}^m \lambda_{jk}^2} = \frac{2}{\sqrt{n}} \|A_k\|_F \leqslant \frac{2\beta}{\sqrt{n}}.$$

and

$$\alpha_* = \frac{4}{n} \max_{j=1,...,m} |\lambda_{jk}| = \frac{4}{n} ||A_k|| \le \frac{4\gamma}{n}.$$

This follows from the standard result that if Y_1,\ldots,Y_N are independent sub-exponential with parameters (ν_i,α_i) , then for any fixed vector $u\in\mathbb{R}^N$, the linear combination $\sum_i u_iY_i$ is sub-exponential with parameters $(\sqrt{\sum_i u_i^2\nu_i^2}, \max_i\alpha_i)$. Standard sub-exponential tail bound (Proposition 2.9 in Wainwright (2019)) imply then that

$$\mathbb{P}(|\Delta_k^{(n)}| \geqslant t) \leqslant \begin{cases} 2e^{-\frac{t^2n}{8\beta^2}} & \text{if } 0 \leqslant t \leqslant \frac{\beta^2}{\gamma}, \\ 2e^{-\frac{tn}{8\gamma}} & \text{if } t > \frac{\beta^2}{\gamma}. \end{cases}$$

The result follows by taking $t = \kappa_{\infty}(\epsilon)$ and using (21).

To conclude our discussion of the statistical properties of the Bregman estimator, we note that our set-up is flexible and S_n could be replaced with any other reasonable estimator. This may be particularly relevant in modelling heavy-tailed distributions; e.g. Lugosi and Mendelson (2019). If the replacement for S_n is an M-estimator then our method still results in an M-estimator and the theory of Section 4.1 applies.

5. Mixed convex constraints. It is evident that our analysis extends to models defined by arbitrary (closed) convex restrictions in $L = \nabla F(\Sigma)$, preserving the convex nature of the problem stated in equation (10). However, in certain scenarios a portion of the restrictions may be easier expressed in Σ , while another part is better represented in L. We now explore how to handle such situations and present several theoretical implications. Our findings heavily rely on the geometric considerations underlying the mixed parametrization in exponential families Barndorff-Nielsen (1978), as well as the study of the mixed convex exponential family setup of Lauritzen and Zwiernik (2022).

5.1. Mixed parametrization. Consider a split of $\Sigma \in \mathbb{S}^m$ into two parts Σ_A and Σ_B and the corresponding split $L = (L_A, L_B)$. For example, Σ_A could consist of all the diagonal entries of Σ and Σ_B be the off-diagonal entries. In this section we consider models that are given by convex restrictions on Σ_A and convex restrictions on L_B ; see Lauritzen and Zwiernik (2022) for the special case $\nabla F_A = -\Sigma^{-1}$. For example, modelling correlations is used commonly in econometric GARCH models. In a recent paper, Archakov and Hansen (2021) considered a model in which $\Sigma_{ii} = 1$ for all $i = 1, \ldots, m$ and potential further linear restrictions are imposed on the off-diagonal entries of $L = \log \Sigma$. Another example could be to impose non-negativity restrictions on some entries of Σ and zero restrictions on the complementary entries of L.

For a given subset of entries of a symmetric matrix, we consider the set of its values that allow for a positive definite completion

$$(\mathbb{S}_+^m)_A := \{\Sigma_A : \Sigma = (\Sigma_A, \Sigma_B) \in \mathbb{S}_+^m\}.$$

We have a similar definition for $\mathbb{L}_+^m = \nabla F(\mathbb{S}_+^m)$

$$(\mathbb{L}_{+}^{m})_{B} := \{L_{B} : L = (L_{A}, L_{B}) \in \mathbb{L}_{+}^{m}\}.$$

THEOREM 5.1. Let $F \in \mathcal{E}^m$ be essentially smooth with $L = \nabla F(\Sigma)$. Then there is a one-to-one map between $\Sigma \in \mathbb{S}^m_+$ and $(\Sigma_A, L_B) \in (\mathbb{S}^m_+)_A \times (\mathbb{L}^m_+)_B$.

The relevant theory was conveniently outlined in Sections 5.3 and 5.4 of Barndorff-Nielsen (1978) and applied to study mixed parametrizations in exponential families.

PROOF. The proof of this result is essentially the same as the Theorem 5.34 in Barndorff-Nielsen (1978). Our result is however slightly different as we do not assume that dom(F) is open. The proof easily adapts however because (F, \mathbb{S}_+^m) is of Legendre type (see the discussion preceding Theorem 3.13).

Like in the standard exponential families, the most surprising part of this result is the following conclusion.

PROPOSITION 5.2 (Variational independence). Assume conditions of Theorem 5.1 and let $\Sigma \in \mathbb{S}_+^m$, $L \in \mathbb{L}_+^m$. There exists a unique positive definite matrix $\hat{\Sigma}$ that agrees with Σ on A-entries and such that $\hat{L} = \nabla F(\hat{\Sigma})$ agrees with L on the B-entries.

For general $F \in \mathcal{E}^m$ the conclusion of Theorem 5.1 does not hold. A counterexample can be recovered from Example 3.14. Take $\Sigma_A = (\Sigma_{11}, \Sigma_{22}, \Sigma_{33}, \Sigma_{12}, \Sigma_{23})$ and $L_B = L_{13}$. Take Σ to be S_n from Example 3.14 and let L be the identity matrix. The corresponding (Σ_A, L_B) is the matrix $\hat{\Sigma}$ in Example 3.14 but this one is *not* positive definite.

Perhaps it is also useful to see explicitly how this result works in a smaller example when Theorem 5.1 can be applied.

EXAMPLE 5.3. Consider example (A) with $\nabla F_A(\Sigma) = -\Sigma^{-1}$. Let m=2 and consider the split $\Sigma_A = (\Sigma_{11}, \Sigma_{22})$, $L_B = -(\Sigma^{-1})_{12}$. Here $(\mathbb{S}^2_+)_A = (0, \infty)^2$ and $(\mathbb{S}^2_+)_B = \mathbb{R}$. Suppose $\Sigma_{11} = \Sigma_{22} = 1$ and denote $x = \Sigma_{12}$ and $y = (\Sigma^{-1})_{12}$. The claim is that y can be chosen arbitrarily but here it follows clearly because $y = -x/(1-x^2)$ is a one-to-one mapping from (-1,1) to \mathbb{R} .

5.2. Unrestricted parametrization of correlations and other models. Motivated by temporal modelling of correlation matrices, Archakov and Hansen (2021) studied ways to map the set of correlation matrices in \mathbb{S}^m_+ into a Euclidean space $\mathbb{R}^{m(m-1)/2}$. It is not immediately obvious that such a mapping exists but the fact that $\log \Sigma$ maps \mathbb{S}^m_+ to \mathbb{S}^m suggested a natural strategy. Their main result states that for any selection of the off-diagonal entries of $L = \log(\Sigma)$ there is a unique correlation matrix R such that $\log R$ has precisely those off-diagonal entries.

Our starting point here is that this result is a special case of our Theorem 5.1. Indeed, $F_C \in \mathcal{E}^m$ is essentially smooth and so this theorem applies. Take Σ_A to be the vector containing the diagonal entries of Σ and L_B to be the vector containing the off-diagonal entries of $L = \log(\Sigma)$. Then there is a one-to-one map from $\Sigma \in \mathbb{S}_+^m$ to $(\Sigma_A, L_B) \in (\mathbb{S}_+^m)_A \times (\mathbb{L}_+^m)_B$. In particular, we can fix $\Sigma_A \in (\mathbb{S}_+^m)_A$ to be the vector of ones and $L_B \in (\mathbb{L}_+^m)_B$ to be an arbitrary real vector to get Theorem 1 in Archakov and Hansen (2021). Note also that in this case $\mathbb{L}_+^m = \mathbb{S}^m$ and so

(22)
$$(\mathbb{S}_{+}^{m})_{A} = (0, \infty)^{m}$$
 and $(\mathbb{L}_{+}^{m})_{B} = \mathbb{R}^{m(m-1)/2}$.

We generalize this result in two ways by first providing a simpler map that also offers an unrestricted parametrization of the set of correlation matrices and, then, by showing how similar ideas can be used for other covariance models.

For the first result we observe that the essential part of the above construction was not that $\mathbb{L}_+^m = \mathbb{S}^m$ (which motivated using the matrix logarithm) but that $(\mathbb{L}_+^m)_B = \mathbb{R}^{m(m-1)/2}$. This latter condition can be obtained for simpler transformations.

PROPOSITION 5.4. Suppose that $F \in \mathcal{E}^m$ is essentially smooth and L_B consists of all off-diagonal entries of $L = \nabla F(\Sigma)$. If $(\mathbb{L}^m_+)_B = \mathbb{R}^{m(m-1)/2}$ then for an arbitrary vector L_B , there exists a unique correlation matrix R such that $\nabla F(R)$ has precisely these off-diagonal entries.

Note that when $L = -\Sigma^{-1}$, it is always possible to choose the off-diagonal entries arbitrarily and adjust the diagonal entries to ensure the negative definiteness of L. Consequently, despite the fact that $\mathbb{L}_+^m = -\mathbb{S}_+^m$, we find that $(\mathbb{L}_+^m)_B = \mathbb{R}^{m(m-1)/2}$, which implies that the matrix inverse serves as an unconstrained parameterization for correlation matrices.

COROLLARY 5.5. For any choice of the off-diagonal entries there exists a unique correlation matrix R whose inverse has precisely these off-diagonal entries.

A clear advantage of working with the inverse is that this is a well-understood algebraic map with efficient methods to compute it. Explicit numerical procedures are provided in Améndola and Zwiernik (2021); Llorens-Terrazas and Brownlees (2022). This can also be done using the techniques discussed in Section 6.1. To see how it works, let \mathcal{L} be the set of all $L \in \mathbb{S}^m$ with fixed off-diagonal entries L_B . Then \mathcal{L}^\perp is the set of matrices with zeros on the diagonal. Take A_0 to be any matrix in \mathcal{L} and $S_n = I_m$. Solving the dual problem in Proposition 3.11 we obtain the unique $\widehat{\Sigma}$ with ones on the diagonal and such that $\widehat{L} \in \mathcal{L}$. In the particular case of $L = -\Sigma^{-1}$ this corresponds to computing the dual MLE subject to the constraints $\Sigma_{ii} = 1$ for $i = 1, \ldots, m$ but exactly the same approach for $\log(\Sigma)$, which was exploited in Archakov and Hansen (2021).

Our second contribution in this section is to observe that similar ideas can be applied for other models. One particular example is the model given by zeros in Σ or its inverse. Suppose that Σ_A is some fixed collection of off-diagonal entries of Σ and fix $\Sigma_A = 0$. We again look for a situation when $(\mathbb{L}_+^m)_B$ is the Euclidean space.

The simplest approach is to take F such that $\mathbb{L}_+^m = \mathbb{S}^m$, which again points to the matrix logarithm. However, theoretical analysis of this situation is quite hard and it would advantageous to have a more tractable alternative.

PROPOSITION 5.6. Consider the map $F_E(\Sigma) = -\log \det(\Sigma) + \frac{\lambda}{2} \operatorname{tr}(\Sigma^2)$ for some $\lambda > 0$. Then $F \in \mathcal{E}^m$ is essentially smooth and $\nabla F_E(\Sigma) = \lambda \Sigma - \Sigma^{-1}$ maps bijectively \mathbb{S}_+^m to \mathbb{S}^m .

PROOF. The underlying function ϕ_E is $-\log(x) + \frac{\lambda}{2}x^2$ when x > 0 and $+\infty$ for all other x. It is strictly convex and differentiable in $(0, +\infty)$. Moreover, $\phi_E'(x) = \lambda x - 1/x$ and so $|\phi_E'(x)| \to \infty$ as $x \to 0^+$. This shows that $F_E \in \mathcal{E}^m$ is essentially smooth. As ϕ_E maps $(0, +\infty)$ to \mathbb{R} , the result follows.

The new mapping can be used and analyzed in various creative ways. Not to overload this paper, we will report on this and relating findings in a separate note.

5.3. Estimation under mixed convex constraints. Suppose now that we fix closed convex restrictions C_A on Σ_A and convex restrictions C_B on L_B . Thus, the model is given by

(23)
$$\{\Sigma \in \mathbb{S}^m : \Sigma_A \in \mathcal{C}_A \cap (\mathbb{S}_+^m)_A \text{ and } L_B \in \mathcal{C}_B \cap (\mathbb{L}_+^m)_B\}.$$

We propose the following 2-step method to fit a model given by convex restriction on Σ_A and convex restrictions on L_B .

- (S1) Minimize the Bregman divergence $D_F(S_n, L) = F(S_n) + F^*(L) \langle L, S_n \rangle$ subject to $L_B \in \mathcal{C}_B \cap (\mathbb{L}_+^m)_B$. This is a convex optimization problem and denote the corresponding unique optimizer (if exists) by \hat{L} .
- (S2) Given \hat{L} , minimize the Bregman divergence $D_F(\Sigma, \hat{L}) = F(\Sigma) + F^*(\hat{L}) \langle \hat{L}, \Sigma \rangle$ subject to $\Sigma_A \in \mathcal{C}_A \cap (\mathbb{S}^m_+)_A$. This is again a convex optimization problem and denote the corresponding minimizer by $\check{\Sigma}$.

It is clear immediately by construction that $\check{\Sigma}_A$ satisfies the given constraints on Σ_A . We also have the following more surprising result.

PROPOSITION 5.7. Let $\check{L} = \nabla F(\check{\Sigma})$ then $\check{L}_B = \hat{L}_B \in \mathcal{C}_B$. In other words, $\check{\Sigma}$ lies in the model (23).

PROOF. If the optimum $\check{\Sigma}$ in (S2) exists, by convexity of the function and the underlying $\mathcal{C}_A \cap (\mathbb{S}^m_+)_A$, $\check{\Sigma}$ must satisfy

$$\langle \widecheck{L} - \widehat{L}, \Sigma - \widecheck{\Sigma} \rangle \geqslant 0$$
 for all Σ s.t. $\Sigma_A \in \mathcal{C}_A$.

Since \mathbb{S}_+^m is open, a small perturbation $\check{\Sigma} + T$ also lies in \mathbb{S}_+^m . Assuming that $T_A = 0$ we can even conclude that $\check{\Sigma}_A + T_A \in \mathcal{C}_A$. Since T with $T_A = 0$ is small but otherwise arbitrary, we conclude that $\check{L}_B = \hat{L}_B$. Moreover, $\hat{L}_B \in \mathcal{C}_B$ because \hat{L} solves (S1).

According to Proposition 5.7, our procedure yields a point satisfying both types of constraints by solving two convex problems (S1) and (S2). Some statistical properties of the corresponding estimator can also be obtained following Section 4 above and Section 6 in Lauritzen and Zwiernik (2022). Let the Bregman estimator (BE) be the estimator $\widetilde{\Sigma}$ obtained by minimizing the Bregman divergence $D_F(S_n, \Sigma)$ subject to $\Sigma_A \in \mathcal{C}_A$ and $L_B \in \mathcal{C}_B$ (this is in general a non-convex optimization problem). In a way analogous to Theorem 6.1 in Lauritzen and Zwiernik (2022) and with essentially the same proof, we expect that the estimations $\widetilde{\Sigma}_n$ and $\widecheck{\Sigma}_n$ are asymptotically equivalent, in the sense that $\sqrt{n}(\widetilde{\Sigma}_n - \widecheck{\Sigma}_n) = o_P(1)$. The importance of this comes from the fact that the Bregman estimator is an M-estimator and so its asymptotics under general restrictions is quite well understood Geyer (1994).

- **6. Some other considerations.** Our modelling setting raises further questions, which require careful study. In this section we briefly describe some of these problems.
- 6.1. Numerical optimization. We start by discussing an algorithm to solve the problem (10) or the dual problem (12). In the specific example when $F(\Sigma) = -\log \det \Sigma$ there exist numerous approaches including coordinate descent and block-coordinate algorithms. Since second order information is in general hard to obtain for most choices of F (c.f. Lewis and Sendov (2001)), we propose a first-order method.

The simplest solution is to perform the gradient descent algorithm for the dual problem (12): minimize $F(\Sigma) - \langle A_0, \Sigma \rangle$ subject to $\Sigma - S_n \in \mathcal{L}^{\perp}$. Note that if \mathcal{L} is a linear subspace, we can take $A_0 = 0$, which simplifies the formulas below.

We initiate the algorithm at $\Sigma^{(0)} = S_n$, which is dually feasible. The gradient of $F(\Sigma)$ is $L - A_0$. Denote by $\Pi^{\perp}_{\mathcal{L}}(L - A_0)$ the orthogonal projection of $L - A_0 \in \mathbb{S}^m$ to \mathcal{L}^{\perp} . We move from $\Sigma^{(t)}$ to $\Sigma^{(t+1)}$ using the formula

$$\Sigma^{(t+1)} = \Sigma^{(t)} - s_t \Pi_{\mathcal{L}}^{\perp} (L^{(t)} - A_0).$$

If $\Sigma^{(t)}$ is feasible, that is, if $\Sigma^{(t)} - S_n \in \mathcal{L}^{\perp}$ then $\Sigma^{(t+1)}$ is also feasible. We can use the step size s_t using backtracking, assuring in this way that the value of the function increases at each step. Since F is strictly convex, this algorithm eventually converges to the optimum. This follows from the fact that the projected gradient descent is a special case of proximal gradient algorithms; see Section 10.4 in Beck (2017) for relevant results.

Alternatively, it is possible to solve the primal problem (10). We start by any feasible $L^{(0)} \in \mathcal{L}$. Then, at each iterate $L^{(t)}$, we project the gradient $-\Sigma^{(t)} + S_n$ onto \mathcal{L} . We denote this projection by $\Pi_{\mathcal{L}}$. Then we move

(24)
$$L^{(t+1)} = L^{(t)} - s_t \Pi_{\mathcal{L}}(\Sigma^{(t)} - S_n).$$

Again, the step size can be chosen using backtracking. Note that here in some situations the choice of a starting point L_0 may be problematic.

The main bottleneck in all these cases is that in each step we need to map between Σ and L. This requires computing the spectral decomposition and so the complexity is at least $O(m^3)$, which may be prohibitive if m is very large. In the special case, when $F(\Sigma) = \operatorname{tr}(\phi(\Sigma))$ is a spectral sum, Han, Avron and Shin (2018) proposed to study the stochastic gradient descent based on stochastic truncation of the Chebyshev expansion of F (or its conjugate). This and other techniques to approximate F are discussed in Section 4.4 of Higham (2008).

Another possible approach is to employ an iterative projection algorithm as discussed by Dhillon and Tropp (2008), which is structurally similar to iterative proportional scaling in exponential families. Observe that minimizer of $D_F(S,L)$ over the hyperplane H given by $\langle B,L\rangle=c$ must satisfy $\hat{\Sigma}-S=\lambda B$ for some $\lambda\in\mathbb{R}$. Equivalently, we can solve the one-dimensional problem

(25) minimize
$$F(S + \lambda B) - \lambda c$$
 $\lambda \in \mathbb{R}$.

Suppose now that $\mathcal{L} = \bigcap_{i=1}^k H_i$, where H_i is a hyperplane $\langle B_i, L \rangle = c_i$. We could iteratively "project" on H_1, \ldots, H_k by minimizing the Bregman divergence. Thus, we could run an iterative algorithm that starts with $\Sigma^{(0)} = S$ and for $t \geqslant 0$

(26)
$$L^{(t+1)} = \arg\min_{L \in H_i} D_F(\Sigma^{(t)}, L), \qquad \Sigma^{(t+1)} = \nabla F^*(L^{(t+1)}),$$

where i cycles around $\{1, \ldots, k\}$. Each step relies on solving the corresponding one-dimensional problem in (25) with $B = B_i$ and $c = c_i$. The following result justifies this algorithm.

PROPOSITION 6.1. If $F \in \mathcal{E}^m$ is essentially smooth and $S \in \mathbb{S}^m_+$ then the algorithm in (26) converges to the global optimum.

The result follows directly from the analogous proof in Section 4 in Dhillon and Tropp (2008). By Lemma 3.9, $D_F(S,L) = D_{F*}(L,S)$ and we apply their result for $D_{F*}(L,S)$. The assumptions are satisfied because (F^*, \mathbb{L}_+^m) is of Legendre type if and only if (F, \mathbb{S}_+^m) is; see Theorem 26.5 in Rockafellar (1970).

EXAMPLE 6.2. For illustration, we show how this could be used in the case when $F(\Sigma) = -\log \det(\Sigma) + \frac{1}{2}\operatorname{tr}(\Sigma^2)$. Fix a graph G and consider the linear space

$$\mathcal{L}_G = \{ L \in \mathbb{S}^m : L_{ij} = 0 \text{ if } i \neq j \text{ and } ij \notin E \}.$$

In this case the hyperplanes on which we project are defined by c=0 and $B=e_ie_j^\top+e_je_i^\top$ for $i\neq j$ and $ij\notin G$. In the t-th iteration we try to minimize $F(\Sigma^{(t)}+\lambda(e_ie_j^\top+e_je_i^\top))$ with respect to $\lambda\in\mathbb{R}$. Let $A=\{i,j\}$ and $C=\{1,\ldots,m\}\backslash\{i,j\}$. We write $\Sigma_{A|B}:=\Sigma_{A,A}-\Sigma_{A,B}\Sigma_{B,B}^{-1}\Sigma_{B,A}$. It is useful to observe that standard Schur complement arguments give that

$$\det(\Sigma^{(t)} + \lambda(e_i e_j^\top + e_j e_i^\top)) = \det(\Sigma_{B,B}^{(t)}) \cdot \det\left(\Sigma_{A|B}^{(t)} + \begin{bmatrix} 0 \ \lambda \\ \lambda \ 0 \end{bmatrix}\right).$$

Moreover,

$$\frac{1}{2}\operatorname{tr}((\Sigma^{(t)} + \lambda(e_i e_i^{\top} + e_j e_i^{\top}))^2) = \frac{1}{2}\operatorname{tr}((\Sigma^{(t)})^2) + 2\lambda\Sigma_{ij}^{(t)} + \lambda^2.$$

Denote $W = \Sigma_{A|B}^{(t)} \in \mathbb{S}^2$. Then

$$\frac{\mathrm{d}}{\mathrm{d}\lambda} F(\Sigma^{(t)} + \lambda (e_i e_j^\top + e_j e_i^\top)) = \frac{2\lambda + 2W_{12}}{\det(\Sigma_{A|B}^{(t)}) - 2\lambda W_{12} - \lambda^2} + 2\Sigma_{ij}^{(t)} + 2\lambda.$$

Equating this to zero results in a cubic polynomial equation, which can be solved exactly.

6.2. Sparsity and positive definite completion. One important concept that has been extensively studied in high-dimensional statistics is sparsity Hastie, Tibshirani and Wainwright (2015). In the context of covariance matrix estimation, Gaussian graphical models have proven to be particularly successful.

EXAMPLE 6.3 (Gaussian graphical models). The multivariate Gaussian distribution $N_m(0,\Sigma)$ forms an exponential family with canonical parameter $K=\Sigma^{-1}$. Given a sample X_1,\ldots,X_n from this model, the sufficient statistics is $S_n=\frac{1}{n}\sum_{i=1}^n X_iX_i^{\top}$. Denote the entries of S_n by S_{ij} . Fix a graph G with m nodes and edges E. Gaussian graphical models are given by imposing zero restrictions on some off-diagonal entries of $K=\Sigma^{-1}$

$$M(G) = \{ \Sigma \in \mathbb{S}_+^m : (\Sigma^{-1})_{ij} = 0 \text{ for } ij \notin E \}.$$

This model is an exponential family itself. The canonical parameters are $((K_{ii})_{i=1}^m, (K_{ij})_{ij \in E})$ and the sufficient statistics is $((S_{ii})_{i=1}^m, (S_{ij})_{ij \in E})$.

Gaussian graphical models have made a significant impact on multivariate statistics and are commonly used even for non-Gaussian data. The elegant SKEPTIC approach introduced by Liu et al. (2012) allows to extend the Gaussian setting to Gaussian copulas with minimal loss of efficiency and no loss of interpretability. However, Gaussian graphical models are also routinely employed beyond this favourable scenario. In such cases, the Gaussian log-likelihood

is considered a suitable loss function, and the zero restrictions correspond to conditional independence assumptions, albeit under the assumption of linear conditional independence. Interestingly, as demonstrated in Rossell and Zwiernik (2020), some distributional settings, such as elliptical distributions, preserve certain non-linear conditional independence information even when partial correlations vanish.

Zero restrictions on Σ have also been explored in the literature, leading to the covariance graph model Pearl and Wermuth (1994); Kauermann (1996); Chaudhuri, Drton and Richardson (2007); Drton and Richardson (2008). More recently, zero restrictions on $\log(\Sigma)$ have been considered in Battey (2017, 2019); Rybak and Battey (2021), with additional geometric motivations presented in Pavlov (2023). In Section 6.3, we introduce a new model that imposes zero restrictions on Σ^{-2} or more generally on Σ^{-p} for $p \geqslant 1$. All of these models fall under the category of entropic models.

Known sparsity: If the sparsity is defined by a graph G, we denote the corresponding linear subspace by \mathcal{L}_G :

$$\mathcal{L}_G := \{ L \in \mathbb{S}^m : L_{ij} = 0 \text{ if } ij \notin E \}.$$

Note that we can take $A_0 = 0$ in this case. The next result follows from Corollary 3.11.

PROPOSITION 6.4. Let S_n be the sample covariance matrix and consider the problem of maximizing $\mathscr{J}_n(L)$ subject to $L \in \mathcal{L}_G \cap \mathbb{L}_+^m$. The dual problem is to minimize $F(\Sigma)$ subject to $\Sigma_{ij} = S_{ij}$ for all $ij \in E$.

EXAMPLE 6.5. Suppose m=3 and suppose that $L_{13}=0$ is the only constraint defining \mathcal{L}_G . Let $S \in \mathbb{S}^3_+$ be given by

$$S = \begin{bmatrix} 4 & 1 & 2 \\ 1 & 4 & 3 \\ 2 & 3 & 4 \end{bmatrix} \quad \text{with} \qquad G = \overset{1}{\bullet} - \overset{2}{\bullet} - \overset{3}{\bullet} \quad \text{and} \qquad \hat{\Sigma} = \begin{bmatrix} 4 & 1 & ? \\ 1 & 4 & 3 \\ ? & 3 & 4 \end{bmatrix}.$$

By Proposition 6.4, irrespective of the form of F, the Bregman estimator $\hat{\Sigma}$ is equal to S on all the entries apart from the entries (1,3) and (3,1). The KKT conditions require that

$$(\nabla F(\widehat{\Sigma}))_{13} = 0.$$

We now show how this equation can be solved for our four running examples together with the new example $F_E(\Sigma) = F_A(\Sigma) + F_B(\Sigma)$ introduced in Proposition 5.6. For $\nabla F_A = -\Sigma^{-1}$ we get $\hat{\Sigma}_{13} = S_{12}S_{22}^{-1}S_{23} = \frac{3}{4}$. For $\nabla F_B(\Sigma) = \Sigma$, $\hat{\Sigma}_{13} = 0$ as the resulting $\hat{\Sigma}$ is positive definite (c.f. Example 3.14). If $F(\Sigma)$ is the negative von Neumann divergence, we need to rely on numerical computations developed in Section 6.1 obtaining

$$\hat{\Sigma} = \begin{bmatrix} 4.0000 & 1.0000 & \mathbf{0.4298} \\ 1.0000 & 4.0000 & 3.0000 \\ \mathbf{0.4298} & 3.0000 & 4.0000 \end{bmatrix} \qquad \hat{L} = \log(\hat{\Sigma}) = \begin{bmatrix} 1.3520 & 0.2721 & \mathbf{0.0000} \\ 0.2721 & 0.9305 & 0.9806 \\ \mathbf{0.0000} & 0.9806 & 0.9695 \end{bmatrix}.$$

For $\nabla F_D(\Sigma) = -\Sigma^{-2}$, $\hat{\Sigma}_{13} = \frac{1}{3}(64 - \sqrt{3754}) \approx 0.91$. Finally, for $\nabla F_E(\Sigma) = \Sigma - \Sigma^{-1}$, $\hat{\Sigma}_{13} \approx 0.105$.

Unknown sparsity: If we are interested in models where $\nabla F(\Sigma)$ is sparse but the zero pattern is unknown, it is natural to consider the optimization problem

(27) minimize
$$F^*(L) - \langle L, S_n \rangle + \lambda \sum_{i \neq j} |L_{ij}|$$

for some $\lambda > 0$. This is a straightforward generalization of the graphical LASSO approach Yuan and Lin (2007); Friedman, Hastie and Tibshirani (2008) and related methods that have been applied to covariance graph models Bien and Tibshirani (2011), and sparse matrix logarithms Deng and Tsui (2013). The dual to this problem is a simple modification of (12).

PROPOSITION 6.6. If $F \in \mathcal{E}^m$ then the dual problem (27) is to minimize $F(\Sigma)$ subject to $\Sigma_{ij} - S_{ij} \in [-\lambda, \lambda]$ for all $i \neq j$.

The proof idea is essentially taken from Banerjee, Ghaoui and d'Aspremont (2008).

PROOF. First note that $\lambda \sum_{i \neq j} |L_{ij}|$ can be rewritten as $\max_{\Gamma} \langle \Gamma, L \rangle$, where Γ is a symmetric matrix with zeros on the diagonal and $-\lambda \leqslant \Gamma_{ij} \leqslant \lambda$ for all $i \neq j$. It follows that

$$\min_{L} F^{*}(L) - \langle L, S_{n} \rangle + \lambda \sum_{i < j} |L_{ij}| = \min_{L} \max_{\Gamma} F^{*}(L) - \langle L, S_{n} - \Gamma \rangle$$

$$= \max_{\Gamma} \min_{L} F^{*}(L) - \langle L, S_{n} - \Gamma \rangle$$

$$= \max_{\Gamma} F^{*}(\nabla F(S_{n} - \Gamma)) - \langle \nabla F(S_{n} - \Gamma), S_{n} - \Gamma \rangle$$

$$= \max_{\Gamma} -F(S_{n} - \Gamma),$$

where swapping max and min in the second line passes to the dual problem, and in the third line we use that ∇F and ∇F^* are inverses of each other. In the last line we used (8) and the fact that $F^{**} = F$, which follows because F is lower semicontinuous. Thus, as claimed, the problem can be rewritten as: minimize $F(\Sigma)$ subject to $-\lambda \leqslant \Sigma_{ij} - S_{ij} \leqslant \lambda$ for all $i \neq j$. \square

REMARK 6.7. A similar reformulation can be found for the general GOLAZO algorithm of Lauritzen and Zwiernik (2022), which is suitable for handling a range of elementwise constraints on L.

6.3. Sparsity in higher powers. One way to motivate the model that imposes zero restrictions on the entries of the higher-order powers of Σ^{-1} is to observe that zeros in Σ^{-2} give us some structural information in the context of Gaussian directed acyclic graph models, which complements the interpretation for zeros in Σ^{-1} given by Pearl and Wermuth (1994).

Consider a directed acyclic graph (DAG) G whose nodes represent components of the random vector $X = (X_1, \ldots, X_m)$. We say that the distribution of X lies in a Gaussian linear structural model over G if

$$X_i = \sum_{j \to i \in G} \lambda_{ij} X_j + \varepsilon_i,$$

where $\lambda_{ij} \in \mathbb{R}$ and ε_i is independent of X_j for each parent j of i in G, and the ε_i 's are mutually independent. Denote by $\Lambda \in \mathbb{R}^{m \times m}$ the matrix with entries λ_{ij} if $j \to i$ in G and zero otherwise. Then the covariance matrix Σ of X satisfies

$$\Sigma = (I - \Lambda)^{-1} \Omega (I - \Lambda)^{-\top},$$

where Ω is the diagonal covariance matrix of ε . Taking the inverse we get $K = L\Omega^{-1}L^{\top}$ (see e.g. Proposition 2.1 in Sullivant, Talaska and Draisma (2010)), where $L = (I - \Lambda)^{\top}$, and so $L_{ij} = 0$ unless i = j or $i \to j$ in the underlying DAG.

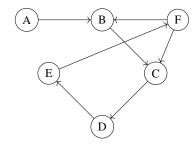


FIG 1.

DEFINITION 6.8. Let $p \in \mathbb{N}$. A p-zig-zag path between i and j in a DAG G is any path of the form

$$i = w_0 \rightarrow u_1 \leftarrow w_1 \rightarrow u_2 \leftarrow w_2 \rightarrow \cdots \leftarrow w_{p-1} \rightarrow u_p \leftarrow w_p = j.$$

Note that each p-zig-zag path contains p "right" and p "left" arrows. A p-zig-zag is called degenerate if some edges are contracted, where by contracting an edge we mean removing the corresponding arrow and equating both nodes.

For example, an edge $i \to j$ is a degenerate p-zig-zag path for every $p \ge 1$. If a path is a p-zig-zag path for some p then it is a degenerate q-zig-zag path for every q > p.

EXAMPLE 6.9. Consider the DAG in Figure 1. Here A is connected by a 1-zig-zag path to F and by a degenerate 1-zig-zag path to B. However, there is no 1-zig-zag path between A and any other node. There is no 2-zig-zag path between A and D (every path has at three arrows going in one direction). Any two nodes are linked by a (degenerate) 3-zig-zag path.

Note that if there is a p-zig-zag path between i and j in G and $X_i \perp \!\!\! \perp X_j | X_S$ for some subset of nodes $S \subseteq \{1, \ldots, m\} \backslash \{i, j\}$ then $|S| \geqslant p$ because S must in particular contain all nodes u_1, \ldots, u_p in the zig-zag.

PROPOSITION 6.10. If there is no (possibly degenerate) 2-zig-zag path between i and j then $(K^2)_{ij} = 0$. More generally, if there is no (possibly degenerate) p-zig-zag path between i and j then $(K^p)_{ij} = 0$.

The proof of this result follows simply by taking $K = L\Omega^{-1}L^{\top}$ and writing the formula for the (i, j)-th entry of K^p . For example,

$$(K^2)_{ij} = (L\Omega^{-1}L^{\top}L\Omega^{-1}L^{\top})_{ij} = \sum_{u,v,w} \frac{L_{iu}L_{vu}L_{vw}L_{jw}}{\Omega_{uu}\Omega_{ww}}.$$

If there is no (possibly degenerate) 2-zig-zag between i and j then each product $L_{iu}L_{vu}L_{vw}L_{jw}$ must be zero.

6.4. *Jordan algebras*. Suppose that $\mathcal{L} \subseteq \mathbb{S}^m$ is a linear space and that it satisfies

$$(28) \forall A, B \in \mathcal{L} AB + BA \in \mathcal{L}.$$

Such a linear subspace is called a Jordan algebra of symmetric matrices Jensen (1988). It is obvious that if $A \in \mathcal{L}$ then $A^2 \in \mathcal{L}$ (or $A^n \in \mathcal{L}$ in general for $n \ge 1$). This condition is in fact equivalent to (28) by the fact that \mathcal{L} is a linear subspace and by the identity $AB + BA = (A+B)^2 - A^2 - B^2$.

Szatrowski showed in a series of papers Szatrowski (1978, 1980, 2004) that the MLE for linear Gaussian covariance models has an explicit representation, i.e., it is a known linear combination of entries of the sample covariance matrix, if and only if \mathcal{L} forms a Jordan algebra. Furthermore, Szatrowski proved that for this restrictive model class the MLE is the arithmetic mean of the corresponding elements of the sample covariance matrix and that Anderson's scoring method Anderson (1973) yields the MLE in one iteration when initiated at any positive definite matrix in the model.

The relevance of this set-up to our considerations comes from the following result.

PROPOSITION 6.11. Suppose $F \in \mathcal{E}^m$ takes the form $F(\Sigma) = \operatorname{tr}(\phi(\Sigma))$ for a function ϕ that is analytic in $(0, +\infty)$. Suppose \mathcal{L} is a linear subspace which satisfies (28) and $I_m \in \mathcal{L}$, then $\Sigma \in \mathcal{L} \cap \mathbb{S}^m_+$ if and only if $\nabla F(\Sigma) \in \mathcal{L} \cap \mathbb{L}^m_+$.

PROOF. Since ϕ is analytic on $(0, +\infty)$, ϕ' is also analytic and we can take its series expansion around 1:

$$\phi'(x) = \sum_{n \ge 0} c_n (x-1)^n$$
 for some $c_n \in \mathbb{R}, n \ge 0$.

In consequence, if $\Sigma \in \mathcal{L}$ and \mathcal{L} satisfies (28) with $I_m \in \mathcal{L}$ then $(\Sigma - I_m)^n \in \mathcal{L}$ for all $n \geqslant 1$ and so

$$\phi'(\Sigma) = c_0 I_m + \sum_{n \ge 1} c_n (\Sigma - I_m)^n \in \mathcal{L}.$$

This shows the right implication. For the left implication we use the fact that $\phi''(x) > 0$ (strict convexity) and so ϕ' is strictly increasing. The inverse of ϕ' is also analytic by the Lagrange Inversion Theorem. Now we can apply exactly the same argument as above to the inverse of ϕ' .

Szatrowski (2004) also gives an overview of interesting linear restrictions that correspond to Jordan algebras. Perhaps the most interesting is given by patterns that are invariant under a permutation subgroup; see also RCOP models defined in Højsgaard and Lauritzen (2008). An extreme version of this is when invariance is under the full symmetric group.

EXAMPLE 6.12. Consider the correlation model with an additional restriction that all off-diagonal entries are equal to each other. This is known as the equicorrelation model Améndola and Zwiernik (2021). In Proposition 2 of Archakov and Hansen (2021), it was shown that the logarithm of an equicorrelation matrix has equal off-diagonal entries. This result is a special case of Proposition 6.11 by observing that the set of matrices with equal diagonal entries and equal off-diagonal entries forms a Jordan algebra.

The following example was motivated by spatial modelling and it has been less studied in the literature.

EXAMPLE 6.13. Consider the subspace

$$\mathcal{L} = \{ L \in \mathbb{S}^m : \exists \alpha \in \mathbb{R} \text{ s.t. } L\mathbf{1}_m = \alpha \mathbf{1}_m \}.$$

This \mathcal{L} satisfies conditions of Proposition 6.11. The MESS model LeSage and Pace (2007) assumes $\log \Sigma \in \mathcal{L}$. Their main motivation for studying this model is that the Gaussian log-likelihood can be explicitly maximized. This again is a special case of the general result on models defined by Jordan algebras.

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APPENDIX A: SPECTRAL FUNCTIONS

A.1. General results. Establishing convexity of a general function $F: \mathbb{S}^m \to \mathbb{R} \cup \{+\infty\}$ and computing its gradient may be in general complicated. We note however that are our running examples are spectral functions Lewis (1996a); Watkins (1974). For reader's convenience we briefly mention relevant results and definitions.

DEFINITION A.1. A function $F: \mathbb{S}^m \to \mathbb{R} \cup \{+\infty\}$ is a spectral function if $F(U^\top \Sigma U) = F(\Sigma)$ for all $\Sigma \in \mathbb{S}^m$ and orthogonal U. In particular, $F(\Sigma)$ depends on the eigenvalues of Σ only.

Associated with any spectral function is a symmetric real-valued function $f: \mathbb{R}^m \to \mathbb{R} \cup \{+\infty\}$. Specifically, we define $f(\lambda) = F(\operatorname{diag}(\lambda))$, where $\operatorname{diag}(\lambda)$ is the diagonal matrix with $\lambda = (\lambda_1, \dots, \lambda_m)$ on the diagonal. Denote by $\lambda(\Sigma) = (\lambda_1(\Sigma), \dots, \lambda_m(\Sigma))$ the spectrum of Σ and by

$$\Lambda(\Sigma) = \operatorname{diag}(\lambda(\Sigma))$$

the diagonal matrix with $(\lambda_1, \dots, \lambda_m)$ on the diagonal. The spectral functions are precisely those of the form $F(\Sigma) = F(\Lambda(\Sigma)) = f(\lambda(\Sigma))$. The following important result appears as Corollary 2.4 in Lewis (1996a); see also Davis (1957).

THEOREM A.2. If $f: \mathbb{R}^m \to \mathbb{R} \cup \{+\infty\}$ is a symmetric, closed convex function then the associated spectral function $F: \mathbb{S}^m \to \mathbb{R} \cup \{+\infty\}$ defined by $F(\Sigma) = f(\lambda(\Sigma))$ is a closed convex function.

Computing the gradient of a spectral function F also relies on computing the gradient of f. The following result will be useful; see Corollary 3.2 Lewis (1996a).

THEOREM A.3. Suppose that the function $f: \mathbb{R}^m \to \mathbb{R} \cup \{+\infty\}$ is a symmetric, closed convex function. If F is the associated spectral function and $\Sigma = U\Lambda(\Sigma)U^{\top}$ for an orthogonal matrix U then for every Σ in the interior of the domain of F

$$\nabla F(\Sigma) = U \operatorname{diag}(\nabla f(\lambda(\Sigma))) U^{\top}.$$

We leave it as an exercise to confirm this result for our running examples in Table 1. We also note that this result is true more generally for spectral functions that are not convex; see Theorem 1.1 in Lewis (1996b). The computation of the second order derivatives is generally much more complicated Lewis and Sendov (2001).

It is worth noting that all our examples have a special form

(29)
$$f(\lambda) = \sum_{i=1}^{m} \phi(\lambda_i)$$

for some smooth function $\phi: \mathbb{R} \to \mathbb{R} \cup \{+\infty\}$. For example, $-\log \det(\Sigma) = -\sum_{i=1}^m \log \lambda_i(\Sigma)$ and $\frac{1}{2}\operatorname{tr}(\Sigma^2) = \frac{1}{2}\sum_{i=1}^m \lambda_i^2(\Sigma)$. Using the matrix function notation (e.g. Higham (2008)) we can write it more elegantly as $F(\Sigma) = \operatorname{tr}(\phi(\Sigma))$. Such functions are also sometimes called spectral sums. The following follows from Theorem A.3.

PROPOSITION A.4. Suppose that ϕ is differentiable in $(0, +\infty)$. Then, for every $\Sigma \in \mathbb{S}_+^m$, we get $\nabla \operatorname{tr}(\phi(\Sigma)) = \phi'(\Sigma)$.

A.2. Running examples. Many results in this paper rely on the fact that the underlying function F is lower semicontinuous. As we said earlier, we normally define F over \mathbb{S}^m_+ and then we extend it to \mathbb{S}^m_+ by taking the lower semicontinuous closure. We now explain how this works for our running examples.

Suppose that ϕ is a proper convex function. Taking $\operatorname{tr}(\phi(\Sigma)) + \operatorname{i}_{\overline{\mathbb{S}}_+^m}(\Sigma)$ in Remark 2.1 corresponds to adding to ϕ the indicator of the closed interval $[0, +\infty)$. Here the semicontinuous closure is easy to calculate directly. Thus, the functions $\phi : \mathbb{R} \to \mathbb{R} \cup \{+\infty\}$ that we consider in this paper take the form

(i)
$$\phi(x) = +\infty$$
 for $x < 0$; (ii) $\phi(x) < +\infty$ for $x > 0$; (iii) $\phi(0) = \lim_{x \to 0^+} \phi(x)$.

We have $dom(\phi) = (0, +\infty)$ or $dom(\phi) = [0, +\infty)$ depending on whether the limit in (iii) is finite or not.

Now we can present our running examples more formally. In example (A) we have:

(30)
$$\phi_A(x) = \begin{cases} -\log(x) & x > 0 \\ +\infty & x \leqslant 0 \end{cases}, \qquad F_A(\Sigma) = \begin{cases} -\log\det(\Sigma) & \Sigma \in \mathbb{S}_+^m \\ +\infty & \Sigma \notin \mathbb{S}_+^m \end{cases}.$$

and so dom $(F_A) = \mathbb{S}^m_+$. In example (B):

(31)
$$\phi_B(x) = \begin{cases} \frac{1}{2}x^2 & x \ge 0 \\ +\infty & x < 0 \end{cases}, \qquad F_B(\Sigma) = \begin{cases} \frac{1}{2}\operatorname{tr}(\Sigma^2) & \Sigma \in \overline{\mathbb{S}}_+^m \\ +\infty & \Sigma \notin \overline{\mathbb{S}}_+^m \end{cases}.$$

and so $\mathrm{dom}(F_B)=\overline{\mathbb{S}}_+^m$. Note that $\lim_{x\to 0^+}\phi_B(x)=0$ so x=0 lies in the domain of ϕ_B . Here the extension was rather trivial because $\frac{1}{2}x^2$ is well defined for all $x\in\mathbb{R}$. Example (C) is slightly more subtle:

(32)
$$\phi_C(x) = \begin{cases} -x(1 - \log(x)) & x > 0 \\ 0 & x = 0, \\ +\infty & x < 0 \end{cases} \quad F_C(\Sigma) = \begin{cases} -\operatorname{tr}(\Sigma - \Sigma \log(\Sigma)) & \Sigma \in \mathbb{S}_+^m \\ +\infty & \Sigma \notin \overline{\mathbb{S}_+^m} \end{cases}$$

and so $\mathrm{dom}(F_C) = \overline{\mathbb{S}}_+^m$. Note that we did not write explicitly what is the value of the map on the boundary of $\overline{\mathbb{S}}_+^m$. This function, similarly to the pseudoinverse, takes the spectral decomposition $\Sigma = U\Lambda U^{\top}$ and applies the transformation ϕ_C only to the non-zero eigenvalues in Λ leaving the zero eigenvalues unchanged. Finally, in example (D):

(33)
$$\phi_D(x) = \begin{cases} \frac{1}{x} & x > 0 \\ +\infty & x \leq 0 \end{cases}, \qquad F_D(\Sigma) = \begin{cases} \operatorname{tr}(\Sigma^{-1}) & \Sigma \in \mathbb{S}_+^m \\ +\infty & \Sigma \notin \mathbb{S}_+^m \end{cases}$$

and so dom $(F_D) = \mathbb{S}^m_+$.

A.3. Convex conjugate. Suppose F is a spectral function we define its conjugate dual as in (7). By Theorem 2.3 in Lewis (1996a), if f is the symmetric function associated to F then F^* is equal to the spectral function defined by the conjugate dual of f. In the special case of spectral sums, f satisfies (29) for some $\phi : \mathbb{R} \to \mathbb{R}$. It is straightforward to see that

$$f^*(y) = \sup_{x \in \mathbb{R}^m} \{ \langle x, y \rangle - \sum_{i=1}^m \phi(x_i) \} = \sum_{i=1}^m \phi^*(y_i).$$

In other words, we have the following result.

LEMMA A.5. If
$$F(\Sigma) = \operatorname{tr}(\phi(\Sigma))$$
 for some $\phi : \mathbb{R} \to \mathbb{R}$ then $F^*(L) = \operatorname{tr}(\phi^*(L))$.

In example (A), ϕ_A is given in (30) and

$$\phi_A^*(y) = \sup_{x \in \mathbb{R}} \{xy - \phi(x)\} = \sup_{x > 0} \{xy + \log(x)\} = \begin{cases} -1 - \log(-y) & \text{if } y < 0, \\ +\infty & \text{otherwise.} \end{cases}$$

This calculation shows that

$$F_A^*(L) = \begin{cases} -m - \log \det(-L) & \text{if } L \in -\mathbb{S}_+^m, \\ +\infty & \text{otherwise} \end{cases}, \quad \operatorname{dom}(F_A^*) = -\mathbb{S}_+^m = \nabla F_A(\mathbb{S}_+^m).$$

Similarly, ϕ_B is given in (31) and

$$\phi_B^*(y) = \sup_{x \ge 0} \{xy - \frac{1}{2}x^2\} = \begin{cases} \frac{1}{2}y^2 & \text{if } y \ge 0, \\ 0 & \text{otherwise.} \end{cases}$$

In particular,

(34)
$$F_B^*(L) = \begin{cases} \frac{1}{2}\operatorname{tr}(L^2) & \text{if } L \in \overline{\mathbb{S}}_+^m, \\ 0 & \text{otherwise.} \end{cases}, \quad \operatorname{dom}(F_B^*) = \mathbb{S}^m \supset \nabla F_B(\mathbb{S}_+^m) = \mathbb{S}_+^m$$

In example (C), ϕ_C is given by (32) and

$$\phi_C^*(y) = \max\{0, \sup_{x>0} \{xy + x - x \log(x)\}\} = e^y.$$

In particular, $F_C^*(L) = \exp(L)$ and $\operatorname{dom}(F_C^*) = \mathbb{S}^m = \nabla F_C(\mathbb{S}_+^m)$. Finally, ϕ_D is given in (33) and its conjugate is

$$\phi_D^*(y) = \sup_{x>0} \{xy - \frac{1}{x}\} = \begin{cases} -2\sqrt{-y} & \text{if } y < 0 \\ +\infty & \text{otherwise} \end{cases}$$

and we have

$$F_D^*(L) = \begin{cases} -2\operatorname{tr}(\sqrt{-L}) & \text{if } L \in -\mathbb{S}_+^m \\ +\infty & \text{otherwise.} \end{cases}, \quad \operatorname{dom}(F_D^*) = -\mathbb{S}_+^m = \nabla F_D(\mathbb{S}_+^m).$$

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