

# A Random Matrix-Theoretic Approach to Handling Singular Covariance Estimates

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**Abstract**—In many practical situations we would like to estimate the covariance matrix of a set of variables from an insufficient amount of data. More specifically, if we have a set of  $N$  independent, identically distributed measurements of an  $M$  dimensional random vector the maximum likelihood estimate is the sample covariance matrix. Here we consider the case where  $N < M$  such that this estimate is singular (noninvertible) and therefore fundamentally bad. We present a radically new approach to deal with this situation based on the idea of dimensionality reduction through an ensemble of isotropically random unitary matrices. We obtain two estimates *cov* and *invcov* which are estimates for the covariance matrix and the inverse covariance matrix respectively. Both estimates retain the original eigenvectors while altering the eigenvalues. We have a closed form analytical expression for *cov* and *invcov* in terms of the eigenvector/eigenvalue decomposition of the sample covariance. We motivate the use of *invcov* through applications to linear estimation, supervised learning, and high-resolution spectral estimation. We also compare the performance of these estimators with other more conventional methods.

**Index Terms**—Curse of dimensionality, isotropically random, limiting distribution, random matrices, sensor networks, singular covariance matrices, Stiefel manifold.

## I. INTRODUCTION

THE estimation of a covariance matrix from an insufficient amount of data is one of the most common multivariate problems in statistics, signal processing, and learning theory. Inexpensive sensors permit ever more measurements to be taken simultaneously. Thus the dimensions of feature vectors are growing. But typically the number of independent measurements of the feature vector are not increasing at a commensurate rate. Consequently, for many problems, the sample covariance matrix is almost always singular (noninvertible). More precisely, given a set of independent multivariate Gaussian feature vectors, the sample covariance matrix is a maximum likelihood estimate. When the number of feature vectors is smaller than their dimension then the estimate is singular, and the sample covariance is a fundamentally bad estimate in the sense that the maximum likelihood principle yields a nonunique estimate

having infinite likelihood. The sample covariance finds linear relations among the random variables when there may be none. The estimates for the larger eigenvalues are typically too big, and the estimates for the small eigenvalues are typically too small.

The conventional treatment of covariance singularity artificially converts the singular sample covariance matrix into an invertible (positive-definite) covariance by the simple expedient of adding a positive diagonal matrix, or more generally, by taking a linear combination of the sample covariance and an identity matrix. This procedure is variously called “diagonal loading” or “ridge regression” [12], [10]. The resulting covariance has the same eigenvectors as the sample covariance, and eigenvalues which are uniformly scaled and shifted versions of the sample covariance eigenvalues. The choice of the loading parameters is a long-standing research problem. The method of Ledoit and Wolf [7] automatically chooses the loading parameters. Others methods as the ones in [22] and [23] have also been considered.

We propose a radically different alternative to diagonal loading which is based on an ensemble of dimensionality reducing random unitary matrices. The concept is that the unitary matrix multiplies the feature vectors to produce shortened feature vectors, having dimension significantly smaller than the number of feature vectors, which produce a statistically meaningful and invertible covariance estimate. The covariance estimate is used to compute an estimate for the ultimate quantity or quantities of interest. Finally this estimate is averaged over the ensemble of unitary matrices. We consider two versions of this scheme which we call *cov* and *invcov*. We show that the estimate *cov* is equivalent to diagonal loading. Both estimates *invcov* and *cov* retain the original eigenvectors and make nonzero the formerly zero eigenvalues. We have a closed form analytical expression for *invcov* in terms of its eigenvector and eigenvalue decomposition. We motivate the use of *invcov* through applications to linear estimation, supervised learning, and high-resolution spectral estimation. We also compare the performance of the estimator *invcov* with respect to diagonal loading.

Throughout the paper we will denote by  $A^*$  the complex conjugate transpose of the matrix  $A$ .  $I_N$  will represent the  $N \times N$  identity matrix. We let  $\text{Tr}$  be the nonnormalized trace for square matrices, defined by,  $\text{Tr}(A) := \sum_{i=1}^N a_{ii}$  where  $a_{ii}$  are the diagonal elements of the  $N \times N$  matrix  $A$ . We also let  $\text{tr}$  be the normalized trace, defined by  $\text{tr}(A) = \frac{1}{N} \text{Tr}(A)$ .

## II. NEW APPROACH TO HANDLING COVARIANCE SINGULARITY

We begin with a set of  $N$  independent identically distributed measurements of an  $M$  dimensional random vector where  $N <$

Manuscript received February 12, 2010; revised May 09, 2011; accepted May 09, 2011. Date of current version August 31, 2011.

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Communicated by A. L. Moustakas, Associate Editor for Communications.

Color versions of one or more of the figures in this paper are available online at <http://ieeexplore.ieee.org>.

Digital Object Identifier 10.1109/TIT.2011.2162175

$M$ . We introduce an ensemble of  $L \times M$  random unitary matrices, such that  $L \leq N$ . The unitary matrix multiplies the feature vectors to produce a set of  $N$  feature vectors of dimension  $L$  from which we obtain an invertible sample covariance matrix. The dimensionality reduction process is reversible (i.e., no information is thrown away) provided it is done for a sufficient multiplicity of independent unitary matrices. The key question is what to do with the ensemble of reduced dimension covariance estimates.

#### A. Notation and Sample Covariance

We are given a  $M \times N$  data matrix  $X$  the columns of which comprise  $N$  independent identically distributed realizations of a random vector. For convenience we assume that the random vector is zero-mean. We also will assume that the random vector is circularly-symmetric complex. The sample covariance is

$$K = \frac{1}{N} X X^*. \quad (1)$$

We are interested in the case where  $N < M$ . Consequently, the sample covariance is singular with rank equal to  $N$ .

#### B. Dimensionality Reducing Ensemble

We introduce an ensemble of  $L \times M$  random unitary matrices,  $\Phi$  where  $L \leq N$  and  $\Phi \Phi^* = I_L$ , where  $I_L$  is the  $L \times L$  identity matrix. The multiplication of the data matrix by the unitary matrix results in a data matrix of reduced dimension  $L \times N$ , which in turn produces a statistically meaningful sample covariance matrix provided that  $L$  is sufficiently small compared with  $N$

$$\frac{1}{N} \Phi X X^* \Phi^* = \Phi K \Phi^*. \quad (2)$$

We need to specify the distribution of the random unitary matrix. One possibility would be to use a random permutation matrix, the effect of which would be to discard all but  $L$  of the  $M$  components of the data vectors. Instead we utilize the Haar measure (sometimes called the “isotropically random” distribution [11]). A fundamental property of the Haar distribution is its invariance to multiplication of the random unitary matrix by an unrelated unitary matrix. Specifically, let  $p(\Phi)$  be the joint probability density for the components of the unitary matrix, and let  $\Theta$  be any unrelated  $M \times M$  unitary matrix (i.e., either  $\Theta$  is deterministic, or it is statistically independent of  $\Phi$ ). Then  $\Phi$  has Haar measure if and only if for all unitary  $\Theta$

$$p(\Phi \Theta) = p(\Phi). \quad (3)$$

Compared with the random permutation matrix, the Haar measure is more flexible as it permits linear constraints to be imposed.

#### C. Two Nonsingular Covariance Estimates

The generation of the ensemble of reduced-dimension covariance estimates (2) is well motivated. It is less obvious what to do with this ensemble. We have investigated two approaches: *cov* which yields directly a nonsingular estimate for the  $M \times M$  covariance matrix, and *invcov* which yields directly an estimate for the inverse  $M \times M$  covariance matrix.

1) *cov*: If we project the  $L \times L$  covariance (2) out to a  $M \times M$  covariance using the same random unitary matrix, and then take the expectation over the unitary ensemble, we obtain the following:

$$\text{cov}_L(K) = \mathbb{E}_\Phi(\Phi^*(\Phi K \Phi^*)\Phi). \quad (4)$$

This expectation can be evaluated in closed form (either by evaluating fourth moments, or by using Schur polynomials as shown later)

$$\text{cov}_L(K) = \frac{L}{(M^2 - 1)M} [(ML - 1)K + (M - L)\text{Tr}(K)I_M]. \quad (5)$$

Thus the procedure *cov* is equivalent to diagonal loading for a particular pair of loading parameters. The dimensionality parameter  $L$  determines the amount of diagonal loading. It is reasonable to rescale the covariance expression (5) by the factor  $M/L$  because the dimensionality reduction yields shortened feature vectors whose energy is typically  $L/M$  times the energy of the original feature vectors. Note that we use the term energy to denote the  $\|x\|_2^2$  of a vector  $x$ . If the covariance is scaled in this manner then the trace of the sample covariance is preserved.

Although it is both interesting and surprising that *cov* is equivalent to diagonal loading, we instead pursue an approach which is better motivated and which promises more compelling action.

2) *invcov*: We first invert the  $L \times L$  covariance (2) (which is invertible with probability one), project out to  $M \times M$  using the same unitary matrix, and then take the expectation over the unitary ensemble to obtain the following:

$$\text{invcov}_L(K) = \mathbb{E}_\Phi(\Phi^*(\Phi K \Phi^*)^{-1}\Phi). \quad (6)$$

The estimate *invcov* (as well as *cov*) preserves the eigenvectors. In other words, if we perform the eigenvector and eigenvalue decomposition

$$K = U D U^* \quad (7)$$

where  $D$  is the  $M \times M$  diagonal matrix, whose diagonals are the eigenvalues, ordered from largest to smallest, and  $U$  is the  $M \times M$  unitary matrix of eigenvectors, then we prove (in Section IV) that

$$\text{invcov}_L(K) = U \text{invcov}_L(D) U^*. \quad (8)$$

Therefore it is enough to compute  $\text{invcov}_L(D)$ . We also show that  $\text{invcov}_L(D)$  is a diagonal matrix. Moreover, if  $D = \text{diag}(D_N, 0_{M-N})$  where  $D_N = \text{diag}(d_1, \dots, d_N)$  is the matrix with the nonzero entries then the matrix  $\text{invcov}_L(D)$  is a diagonal matrix that can be decomposed as

$$\text{invcov}_L(D) = \text{diag}(\lambda_1, \dots, \lambda_N, \mu I_{M-N}). \quad (9)$$

In other words all the zero-eigenvalues are transformed to a nonzero constant  $\mu$ , while the nonzero eigenvalues are altered

in a nontrivial way. In Section VI we prove an exact expression for the entries of  $\text{invcov}_L(D)$ . More specifically we prove that

$$\mu = \text{Tr}[\mathbb{E}((Z^* D_N Z)^{-1})] \quad (10)$$

where the average is taken over the ensemble of all  $N \times L$  Gaussian random matrices  $Z$  with independent and complex entries with zero mean and unit variance. Proposition 1 (in Section VI) gives us an explicit formula for  $\mu$ . Also, using Lemma 1 (in the same Section) we prove that

$$\lambda_k = \frac{\partial}{\partial d_k} \int_{\Omega_{L,N}} \text{Tr} \log(\Phi^* D_N \Phi) d\phi \quad (11)$$

where  $d\phi$  is integration with respect to the isotropic measure on  $\Omega_{L,N}$ . We also show that the integral

$$\int_{\Omega_{L,N}} \text{Tr} \log(\Phi^* D_N \Phi) d\phi \quad (12)$$

can be computed explicitly using Theorem 1 in Section VI. Therefore, given  $D$  we obtain closed form expressions for all the entries of the matrix  $\text{invcov}_L(D)$  for every  $M, N$  and  $L$ .

In Section VIII using Free Probability techniques we prove asymptotic formulas for the entries of  $\text{invcov}_L(D)$  for large values of  $N$ .

We focus the remainder of the paper on some potential applications of  $\text{invcov}$ , the derivation of its fundamental properties, and how to compute it.

### III. POTENTIAL APPLICATIONS OF INVCOV

Typically neither the covariance matrix nor its inverse is of direct interest. Rather some derived quantity is desired. Here we discuss three potential applications where  $\text{invcov}$  arises in a natural way.

#### A. Design of a Linear Estimator From Training Data

The problem is to design a minimum mean square linear estimator for a  $M_x \times 1$  random vector  $x$  given an observation of a  $M_y \times 1$  random vector  $y$ . Exact statistics are not available; instead we have to work with statistics that are estimated from a set of training data. If the statistics were available then the optimum estimator would be (assuming that the vectors have zero-mean)

$$\hat{x}(y) = K_{xy} K_y^{-1} y \quad (13)$$

where  $K_y$  is the covariance matrix of vector  $y$  and  $K_{xy}$  is the cross-covariance matrix of vectors  $x$  and  $y$ . In this case, the mean-square error matrix is given by

$$\begin{aligned} \text{MMSE} &= \mathbb{E}((\hat{x}(y) - x)(\hat{x}(y) - x)^*) \\ &= K_x - K_{xy} K_y^{-1} K_{yx}. \end{aligned} \quad (14)$$

The trace of this matrix give us the mean-square error. For the design of the estimator we have training data comprising  $N$  independent joint realizations of  $x$  and  $y$ :  $X$  ( $M_x \times N$ ) and  $Y$  ( $M_y \times N$ ), where  $N < M_y$ .

We introduce an ensemble of  $L \times M_y$  isotropically random unitary matrices,  $\Phi$ , where  $L \leq N$ . We reduce the dimen-

sionality of the observed vector,  $y \rightarrow \Phi y$ , and the training set  $Y \rightarrow \Phi Y$  and we estimate the relevant covariances as follows:

$$K_{x,\Phi y} = \frac{1}{N} X Y^* \Phi^* \quad (15)$$

$$K_{\Phi y} = \frac{1}{N} \Phi Y Y^* \Phi^*. \quad (16)$$

We estimate  $x$  given the reduced observation  $\Phi y$  by treating the covariance estimates (15) and (16) as if they were correct

$$\begin{aligned} \hat{x}(\Phi y) &= K_{x,\Phi y} K_{\Phi y}^{-1} \Phi y \\ &= X Y^* \Phi^* (\Phi Y Y^* \Phi^*)^{-1} \Phi y. \end{aligned} \quad (17)$$

The mean-square error of this estimator conditioned on the random unitary matrix,  $\Phi$ , is found by taking an expectation with respect to the training data  $\{X, Y\}$ , the observation  $y$ , (which is independent of the training data), and the true value of the unknown vector  $x$

$$\begin{aligned} \mathbb{E}\{[\hat{x}(\Phi y) - x][\hat{x}(\Phi y) - x]^* | \Phi\} &= \\ &= [K_x - K_{xy} \Phi^* (\Phi K_y \Phi^*)^{-1} \Phi K_{yx}] \cdot \\ &= [1 + \mathbb{E}_V (\text{Tr}(V^* V)^{-1})] \end{aligned} \quad (18)$$

where  $V$  is a  $N \times L$  random matrix with independent, complex Gaussian random entries, with zero mean and unit variance.

To obtain the mean-square error expression (18) we let  $z = \Phi y$ , and  $Z = \Phi Y$ , and proceed as follows:

$$\begin{aligned} \mathbb{E}\{[\hat{x}(z) - x][\hat{x}(z) - x]^* | \Phi\} &= \\ \mathbb{E}\{[K_{xz} K_z^{-1} z - x][K_{xz} K_z^{-1} z - x]^*\} &+ \\ \mathbb{E}\{[\hat{x}(z) - K_{xz} K_z^{-1} z][\hat{x}(z) - K_{xz} K_z^{-1} z]^* | \Phi\}. \end{aligned} \quad (19)$$

The first term in the above expression is the optimum error covariance as if the exact statistics were known

$$\begin{aligned} \mathbb{E}\{[K_{xz} K_z^{-1} z - x][K_{xz} K_z^{-1} z - x]^*\} &= \\ K_x - K_{xz} K_z^{-1} K_{zx}. \end{aligned} \quad (20)$$

We treat the second term in (19) as follows:

$$\begin{aligned} [\hat{x}(z) - K_{xz} K_z^{-1} z] &= \\ [X Z^* (Z Z^*)^{-1} z - K_{xz} K_z^{-1} z] &= \\ [(X - K_{xz} K_z^{-1} Z) Z^* (Z Z^*)^{-1} z]. \end{aligned} \quad (21)$$

We take first, the expectation with respect to  $y$ , and then the conditional expectation over  $X$  given  $Z$  to obtain the following:

$$\begin{aligned} \mathbb{E}\{[\hat{x}(z) - K_{xz} K_z^{-1} z][\hat{x}(z) - K_{xz} K_z^{-1} z]^* | Z, \Phi\} &= \\ [K_x - K_{xz} K_z^{-1} K_{zx}] \cdot \text{Tr}\{A\} \end{aligned} \quad (22)$$

where

$$A = Z^* (Z Z^*)^{-1} K_z (Z Z^*)^{-1} Z. \quad (23)$$

Finally, we take the conditional expectation of (22) with respect to  $Z$  given  $\Phi$ , which combined with (20) and (19) gives (18).

Recall from random matrix theory the following result (see [6] for more details)

$$\mathbb{E}\left(\text{tr}((V^*V)^{-1})\right) = \frac{L}{N-L}. \quad (24)$$

The mean-square error (18) is equal to the product of two terms: the mean-square error which results from performing estimation with a reduced observation vector and with exact statistics available, and a penalty term which account for the fact that exact statistics are not available. The first term typically decreases with increasing dimensionality parameter  $L$ , which the second term increases with  $L$ .

Instead of performing the estimation using one value of the dimensionality-reducing matrix,  $\Phi$ , one can average the estimator (17) over the unitary ensemble

$$\begin{aligned} \hat{x}(y) &= \mathbb{E}_\Phi(\hat{x}(\Phi y)) \\ &= XY^* \mathbb{E}_\Phi(\Phi^*(\Phi YY^* \Phi^*)^{-1} \Phi) y \\ &= XY^* \cdot \text{invcov}_L(YY^*) \cdot y. \end{aligned} \quad (25)$$

Jensen's inequality implies that the ensemble-averaged estimator (25) has better performance than the estimator (17) that is based on a single realization of  $\Phi$

$$\begin{aligned} \mathbb{E}([ \mathbb{E}_\Phi(\hat{x}(\Phi y)) - x ] \cdot [ \mathbb{E}_\Phi(\hat{x}(\Phi y)) - x ]^*) &\leq \\ \mathbb{E}_\Phi(\mathbb{E}([ \hat{x}(\Phi y) - x ] [ \hat{x}(\Phi y) - x ]^*)). \end{aligned} \quad (26)$$

### B. Supervised Learning: Design of a Quadratic Classifier From Training Data

The problem is to design a quadratic classifier from labeled training data. Given an observation of a  $M \times 1$  zero-mean complex Gaussian random vector, the classifier has to choose one of two hypotheses. Under hypothesis  $H_j$ ,  $j = 0, 1$ , the observation is distributed as  $\text{CN}(0, K_j)$ ,  $j = 0, 1$ . If the two covariance matrices were known the optimum classifier is a likelihood ratio test [15]

$$\begin{aligned} &H_1 \\ -x^* (K_1^{-1} - K_0^{-1}) x &\stackrel{H_1}{>} \gamma \\ &\stackrel{H_0}{<} \end{aligned} \quad (27)$$

where  $\gamma$  is a threshold. Instead the covariances have to be estimated from two  $M \times N$  matrices of labeled training data,  $X_j$ ,  $j = 0, 1$ , each of which comprises  $N < M$  independent observations of the random vector under their respective hypotheses.

We introduce an ensemble of  $L \times M$  random unitary matrices  $\Phi$  where  $L \leq N$ . For a given  $\Phi$  we reduce the dimension of both sets of training data and then estimate the reduced covariance matrices

$$K_j = \frac{1}{N} \Phi X_j X_j^* \Phi^*, \quad j = 0, 1. \quad (28)$$

For any  $\Phi$  we could implement a likelihood ratio test based on the estimated reduced covariances (28) and the reduced observation,  $\Phi x$ . Alternatively we could base the hypothesis test on

the expectation of the log-likelihood ratio with respect to the unitary ensemble

$$\begin{aligned} -x^* \mathbb{E}_\Phi(\Phi^*((\Phi X_1 X_1^* \Phi^*)^{-1} - (\Phi X_0 X_0^* \Phi^*)^{-1}) \Phi) x = \\ H_1 \\ -x^* (\text{invcov}_L(X_1 X_1^*) - \text{invcov}_L(X_0 X_0^*)) x \stackrel{H_1}{>} \gamma. \end{aligned} \quad (29)$$

This classifier is of the “naive Bayes” type [16], in which statistical dependencies (in this case the individual likelihood ratios are not statistically dependent) are ignored in order to simplify the construction of the classifier.

### C. Capon MVDR Spectral Estimator

The Capon MVDR (minimum variance distortionless response) spectral estimator estimates power as a function of angle-of-arrival given  $N$  independent realizations of a  $M$ -dimensional measurement vector from an array of sensors [17]. Let  $X$  be the  $M \times N$  vector of measurements,  $M < N$ , and let the “steering vector”  $a$  be the  $M$  dimensional unit vector which describes the wavefront at the array. The conventional power estimate, as a function of the steering vector, is

$$P_{\text{conv}} = a^* K a \quad (30)$$

where  $K$  is the sample covariance matrix. The Capon MVDR power estimate is

$$P_{\text{Capon}} = \frac{1}{a^* K^{-1} a}. \quad (31)$$

A justification for the Capon estimator is the following: one considers the estimated covariance matrix to be the sum of two terms, the first corresponding to power arriving from the direction that is specified by the steering vector, and the second corresponding to power arriving from all other directions

$$K = P \cdot aa^* + K_{\text{other}}. \quad (32)$$

It can be shown that the Capon power estimate (31) is equal to the largest value of power  $P$  such that, in the decomposition (32),  $K_{\text{other}}$  is nonnegative definite [1]. In other words the decomposition (32) is nonunique, and the Capon power estimate is an upper bound on the possible value that the power can take.

We deal with the singularity of the covariance matrix by introducing an ensemble of  $L \times M$  unitary matrices,  $\Phi$ . Since we are looking for power that arrives from a particular direction we constrain the unitary matrices to preserve the energy of the steering vector, i.e.,  $a^* \Phi^* \Phi a = a^* a = 1$ . This is readily done through a Householder unitary matrix,  $Q$ , such that

$$Q = \begin{bmatrix} a^* \\ A_\perp \end{bmatrix} \quad (33)$$

where  $A_\perp$  is a  $M - 1 \times M$  unitary matrix whose rows are orthogonal to  $a$ . We represent the ensemble  $\Phi$  as follows:

$$\Phi = \begin{bmatrix} a^* \\ \Theta A_\perp \end{bmatrix} \quad (34)$$

where  $\Theta$  is a  $L - 1 \times M - 1$  isotropically random unitary matrix. We now use the constrained unitary matrix  $\Phi$  to reduce the dimensionality of the sample covariance matrix and the steering vector, we compute the Capon power estimate from the reduced quantities, and finally we average the power with respect to the unitary ensemble [2]

$$\begin{aligned}\hat{P} &= \mathbb{E}_{\Phi} \left[ \frac{1}{a^* \Phi^* (\Phi K \Phi^*)^{-1} \Phi a} \right] \\ &= a^* K a - a^* K A_{\perp}^* \text{invcov}_{L-1}(A_{\perp} K A_{\perp}^*) A_{\perp} K a\end{aligned}\quad (35)$$

where

$$\text{invcov}_{L-1}(A_{\perp} K A_{\perp}^*) = \mathbb{E}_{\Theta}(\Theta^*(\Theta A_{\perp} K A_{\perp}^* \Theta^*)^{-1} \Theta). \quad (36)$$

#### D. Distantly Related Research

Our approach to handling covariance singularity is based on an ensemble of dimensionality-reducing random unitary matrices. Here we mention some other lines of research which also involve random dimensionality reduction.

1) *Johnson-Lindenstrauss Lemma*: In qualitative terms, the Johnson-Lindenstrauss Lemma [13] has the following implication: the angle between two vectors of high dimension tends to be preserved accurately when the vectors are shortened through multiplication by a random unitary dimensionality-reducing matrix.

2) *Compressed Sampling or Sensing*: Compressive sampling or sensing permits the recovery of a sparsely-sampled data vector (for example, obtained by multiplying the original vector by a random dimensionality-reducing matrix), provided the original data vector can be linearly transformed to a domain in which it has sparse support [14]. The classical compressive sampling theory utilizes only one dimensionality-reducing matrix. In contrast our approach to handling covariance singularity utilizes an *ensemble* of random dimensionality-reducing matrices. We note that since the completion of this research some recent work in compressed sensing addresses information-theoretic questions using an ensemble of random dimensionality reducing matrices (see [24] and [25] for more details).

#### IV. DERIVATION OF SOME BASIC PROPERTIES OF INVCOV

In this section, we state and prove two basic and fundamental properties of  $\text{invcov}_L(K)$ . We perform the eigenvector and eigenvalue decomposition of the sample covariance (7) where  $D$  is the  $M \times M$  diagonal matrix, whose diagonals are the eigenvalues, ordered from largest to smallest, and  $U$  is the  $M \times M$  unitary matrix of eigenvectors.

##### A. Eigenvectors of Sample Covariance are Preserved

We substitute the eigenvalue decomposition (7) into the expression (6) for  $\text{invcov}_L(K)$  to obtain the following:

$$\begin{aligned}\text{invcov}_L(K) &= \mathbb{E}_{\Phi}(\Phi^*(\Phi K \Phi^*)^{-1} \Phi) \\ &= \mathbb{E}_{\Phi}(U(\Phi U)^*(\Phi U D U^* \Phi^*)^{-1}(\Phi U)U^*) \\ &= U \mathbb{E}_{\Phi}(\Phi^*(\Phi D \Phi^*)^{-1} \Phi) U^* \\ &= U \text{invcov}_L(D) U^*\end{aligned}\quad (37)$$

where we have used the fundamental definition of the isotropic distribution (3), i.e., that the product  $\Phi U$  has the same distribution as  $\Phi$ . We intend to show that  $\text{invcov}_L(D)$  is itself diagonal. We utilize the fact that a matrix  $A$  is diagonal if and only if, for all diagonal unitary matrices  $\Omega$ ,  $\Omega A \Omega^* = A$ . Let  $\Omega$  be a diagonal unitary matrix; we have

$$\begin{aligned}\Omega \text{invcov}_L(D) \Omega^* &= \\ &= \mathbb{E}_{\Phi}((\Phi \Omega^*)^*(\Phi \Omega^*) \Omega D \Omega^* (\Phi \Omega^*)^*)^{-1} (\Phi \Omega^*) \\ &= \mathbb{E}_{\Phi}(\Phi^*(\Phi D \Phi^*)^{-1} \Phi) \\ &= \text{invcov}_L(D)\end{aligned}\quad (38)$$

where we used the fact that  $\Phi \Omega^*$  has the same distribution as  $\Phi$ , and that  $\Omega D \Omega^* = D$ . Therefore we have established that the final expression in (37) is the eigenvector/eigenvalue decomposition of  $\text{invcov}_L(K)$ , for which the eigenvector matrix is  $U$  and the diagonal matrix of eigenvalues is  $\text{invcov}_L(D)$ . Hence, we need only consider applying  $\text{invcov}$  to diagonal matrices.

##### B. The Zero-Eigenvalues of the Sample Covariance are Converted to Equal Positive Values

When the rank of the covariance matrix is equal to  $N < M$ , the eigenvalue matrix of  $K$  has the form

$$D = \begin{bmatrix} D_N & 0 \\ 0 & 0_{M-N} \end{bmatrix}. \quad (39)$$

We want to establish that the last  $M - N$  eigenvalues of  $\text{invcov}_L(K)$  are equal. To that end, we introduce a unitary matrix  $\Xi$

$$\Xi = \begin{bmatrix} I_N & 0 \\ 0 & P_{M-N} \end{bmatrix} \quad (40)$$

where  $P_{M-N}$  is an arbitrary  $M - N \times M - N$  permutation matrix. We now pre- and postmultiply  $\text{invcov}_L(D)$  by  $\Xi$  and  $\Xi^*$  respectively: it will be shown that this does not change the diagonal matrix, so consequently the last  $M - N$  eigenvalues are equal. We have

$$\begin{aligned}\Xi \text{invcov}_L(D) \Xi^* &= \Xi \mathbb{E}_{\Phi}(\Phi^*(\Phi D \Phi^*)^{-1} \Phi) \Xi^* \\ &= \mathbb{E}_{\Phi}(\Phi^*(\Phi \Xi D \Xi^* \Phi^*)^{-1} \Phi) \\ &= \mathbb{E}_{\Phi}(\Phi^*(\Phi D \Phi^*)^{-1} \Phi) \\ &= \text{invcov}_L(D),\end{aligned}\quad (41)$$

where we used the fact that  $\Phi \Xi^*$  has the same distribution as  $\Phi$ , and that  $\Xi D \Xi^* = D$ .

#### V. FUNCTIONAL EQUATION

In this section, we will prove a functional equation for the inverse covariance estimate  $\text{invcov}_L(K)$ .

Let  $K$  be an  $M \times M$  sample covariance matrix  $K$  of rank  $N$ . Since  $K$  is positive definite there exists  $U$  an  $M \times M$  unitary and  $D$  an  $M \times M$  diagonal matrix of rank  $N$  such that  $K = U D U^*$ . Fix  $L \leq N$ . We would like to compute

$$\text{invcov}_L(K) = \mathbb{E}(\Phi^*(\Phi K \Phi^*)^{-1} \Phi) \quad (42)$$

where  $\Phi$  is an  $L \times M$  unitary matrix and the average is taken with respect to the isotropic measure. Let  $Z$  be an  $L \times M$  Gaussian random matrix with complex, independent and identically distributed entries with zero mean and variance 1. It is a well known result in random matrix theory (see [6]) that we can decompose  $Z = C\Phi$  where  $C$  is an  $L \times L$  positive definite and invertible matrix (with probability one). Hence

$$\mathbb{E}(\Phi^*(\Phi K \Phi^*)^{-1}\Phi) = \mathbb{E}(Z^*(Z K Z^*)^{-1}Z)$$

Therefore

$$\text{invcov}_L(K) = \mathbb{E}(Z^*(Z K Z^*)^{-1}Z). \quad (43)$$

Moreover, as shown in the previous section

$$\text{invcov}_L(K) = U\mathbb{E}(Z^*(Z D Z^*)^{-1}Z)U^*. \quad (44)$$

Therefore it is enough to compute  $\mathbb{E}(Z^*(Z D Z^*)^{-1}Z)$ . Decompose  $Z$  as  $Z = [V, W]$  where  $V$  is  $L \times N$  and  $W$  is  $L \times (M - N)$ . Now performing the block matrix multiplications and taking the expectation we obtain that  $\text{invcov}_L(D)$  is equal to

$$\begin{bmatrix} \mathbb{E}(V^*(V D_N V^*)^{-1}V) & 0 \\ 0 & \mathbb{E}(W^*(V D_N V^*)^{-1}W) \end{bmatrix} \quad (45)$$

where  $D = \text{diag}(D_N, 0_{M-N})$  and  $D_N$  an  $N \times N$  diagonal matrix of full rank.

Let us first focus on the  $N \times N$  matrix  $\mathbb{E}(V^*(V D_N V^*)^{-1}V)$ , denote this matrix by

$$\Lambda_L(D_N) := \mathbb{E}(V^*(V D_N V^*)^{-1}V). \quad (46)$$

Let  $T$  be the matrix  $T = V D_N^{1/2}$ . Then

$$\begin{aligned} \Lambda_L(D_N) &= \mathbb{E}(V^*(V D_N V^*)^{-1}V) \\ &= D_N^{-1/2} \mathbb{E}(T^*(T T^*)^{-1}T) D_N^{-1/2} \end{aligned} \quad (47)$$

and

$$\begin{aligned} \mathbb{E}(T^*(T T^*)^{-1}T) &= \\ &= \lim_{\gamma \rightarrow 0} \mathbb{E}[T^*(\gamma I_L + T T^*)^{-1}T] \\ &= I_N - \lim_{\gamma \rightarrow 0} \mathbb{E} \left[ \left( I_N + \frac{1}{\gamma} T^* T \right)^{-1} \right]. \end{aligned} \quad (48)$$

Therefore it is enough to compute

$$\lim_{\gamma \rightarrow 0} \mathbb{E} \left[ \left( I_N + \frac{1}{\gamma} T^* T \right)^{-1} \right] \quad (49)$$

which is equal to

$$\lim_{\gamma \rightarrow 0} D_N^{-1/2} \mathbb{E} \left[ \left( D_N^{-1} + \frac{1}{\gamma} V^* V \right)^{-1} \right] D_N^{-1/2}. \quad (50)$$

Let us decompose  $V^* V = \Omega D_x \Omega^*$  where  $\Omega$  is an  $N \times N$  unitary matrix and  $D_x$  is an  $N \times N$  diagonal matrix of rank  $L$ . Then

$D_x = \text{diag}(D_0, 0_{N-L})$ . It is a straightforward calculation to see that

$$D_N^{-1/2} \mathbb{E} \left[ \left( D_N^{-1} + \frac{1}{\gamma} V^* V \right)^{-1} \right] D_N^{-1/2} \quad (51)$$

is equal to

$$D_N^{-1/2} \mathbb{E} \left[ \Omega \left( \Omega^* D_N^{-1} \Omega + \frac{1}{\gamma} D_x \right)^{-1} \Omega^* \right] D_N^{-1/2}. \quad (52)$$

Doing the block matrix decomposition

$$\Omega^* D_N^{-1} \Omega = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \quad (53)$$

where  $A_{11}$  is  $L \times L$  and  $A_{22}$  is  $(N - L) \times (N - L)$  we see that

$$\begin{aligned} \left( \Omega^* D_N^{-1} \Omega + \frac{1}{\gamma} D_x \right)^{-1} &= \begin{bmatrix} A_{11} + \frac{1}{\gamma} D_0 & A_{12} \\ A_{21} & A_{22} \end{bmatrix}^{-1} \\ &= \begin{bmatrix} P & Q \\ R & S \end{bmatrix} \end{aligned} \quad (54)$$

where  $P = \left( A_{11} + \frac{1}{\gamma} D_0 - A_{12} A_{22}^{-1} A_{21} \right)^{-1}$ ,  $Q = -P A_{12} A_{22}^{-1}$ ,  $R = -A_{22}^{-1} A_{21} P$ , and  $S = A_{22}^{-1} + A_{22}^{-1} A_{21} P A_{12} A_{22}^{-1}$ . Since the limit  $\lim_{\gamma \rightarrow 0} P = 0$  we see that

$$\lim_{\gamma \rightarrow 0} \left( \Omega^* D_N^{-1} \Omega + \frac{1}{\gamma} D_x \right)^{-1} = \begin{bmatrix} 0 & 0 \\ 0 & A_{22}^{-1} \end{bmatrix}. \quad (55)$$

Putting all the pieces together we obtain that

$$\Lambda_L(D_N) = D_N^{-1} - D_N^{-1} \cdot \mathbb{E} \left( \Omega \begin{bmatrix} 0 & 0 \\ 0 & A_{22}^{-1} \end{bmatrix} \Omega^* \right) \cdot D_N^{-1} \quad (56)$$

where  $\Omega$  is an isotropically distributed  $N \times N$  unitary matrix and

$$\Omega^* D_N^{-1} \Omega = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}. \quad (57)$$

Let us decompose the unitary matrix  $\Omega$  as  $\Omega = [\Omega_1 \ \Omega_2]$ , where  $\Omega_1$  is  $N \times L$  and  $\Omega_2$  is  $N \times (N - L)$  and both are isotropically distributed unitaries. Then  $\Omega_1^* \Omega_1 = I_L$  and  $\Omega_2^* \Omega_2 = I_{N-L}$ . It is an easy calculation to see that

$$\begin{aligned} \mathbb{E} \left( \Omega \begin{bmatrix} 0 & 0 \\ 0 & A_{22}^{-1} \end{bmatrix} \Omega^* \right) &= \mathbb{E} \left( \Omega_2 (\Omega_2^* D_N^{-1} \Omega_2)^{-1} \Omega_2^* \right) \\ &= \Lambda_{N-L} (D_N^{-1}). \end{aligned} \quad (58)$$

Therefore, using (56) and (58) we find the following functional equation

$$D_N \Lambda_L(D_N) + D_N^{-1} \Lambda_{N-L} (D_N^{-1}) = I_N. \quad (59)$$

*Remark 1:* Here we list a few results on  $\Lambda_L(D_N)$ .

- 1) If  $N = L$  then  $D_N \Lambda_N(D_N) = I_N$  and therefore  $\Lambda_N(D_N) = D_N^{-1}$ .

- 2) It is not difficult to see, and well-known result on random matrices, see [6], that  $\Lambda_L(I_N) = \frac{L}{N}I_N$ . Therefore

$$\Lambda_L(\alpha I_N) = \frac{L}{\alpha N}I_N. \quad (60)$$

Hence,

$$\alpha I_N \Lambda_L(\alpha I_N) + \alpha^{-1} I_N \Lambda_{N-L}(\alpha^{-1} I_N) = I_N$$

which agrees with (59).

- 3)  $\text{Tr}(D_N \Lambda_L(D_N)) = \text{Tr}(\mathbb{E}(D_N V^* (V D_N V^*)^{-1} V)) = L$  where in the last equality we used the trace property.

As we saw in (45) the other important term in  $\text{invcov}_L(D)$  is

$$\mathbb{E}(W^* (V D_N V^*)^{-1} W). \quad (61)$$

Let us define  $\mu > 0$  as

$$\mu := \text{Tr}[\mathbb{E}((V D_N V^*)^{-1})]. \quad (62)$$

Since  $V$  and  $W$  are Gaussian independent random matrices it is clear that

$$\begin{aligned} \mathbb{E}(W^* (V D_N V^*)^{-1} W) &= \text{Tr}[\mathbb{E}((V D_N V^*)^{-1})] I_{M-N} \\ &= \mu I_{M-N} \end{aligned} \quad (63)$$

where  $I_{M-N}$  is the identity matrix of dimension  $M-N$ . Putting all the pieces together we see that the estimate  $\text{invcov}_L(D)$  is equal to

$$\text{invcov}_L(D) = \text{diag}(\Lambda_L(D_N), \mu I_{M-N}). \quad (64)$$

## VI. CLOSED FORM EXPRESSION

In this section, we will prove an exact and closed form expression for the entries of  $\text{invcov}_L(D)$ . We will treat separately the entries of  $\Lambda_L(D_N)$  and the constant term  $\mu$ . As a matter of fact the analysis developed in this Section will allow us to obtain closed form expressions for more general averages.

Recall that we say a matrix  $A$  is said to be normal if it commutes with its conjugate transpose  $AA^* = A^*A$ . Given a normal matrix  $A$  and  $f : \mathbb{C} \rightarrow \mathbb{C}$  a continuous function we can always define  $f(A)$  using functional calculus. Being more precise, we know by the Spectral Theorem that there exists  $U$  unitary and  $D = \text{diag}(d_1, \dots, d_N)$  diagonal such that

$$A = U D U^*.$$

We then define

$$f(A) = U D_f U^*$$

where  $D_f = \text{diag}(f(d_1), \dots, f(d_N))$ . In particular, let  $D$  be as before and let  $f$  be a continuous function, we will obtain an exact expression for

$$\text{fcov}_L(D) := \mathbb{E}(\Phi^* f(\Phi D \Phi^*) \Phi) \quad (65)$$

where  $\Phi$  is an  $L \times N$  unitary isotropically random. Note that our covariance estimate  $\text{invcov}_L(D)$  is a particular case of the last expression when  $f(x) = x^{-1}$ .

Let  $\Omega_{L,N} = \{\Phi \in \mathbb{C}^{N \times L} : \Phi^* \Phi = I_L\}$  be the Stiefel manifold with the isotropic measure  $d\phi$ . By [3, eq. (18)], we know that

$$\int_{\Omega_{L,N}} s_\lambda(\Phi^* D_N \Phi) d\phi = \frac{s_\lambda(D_N) s_\lambda(I_L)}{s_\lambda(I_N)} \quad (66)$$

where  $s_\lambda$  is the Schur polynomial associated with the partition  $\lambda$ . The latter are explicitly defined for any  $N \times N$  matrix  $A$  in terms of the eigenvalues  $a_1, \dots, a_N$  as

$$s_\lambda(A) = s_\lambda(a_1, \dots, a_N) = \frac{\det(a_i^{N+\lambda_j-j})_{i,j=1}^N}{\det(a_i^{N-j})_{i,j=1}^N} \quad (67)$$

with  $\lambda$  being a partition, i.e., a nonincreasing sequence of non-negative integers  $\lambda_j$ . For an introduction to the theory of symmetric functions and properties of the Schur polynomials see [4] and [5].

Denote by  $(n-k, 1^k)$  the partition  $(n-k, 1, \dots, 1)$  with  $k$  ones. One of the properties of the Schur polynomials is that

$$\text{Tr}(A^n) = \sum_{k=0}^{N-1} (-1)^k s_{(n-k, 1^k)}(A). \quad (68)$$

Using (66) and (68) we see that

$$\int_{\Omega_{L,N}} \text{Tr}((\Phi^* D_N \Phi)^n) d\phi \quad (69)$$

is equal to

$$\sum_{k=0}^{L-1} (-1)^k \frac{s_{(n-k, 1^k)}(D_N) s_{(n-k, 1^k)}(I_L)}{s_{(n-k, 1^k)}(I_N)} \quad (70)$$

where the constant  $s_{(n-k, 1^k)}(I_p)$  is equal to  $\frac{(n+p-k-1)!}{k!(p-k-1)!(n-k-1)!n}$  (see [4]). Therefore

$$\frac{s_{(n-k, 1^k)}(I_L)}{s_{(n-k, 1^k)}(I_N)} = \frac{(n+L-(k+1))!}{(n+N-(k+1))!} \cdot \frac{(N-(k+1))!}{(L-(k+1))!}. \quad (71)$$

Given a diagonal matrix  $A = \text{diag}(a_1, a_2, \dots, a_n)$  we denote by  $\Delta(A)$  the Vandermonde matrix associated with the matrix  $A$ . This one is defined as

$$\Delta(A) := \begin{pmatrix} 1 & 1 & \dots & 1 \\ a_1 & a_2 & \dots & a_n \\ \vdots & \vdots & \ddots & \vdots \\ a_1^{n-1} & a_2^{n-1} & \dots & a_n^{n-1} \end{pmatrix}. \quad (72)$$

For each positive integer  $p$  consider the operator  $I^{(p)}$  defined in  $x^n$  by

$$I^{(p)}(x^n) = \frac{x^{n+p}}{(n+1) \dots (n+p)}.$$

This operator extends linearly and continuously to a well-defined linear operator  $I^{(p)} : C[0, r] \rightarrow C[0, r]$  where  $C[0, r]$  are the continuous functions in the interval  $[0, r]$ . Now we are ready to state the main theorem of this section.

*Theorem 1:* Let  $D_N$  be an  $N \times N$  diagonal matrix of rank  $N$ . For any continuous (complex or real valued) function  $f \in C[d_{\min}, d_{\max}]$

$$\int_{\Omega_{L,N}} \text{Tr}(f(\Phi^* D_N \Phi)) d\phi \quad (73)$$

is equal to

$$\sum_{k=0}^{L-1} \frac{(N - (k+1))!}{(L - (k+1))!} \cdot \frac{\det(G_k)}{\det(\Delta(D_N))} \quad (74)$$

where  $\Delta(D_N)$  is the Vandermonde matrix associated to  $D_N$  and  $G_k$  is the matrix defined by replacing the  $(k+1)$  row of the Vandermonde matrix  $\Delta(D_N)$ ,  $\{d_i^{N-(k+1)}\}_{i=1}^N$ , by the row

$$\left\{ I^{(N-L)} \left( x^{(L-(k+1))} f(x) \right) \Big|_{x=d_i} \right\}_{i=1}^N. \quad (75)$$

*Proof:* By linearity and continuity (polynomials are dense in the set of continuous functions) it is enough to prove (73) in the case  $f(x) = x^n$ . By (70) and (71) we know that

$$\int_{\Omega_{L,N}} \text{Tr}((\Phi^* D_N \Phi)^n) d\phi \quad (76)$$

is equal to

$$\sum_{k=0}^{L-1} (-1)^k c_k^{(N,L)} \cdot s_{(n-k,1^k)}(D_N) \quad (77)$$

where

$$c_k^{(N,L)} := \frac{(N - (k+1))!}{(L - (k+1))!} \cdot \frac{(n + L - (k+1))!}{(n + N - (k+1))!}. \quad (78)$$

By definition of the Schur polynomials (see [4])

$$s_{(n-k,1^k)}(D_N) = \frac{\det(S_k)}{\det(\Delta(D_N))} \quad (79)$$

where the  $i$ th-column of the matrix  $S_k$  is

$$\begin{pmatrix} d_i^{N-1+n-k} \\ d_i^{N-2+1} \\ d_i^{N-3+1} \\ \vdots \\ d_i^{N-(k+1)+1} \\ d_i^{N-(k+2)} \\ \vdots \\ d_i^{N-(N-1)} \\ 1 \end{pmatrix}.$$

Doing  $k$  row transpositions on the rows of the matrix  $S_k$  we obtain a new matrix  $\tilde{S}_k$  where the  $i$ th-column of this new matrix is

$$\begin{pmatrix} d_i^{N-1} \\ d_i^{N-2} \\ d_i^{N-3} \\ \vdots \\ d_i^{N-k} \\ d_i^{N+n-(k+1)} \\ d_i^{N-(k+2)} \\ \vdots \\ d_i^{N-(N-1)} \\ 1 \end{pmatrix}.$$

Note that this matrix  $\tilde{S}_k$  is identical to  $\Delta(D_N)$  except of the  $(k+1)$  row which was replaced by the row  $\{d_i^{N+n-(k+1)}\}_{i=1}^N$  instead of  $\{d_i^{N-(k+1)}\}_{i=1}^N$  as in  $\Delta(D_N)$ . Therefore

$$\int_{\Omega_{L,N}} \text{Tr}((\Phi^* D_N \Phi)^n) d\phi \quad (80)$$

is equal to

$$\sum_{k=0}^{L-1} c_k^{(N,L)} \cdot \frac{\det(\tilde{S}_k)}{\det(\Delta(D_N))}. \quad (81)$$

Using the fact that

$$I^{(N-L)} \left( x^{n+L-(k+1)} \right) \Big|_{x=d_i} = \frac{(n + L - (k+1))!}{(n + N - (k+1))!} d_i^{N+n-(k+1)} \quad (82)$$

we obtain that

$$G_k = \frac{(n + L - (k+1))!}{(n + N - (k+1))!} \cdot \tilde{S}_k. \quad (83)$$

Putting all the pieces together we obtain that

$$\int_{\Omega_{L,N}} \text{Tr}((\Phi^* D_N \Phi)^n) d\phi \quad (84)$$

is equal to

$$\sum_{k=0}^{L-1} \frac{(N - (k+1))!}{(L - (k+1))!} \cdot \frac{\det(G_k)}{\det(\Delta(D_N))}. \quad (85)$$

■

The next Proposition gives us, in particular, an exact and closed form expression for the term  $\mu$  in (62) discussed previously.

*Proposition 1:* Let  $D_N$  be an  $N \times N$  diagonal matrix of rank  $N$ . Let  $1 \leq L < N$  and  $Z$  be an  $N \times L$  Gaussian random



matrix with independent and identically distributed entries with zero mean and variance 1. Then

$$\int_{\Omega_{L,N}} \text{Tr}((\Phi^* D_N \Phi)^{-1}) d\phi = (N - L) \cdot \frac{\det(G)}{\det(\Delta(D_N))} \quad (86)$$

and

$$\mu := \mathbb{E}[\text{Tr}((Z^* D_N Z)^{-1})] = \frac{\det(G)}{\det(\Delta(D_N))} \quad (87)$$

where  $G$  is the matrix constructed by replacing the  $L$ th row of the Vandermonde matrix  $\Delta(D_N)$  by the row

$$(d_1^{N-(L+1)} \log(d_1), \dots, d_N^{N-(L+1)} \log(d_N)). \quad (88)$$

*Proof:* Let  $1 \leq L < N$  and let us consider  $f(x) = x^{-1}$  then for each  $0 \leq k \leq L - 2$  we see that

$$I^{(N-L)} \left( x^{L-(k+1)} x^{-1} \right) \Big|_{x=d_i} = \frac{d_i^{N-(k+2)}}{(L-k-1) \dots (N-k-2)} \quad (89)$$

since this is a multiple of the  $(k+2)$ th row of the Vandermonde matrix  $\Delta(D_N)$  we see that  $\det(G_k) = 0$  for all  $0 \leq k \leq L - 2$ .

It is not difficult to see that for  $k = L - 1$

$$I^{(N-L)}(x^{-1})|_{x=d_i} = \frac{d_i^{N-(L+1)} \log(d_i)}{(N - (L + 1))!}. \quad (90)$$

Therefore using Theorem 1 we see that

$$\int_{\Omega_{L,N}} \text{Tr}((\Phi^* D_N \Phi)^{-1}) d\phi = (N - L) \cdot \frac{\det(G)}{\det(\Delta(D_N))} \quad (91)$$

where  $G$  is constructed by replacing the  $L$ th row of the Vandermonde matrix by the row

$$(d_1^{N-(L+1)} \log(d_1), \dots, d_N^{N-(L+1)} \log(d_N)). \quad (92)$$

Now we will prove the second part of the Proposition. Given  $Z$  an  $N \times L$  random matrix as in the hypothesis we can decompose  $Z$  as

$$Z = \Phi C \quad (93)$$

where  $\Phi$  is an isotropically random  $N \times L$  unitary and  $C$  is a positive definite  $L \times L$  independent from  $\Phi$  (see [6, Sect. 2.1.5]). The matrix  $C$  is invertible with probability 1. Hence

$$(Z^* D_N Z)^{-1} = (C \Phi^* D_N \Phi C)^{-1} = C^{-1} (\Phi^* D_N \Phi)^{-1} C^{-1}. \quad (94)$$

Therefore

$$\begin{aligned} \mathbb{E}[\text{Tr}((Z^* D_N Z)^{-1})] &= \mathbb{E}[\text{Tr}(C^{-1} (\Phi^* D_N \Phi)^{-1} C^{-1})] \\ &= \mathbb{E}[\text{Tr}(C^{-2} (\Phi^* D_N \Phi)^{-1})] \end{aligned} \quad (95)$$

where in the second equality we used the trace property. Recall from random matrix theory that if  $A, B$  are independent  $n \times n$  random matrices then

$$\mathbb{E}[\text{Tr}(AB)] = \frac{1}{n} \mathbb{E}[\text{Tr}(A)] \mathbb{E}[\text{Tr}(B)]. \quad (96)$$

Since the matrix  $C$  is independent with respect to  $\Phi$  and  $D_N$  we conclude that

$$\mathbb{E}[\text{Tr}((Z^* D_N Z)^{-1})] \quad (97)$$

is equal to

$$\frac{1}{L} \mathbb{E}[\text{Tr}(C^{-2})] \mathbb{E}[\text{Tr}((\Phi^* D_N \Phi)^{-1})]. \quad (98)$$

Let  $D_N = I_N$  then  $(Z^* D_N Z)^{-1} = (Z^* Z)^{-1} = C^{-2}$  and it is known (see [6, Lemma 2.10]) that

$$\mathbb{E}[\text{Tr}(C^{-2})] = \frac{L}{N - L}. \quad (99)$$

Putting all the pieces together we see that

$$\mu := \mathbb{E}[\text{Tr}((Z^* D_N Z)^{-1})] = \frac{\det(G)}{\det(\Delta(D_N))} \quad (100)$$

finishing the proof.  $\blacksquare$

#### A. Application of the Main Results to $\text{cov}_L(D)$

Using Theorem 1 we can compute several averages over the Stiefel manifold. As an application let us compute

$$\text{cov}_L(D) = \int_{\Omega_{L,M}} \Phi(\Phi^* D \Phi) \Phi^* d\phi = \text{diag}(t_1, \dots, t_M). \quad (101)$$

The following is a useful result.

*Lemma 1:* Let  $f$  be a differentiable function in the interval  $[d_{\min}, d_{\max}]$  where  $d_{\min} = \min\{d_i\}$  and  $d_{\max} = \max\{d_i\}$ . Then the following formula holds:

$$\frac{\partial}{\partial d_k} \int_{\Omega_{L,N}} \text{Tr}(f(\Phi^* D_N \Phi)) d\phi \quad (102)$$

is equal to

$$\left[ \int_{\Omega_{L,N}} \Phi f'(\Phi^* D_N \Phi) \Phi^* d\phi \right]_{kk} \quad (103)$$

where  $A_{kk}$  means the  $(k, k)$  entry of the matrix  $A$ .

We will defer the proof of this Lemma to the next section where virtually the same proof gives us Lemma 2.

Let  $D$  an  $M \times M$  diagonal matrix of rank  $N$  and let  $L \leq N$ . By (101) and Lemma 1, we know that

$$t_k = \frac{1}{2} \cdot \frac{\partial}{\partial d_k} \int_{\Omega_{L,M}} \text{Tr}((\Phi^* D \Phi)^2) d\phi.$$

Since

$$\int_{\Omega_{L,M}} \text{Tr}((\Phi^* D \Phi)^2) d\phi = \frac{L}{M} \cdot \frac{L+1}{M+1} s_{(2,0)}(D) - \frac{L}{M} \cdot \frac{L-1}{M-1} s_{(1,1)}(D)$$

where

$$s_{(2,0)}(D) = \sum_{i=1}^M d_i^2 + \sum_{i < j} d_i d_j$$

and

$$s_{(1,1)}(D) = \sum_{i < j} d_i d_j.$$

Then

$$\frac{\partial s_{(2,0)}(D)}{\partial d_k} = \text{Tr}(D) + d_k \quad \text{and} \quad \frac{\partial s_{(1,1)}(D)}{\partial d_k} = \text{Tr}(D) - d_k.$$

Therefore  $t_k$  is equal to

$$\frac{1}{2} \cdot \frac{L}{M} \left[ \frac{L+1}{M+1} (d_k + \text{Tr}(D)) - \frac{L-1}{M-1} (\text{Tr}(D) - d_k) \right]$$

hence

$$t_k = \frac{L}{M} \left[ \frac{M-L}{M^2-1} \text{Tr}(D) + \frac{ML-1}{M^2-1} d_k \right].$$

Therefore

$$\begin{aligned} \text{cov}_L(D) &= \int_{\Omega_{L,M}} \Phi(\Phi^* D \Phi) \Phi^* d\phi \\ &= \frac{L}{M} \left[ \frac{M-L}{M^2-1} \text{Tr}(D) \cdot I_M + \frac{ML-1}{M^2-1} \cdot D \right]. \end{aligned}$$

### B. Application of the Main Results to $\text{invcov}_L(D)$

As aforementioned in the Introduction and subsequent sections, the problem we are mainly interested is to compute  $\text{invcov}_L(D)$  when  $D$  is an  $M \times M$  diagonal matrix of rank  $N$  and  $L \leq N$ . Let  $D = \text{diag}(D_N, 0_{M-N})$  where  $D_N = \text{diag}(d_1, \dots, d_N)$ . As we previously saw in (64), the matrix  $\text{invcov}_L(D)$  is diagonal and can be decomposed as

$$\text{invcov}_L(D) = \text{diag}(\Lambda_L(D_N), \mu I_{M-N})$$

where

$$\Lambda_L(D_N) = \int_{\Omega_{L,N}} \Phi(\Phi^* D_N \Phi)^{-1} \Phi^* d\phi = \text{diag}(\lambda_1, \dots, \lambda_N)$$

and

$$\mu = \text{Tr}[\mathbb{E}((Z^* D_N Z)^{-1})]$$

where the average is taken over the ensemble of all  $N \times L$  Gaussian random matrices  $Z$  with independent and complex entries with zero mean and unit variance.

Using Lemma 1 we see that

$$\lambda_k = \frac{\partial}{\partial d_k} \int_{\Omega_{L,N}} \text{Tr} \log(\Phi^* D_N \Phi) d\phi.$$

where

$$\int_{\Omega_{L,N}} \text{Tr} \log(\Phi^* D_N \Phi) d\phi$$

can be explicitly computed using Theorem 1. On the other hand, Proposition 1 gives us an explicit formula for  $\mu$ . Therefore, given  $D$  we obtained closed form expressions for all the entries of the matrix  $\text{invcov}_L(D)$  for every  $M, N$  and  $L$ .

### C. Small Dimension Example

In this subsection we will compute  $\text{invcov}_L(D)$  for a small dimensional example. Let  $M = 4$ ,  $N = 2$  and  $L = 1$  and  $D = \text{diag}(d_1, d_2, 0, 0)$ . Hence following our previous notation  $D_2 = \text{diag}(d_1, d_2)$ . Let us first consider the case  $d_1 = d_2 = d$ . In this case using (60) and (127) we see that

$$\text{invcov}_1(D) = \text{diag}(d^{-1}/2, d^{-1}/2, d^{-1}, d^{-1}).$$

The more interesting case is  $d_1 \neq d_2$ . Applying Theorem 1 and Lemma 1 we see that

$$\text{invcov}_1(D) = \text{diag}(\lambda_1, \lambda_2, \mu, \mu)$$

where

$$\begin{aligned} \lambda_i &= \frac{\partial}{\partial d_i} \int_{\Omega_{1,2}} \text{Tr} \log(\Phi^* D_2 \Phi) d\phi \\ &= \frac{\partial}{\partial d_i} \left( \frac{\det(H)}{\det(\Delta(D_2))} \right) \end{aligned}$$

where

$$\begin{aligned} \Delta(D_2) &= \begin{bmatrix} d_1 & d_2 \\ 1 & 1 \end{bmatrix} \\ &\text{and} \\ H &= \begin{bmatrix} d_1 \log d_1 - d_1 & d_2 \log d_2 - d_2 \\ 1 & 1 \end{bmatrix}. \end{aligned}$$

Doing the calculations we see that

$$\lambda_1 = \frac{d_2 \log d_2 - d_2 \log d_1 + d_1 - d_2}{(d_1 - d_2)^2} \quad (104)$$

$$\lambda_2 = \frac{d_1 \log d_1 - d_1 \log d_2 + d_2 - d_1}{(d_1 - d_2)^2}. \quad (105)$$

On the other hand using Proposition 1

$$\mu = \text{Tr}[\mathbb{E}((Z D_2 Z^*)^{-1})] = \frac{\det(G)}{\det(\Delta(D_2))}$$

where

$$G = \begin{bmatrix} \log d_1 & \log d_2 \\ 1 & 1 \end{bmatrix}.$$

Therefore,

$$\mu = \frac{\log d_1 - \log d_2}{d_1 - d_2}. \quad (106)$$

To summarize, computation of  $\text{invcov}$  is facilitated by first taking the eigenvector and eigenvalue decomposition of the sample covariance matrix and then applying  $\text{invcov}$  to the diagonal eigenvalue matrix. At that point there are three alternatives: a straight Monte Carlo expectation, the asymptotic expressions given in Section VIII, or the closed form analytical expressions according to Proposition 1 and Theorem 1.

## VII. PRELIMINARIES ON THE LIMIT OF LARGE RANDOM MATRICES

A random matrix is a measurable map  $Z$ , defined on some probability space  $(\Omega, P)$  and which takes values in a matrix algebra,  $M_n(\mathbb{C})$  say. In other words,  $Z$  is a matrix whose entries are (complex) random variables on  $(\Omega, P)$ . One often times identifies  $Z$  with the probability measure  $Z(P)$  it induces on  $M_n(\mathbb{C})$  and forgets about the underlying space  $(\Omega, P)$ . Random matrices appear in a variety of mathematical fields and in physics too. For a more complete and detailed discussion of random matrix limits and free probability see [21], [20], [18], [19], and [6]. Here we will review only some key points.

Let us consider a sequence  $\{A_N\}_{N \in \mathbb{N}}$  of self-adjoint  $N \times N$  random matrices  $A_N$ . In which sense can we talk about the limit of these matrices? It is evident that such a limit does not exist as an  $\infty \times \infty$  matrix and there is no convergence in the usual topologies. What converges and survives in the limit are the moments of the random matrices. Let  $A = (a_{ij}(\omega))_{i,j=1}^N$  where the entries  $a_{ij}$  are random variables on some probability space  $\Omega$  equipped with a probability measure  $P$ . Therefore

$$\mathbb{E}(\text{tr}_N(A_N)) := \frac{1}{N} \sum_{i=1}^N \int_{\Omega} a_{ii}(\omega) dP(\omega) \quad (107)$$

and we can talk about the  $k$ th moment  $\mathbb{E}(\text{tr}_N(A_N^k))$  of our random matrix  $A_N$ , and it is well known that for nice random matrix ensembles these moments converge for  $N \rightarrow \infty$ . So let us denote by  $\alpha_k$  the limit of the  $k$ th moment

$$\alpha_k := \lim_{N \rightarrow \infty} \mathbb{E}(\text{tr}_N(A_N^k)). \quad (108)$$

Thus we can say that the limit consists exactly of the collection of all these numbers  $\alpha_k$ . However, instead of talking about a collection of numbers we prefer to identify these numbers as moments of some random variable  $A$ . Now we can say that our random matrices  $A_N$  converge to a variable  $A$  in distribution (which just means that the moments of  $A_N$  converge to the moments of  $A$ ). We will denote this by  $A_N \rightarrow A$ .

One should note that for a self-adjoint  $N \times N$  matrix  $A = A^*$ , the collection of moments corresponds also to a probability measure  $\mu_A$  on the real line, determined by

$$\text{tr}_N(A^k) = \int_{\mathbb{R}} t^k d\mu_A(t). \quad (109)$$

This measure is given by the eigenvalue distribution of  $A$ , i.e., it puts mass  $\frac{1}{N}$  on each of the eigenvalues of  $A$  (counted with multiplicity)

$$\mu_A = \frac{1}{N} \sum_{i=1}^N \delta_{\lambda_i} \quad (110)$$

where  $\lambda_1, \dots, \lambda_N$  are the eigenvalues of  $A$ . In the same way, for a random matrix  $A$ ,  $\mu_A$  is given by the averaged eigenvalue distribution of  $A$ . Thus, moments of random matrices with respect to the averaged trace contain exactly that type of information in which one is usually interested when dealing with random matrices.

*Example 1:* Let us consider the basic example of random matrix theory. Let  $G_N$  be an  $N \times N$  self-adjoint random matrix whose upper-triangular entries are independent zero-mean random variables with variance  $\frac{1}{N}$  and fourth moments of order  $O(\frac{1}{N^2})$ . Then the famous Theorem of Wigner can be stated in our language as

$$G_N \rightarrow s, \text{ where } s \text{ is a semicircular random variable} \quad (111)$$

where semicircular just means that the measure  $\mu_s$  is given by the semicircular distribution (or, equivalently, the even moments of the variable  $s$  are given by the Catalan numbers).

*Example 2:* Another important example in random matrix theory is the Wishart ensemble. Let  $Z$  be an  $N \times K$  random matrix whose entries are independent zero-mean random variables with variance  $\frac{1}{N}$  and fourth moments of order  $O(\frac{1}{N^2})$ . As  $K, N \rightarrow \infty$  with  $\frac{K}{N} \rightarrow \beta$ ,

$$Z^* Z \rightarrow z_{\beta} \quad (112)$$

where  $z_{\beta}$  is a random variable with the Marcenko-Pastur law  $\mu_{\beta}$  with parameter  $\beta$ .

The empirical cumulative eigenvalue distribution function of an  $N \times N$  self-adjoint random matrix  $A$  is defined by the random function

$$F_A^N(\omega, x) := \frac{\#\{k : \lambda_k \leq x\}}{N}$$

where  $\lambda_k$  are the (random) eigenvalues of  $A(\omega)$  for each realization  $\omega$ . For each  $\omega$  this function determines a probability measure  $\mu_N(\omega)$  supported on the real line. These measures  $\{\mu_N(\omega)\}_{\omega}$  define a Borel measure  $\mu_N$  in the following way. Let  $B \subset \mathbb{R}$  be a Borel subset then

$$\mu_N(B) := \mathbb{E}(\mu_N(\omega)(B)).$$

A new and crucial concept, however, appears if we go over from the case of one variable to the case of more variables.

*Definition 1:* Consider  $N \times N$  random matrices  $A_N^{(1)}, \dots, A_N^{(m)}$  and variables  $A_1, \dots, A_m$  (living in some abstract algebra  $\mathcal{A}$  equipped with a state  $\varphi$ ). We say that

$$(A_N^{(1)}, \dots, A_N^{(m)}) \rightarrow (A_1, \dots, A_m)$$

in distribution if and only if

$$\lim_{N \rightarrow \infty} \mathbb{E} \left( \text{tr}_N \left( A_N^{(i_1)} \cdots A_N^{(i_k)} \right) \right) = \varphi \left( A^{(i_1)} \cdots A^{(i_k)} \right) \quad (113)$$

for all choices of  $k, 1 \leq i_1, \dots, i_k \leq m$ .

The  $A_1, \dots, A_m$  arising in the limit of random matrices are *a priori* abstract elements in some algebra  $\mathcal{A}$ , but it is good to know that in many cases they can also be concretely realized by some kind of creation and annihilation operators on a full Fock space. Indeed, free probability theory was introduced by Voiculescu for investigating the structure of special operator algebras generated by these type of operators. In the beginning, free probability had nothing to do with random matrices.

*Example 3:* Let us now consider the example of two independent Gaussian random matrices  $G_N^{(1)}, G_N^{(2)}$  (i.e., each of them is a self-adjoint Gaussian random matrix and all entries of  $G_N^{(1)}$  are independent from all entries of  $G_N^{(2)}$ ). Then one knows that all joint moments converge, and we can say that

$$(G_N^{(1)}, G_N^{(2)}) \rightarrow (s_1, s_2) \quad (114)$$

where Wigner's Theorem tells us that both  $s_1$  and  $s_2$  are semi-circular. The question is: What is the relation between  $s_1$  and  $s_2$ ? Does the independence between  $G_N^{(1)}$  and  $G_N^{(2)}$  survive in some form also in the limit? The answer is yes and is provided by a basic theorem of Voiculescu which says that  $s_1$  and  $s_2$  are free. For a formal definition of freeness and more results in free probability see [21], [20], [18], and [19].

## VIII. ASYMPTOTIC RESULTS

In practical application when the values of  $M$  and  $N$  are too large the expressions of the previous section could be difficult to evaluate and we need simpler mathematical formulas. It is for this reason that in this Section we will provide asymptotic results for the entries of  $\text{invcov}_L(D)$ . As we previously saw in (45)  $\text{invcov}_L(D)$  is equal to

$$\begin{bmatrix} \mathbb{E}(V^*(VD_NV^*)^{-1}V) & 0 \\ 0 & \mathbb{E}(W^*(VD_NV^*)^{-1}W) \end{bmatrix}$$

where  $D = \text{diag}(D_N, 0_{M-N})$  and  $D_N$  an  $N \times N$  diagonal matrix of full rank. Here, we will get asymptotic results for both terms  $\mathbb{E}(V^*(VD_NV^*)^{-1}V)$  and  $\mathbb{E}(W^*(VD_NV^*)^{-1}W)$  as  $N, L \rightarrow \infty$  with  $\lim_{N \rightarrow \infty} \frac{N}{L} = \beta$ .

Recall that  $\mu > 0$  was defined as

$$\mu = \text{Tr}[\mathbb{E}((VD_NV^*)^{-1})]. \quad (115)$$

As we already observed, if  $V$  and  $W$  are Gaussian independent random matrices then

$$\begin{aligned} \mathbb{E}(W^*(VD_NV^*)^{-1}W) &= \text{Tr}[\mathbb{E}((VD_NV^*)^{-1})]I_{M-N} \\ &= \mu I_{M-N}. \end{aligned} \quad (116)$$

Let us introduce the  $\eta$ -transform of an  $N \times N$  random matrix  $A$  as

$$\eta_A(\gamma) := \frac{1}{N} \text{Tr}[\mathbb{E}((1 + \gamma A)^{-1})] \quad \text{for } \gamma > 0. \quad (117)$$

Analogously, given  $\nu$  a probability measure on  $\mathbb{R}$  we can define the  $\eta$ -transform of  $\nu$  as

$$\eta_\nu(\gamma) = \int_{\mathbb{R}} \frac{1}{1 + \gamma t} d\nu(t). \quad (118)$$

It is not difficult to see that (see [6] for more details)

$$\lim_{\gamma \rightarrow \infty} \eta_\nu(\gamma) = \nu(\{0\}) \quad (119)$$

and

$$\lim_{\gamma \rightarrow \infty} \gamma \eta_\nu(\gamma) = \int_{\mathbb{R}} t^{-1} d\nu(t). \quad (120)$$

Consider  $D = (D_N)_{N \in \mathbb{N}}$  a collection of diagonal  $N \times N$  diagonal matrices such that  $D_N$  converge in distribution to a probability measure  $\nu$ , i.e., for all  $k \geq 0$

$$\lim_{N \rightarrow \infty} \frac{1}{N} \mathbb{E}(\text{Tr}(D_N^k)) = \int_0^\infty t^k d\nu(t). \quad (121)$$

Let  $(V_N)_{N \in \mathbb{N}}$  be a sequence of  $L \times N$  complex Gaussian random matrices with standard i.i.d. entries. Then by Theorem 2.39 in [6] we know that  $\frac{1}{L} V_N D_N V_N^*$  converges in distribution (moreover, almost surely) as  $N, L \rightarrow \infty$  with  $\lim_{N \rightarrow \infty} \frac{N}{L} = \beta$  to a probability distribution whose  $\eta$ -transform satisfies

$$\beta(1 - \eta_\nu(\gamma\eta)) = 1 - \eta(\gamma) \quad (122)$$

where  $\eta_\nu$  is the  $\eta$ -transform of the limit in distribution of  $D = (D_N)_{N \in \mathbb{N}}$ . Note that  $\lim_{\gamma \rightarrow \infty} \eta(\gamma) = 0$  and  $\lim_{\gamma \rightarrow \infty} \gamma\eta(\gamma) = \mu$ . Therefore, taking limit as  $\gamma$  goes to infinity on both sides of (122) we get

$$\eta_\nu(\mu) = \frac{\beta - 1}{\beta} \quad (123)$$

since by definition and the convergence in distribution for  $N$  sufficiently large we have that

$$\eta_\nu(\mu) \approx \frac{1}{N} \text{Tr}[\mathbb{E}(1 + \mu D_N)^{-1}] \quad (124)$$

$$\frac{N-L}{N} \approx \frac{\beta - 1}{\beta}. \quad (125)$$

The symbol  $\approx$  denotes that equality holds in the limit.

Using (123) and (124) we obtain

$$\frac{N-L}{N} \approx \frac{1}{N} \sum_{k=1}^N \frac{1}{1 + \mu d_k} \quad (126)$$

where  $D_N = \text{diag}(d_1, \dots, d_N)$ . Note that this equation implicitly and uniquely defines  $\mu > 0$ .

*Remark 2:*

1) If  $N = L$  then  $\mu = \infty$  (which is not surprising).

- 2) If  $d_1 = \dots = d_N = \alpha$  then  $\mu = \alpha^{-1} \text{Tr} \mathbb{E}((VV^*)^{-1})$ . Using [6, Lemma 2.10] we know that  $\text{Tr} \mathbb{E}((VV^*)^{-1}) = \frac{L}{N-L}$ . Therefore for this case

$$\mu = \frac{L}{\alpha(N-L)} \quad (127)$$

which agrees exactly (without the approximation) with (126).

Now we will compute the asymptotics of the other, and more complicated, term

$$\Lambda_L(D_N) = \mathbb{E}(V^*(VD_N V^*)^{-1}V) = \text{diag}(\lambda_1, \dots, \lambda_N).$$

*Lemma 2:* Let  $f$  be a differentiable function on the interval  $[d_{\min}, d_{\max}]$  where  $d_{\min} = \min\{d_i\}$  and  $d_{\max} = \max\{d_i\}$ . Then the following formula holds:

$$\frac{\partial}{\partial d_k} \mathbb{E}[\text{Tr}(f(VDV^*))] = \mathbb{E}[V^* f'(VDV^*) V]_{kk}. \quad (128)$$

*Proof:* It is enough to prove this Lemma for the case  $f$  is a polynomial and by linearity it is enough to prove it for the case  $f(x) = x^n$ . Let  $E_k$  be the  $N \times N$  matrix whose entries are all zero except the entry  $E_{kk}$  which is equal to 1. Note that  $\frac{\partial}{\partial d_k}(D) = E_k$ . If  $f(x) = x^n$  then  $f(VDV^*) = (VDV^*)^n$  and for each  $k$  it is easy to see that

$$\frac{\partial}{\partial d_k} (VDV^*)^n = \sum_{i=0}^{n-1} (VDV^*)^i V E_k V^* (VDV^*)^{n-(i+1)}.$$

Therefore

$$\begin{aligned} \text{Tr} \left( \frac{\partial}{\partial d_k} f(VDV^*) \right) &= n \text{Tr}(V E_k V^* (VDV^*)^{n-1}) \\ &= \text{Tr}(E_k V^* f'(VDV^*) V E_k) \\ &= (V^* f'(VDV^*) V)_{kk} \end{aligned}$$

where we use the trace property and the fact that  $E_k^2 = E_k$ . Taking expectation on both sides we finish the proof. ■

As a corollary we obtain the following.

*Corollary 1:* If

$$\Lambda_L(D_N) = \mathbb{E}(V^*(VD_N V^*)^{-1}V) = \text{diag}(\lambda_1, \dots, \lambda_N)$$

then  $\lambda_k = \frac{\partial}{\partial d_k} \mathbb{E}[\text{Tr} \log(VD_N V^*)]$ .

Before continuing let us define the Shannon transform of a probability distribution. Given  $\nu$  a probability distribution supported in  $\mathbb{R}$  we define

$$\vartheta_\nu(\gamma) = \int_{\mathbb{R}} \log(1 + \gamma t) d\nu.$$

It is easy to see that  $\lim_{\gamma \rightarrow \infty} \vartheta_\nu(\gamma) - \log(\gamma) = \int_{\mathbb{R}} \log(t) d\nu$ . Consider, as before,  $D = (D_N)_{N \in \mathbb{N}}$  a collection of diagonal  $N \times N$  diagonal matrices such that  $D_N$  converge in distribution to a probability measure  $\nu$ . Let  $(V_N)_{N \in \mathbb{N}}$  be a sequence of  $L \times N$  complex Gaussian random matrices with standard i.i.d. entries. Then by [6, eq. (2.167)] we know that  $\frac{1}{L} V_N D_N V_N^*$  converges in distribution (moreover, almost surely) as  $N, L \rightarrow$

$\infty$  with  $\lim_{N \rightarrow \infty} \frac{N}{L} = \beta$  to a probability distribution  $\eta_\beta$  whose Shannon-transform  $\vartheta$  satisfies

$$\vartheta(\gamma) = \beta \vartheta_\nu(\gamma \eta(\gamma)) - \log \eta(\gamma) + \eta(\gamma) - 1. \quad (129)$$

Subtracting  $\log(\gamma)$  on both sides and taking the limit  $\gamma \rightarrow \infty$  we obtain

$$\int_0^\infty \log(t) d\nu_\beta = \beta \vartheta_\nu(\mu) - \log(\mu) - 1. \quad (130)$$

For  $N$  and  $L$  sufficiently large

$$\int_0^\infty \log(t) d\nu_\beta = \lim_{L \rightarrow \infty} \frac{1}{L} \mathbb{E} \left[ \text{Tr} \log \left( \frac{1}{L} V_N D_N V_N^* \right) \right] \quad (131)$$

$$\approx \frac{1}{L} (\mathbb{E}[\text{Tr} \log(V_N D_N V_N^*)] - L \log(L))$$

$$\text{and} \quad \beta \vartheta_\nu(\mu) = \beta \lim_{N \rightarrow \infty} \frac{1}{N} \mathbb{E}[\text{Tr} \log(1 + \mu D_N)] \quad (132)$$

$$\approx \frac{\beta}{N} \sum_{k=1}^N \log(1 + \mu d_k).$$

Hence, for  $N$  sufficiently large

$$\mathbb{E}[\text{Tr} \log(V_N D_N V_N^*)] \approx \sum_{k=1}^N \log(1 + \mu d_k) + L \log \left( \frac{L}{e\mu} \right).$$

Taking partial derivatives on both sides with respect to  $d_k$  we obtain

$$\lambda_k \approx \frac{\partial \mu}{\partial d_k} \cdot \sum_{i=1}^N \frac{d_i}{1 + \mu d_i} + \frac{\mu}{1 + \mu d_k} - \frac{L}{\mu} \frac{\partial \mu}{\partial d_k}. \quad (133)$$

## IX. SIMULATIONS

In this section we present some of the simulations performed. Let  $\Sigma$  be a  $100 \times 100$  true covariance matrix with Toeplitz with entries  $\Sigma_{i,j} = \exp(-\frac{1}{3}|i-j|)$ . Assume we take  $N = 50$  measurements and we want recover  $\Sigma$  to the best of our knowledge. After performing the measurements we construct the sample covariance matrix  $K_x$ . In Fig. 1 we can see the eigenvalues of the true matrix, the eigenvalues of the sample covariance matrix (raw data) and the eigenvalues of the new matrix after performing the randomization to the sample covariance for different values of  $L$ . In other words we are comparing the eigenvalues of  $\Sigma$ ,  $K_x$  and of  $\text{invcov}_L(K_x)^{-1}$  for different values of  $L$ . Recall that  $\text{invcov}_L(K_x)$  is an estimate for  $\Sigma^{-1}$  and therefore  $\text{invcov}_L(K_x)^{-1}$  is an estimate for  $\Sigma$ . We also performed the same experiment for the case that the true covariance matrix is a multiple of the identity. This corresponds to the case in which the sensors are uncorrelated. See Fig. 2.

Let  $A$  be an  $N \times N$  matrix we define the Frobenius norm as  $\|A\|_F^2 = \frac{1}{N} \text{Tr}(A^* A)$ . In Figs. 3, 4, and 5 we compare the performance of our estimator with the more standard estimator of Ledoit and Wolf [7]. The experiment was performed with a  $60 \times 60$  true covariance matrix  $\Sigma$  with Toeplitz entries  $\Sigma_{i,j} = \exp(-\frac{1}{\beta}|i-j|)$  and  $N = 30$ . We compute the Frobenius norm

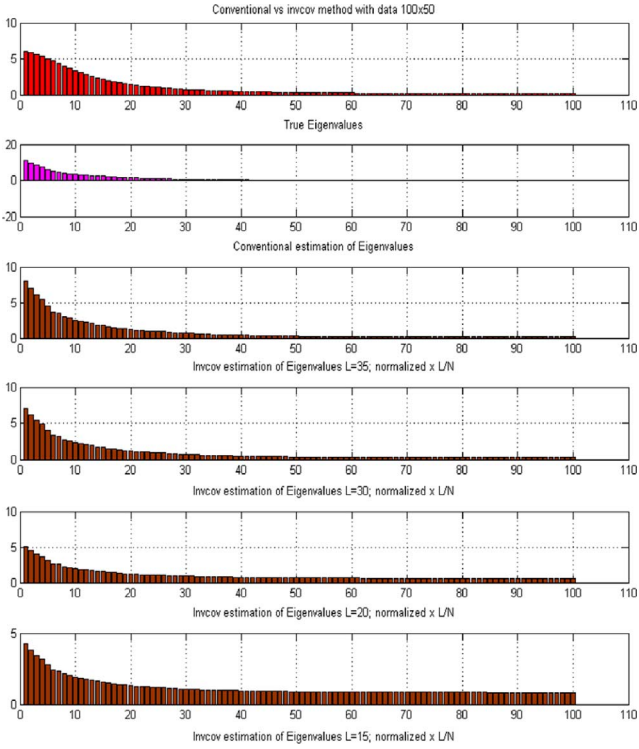


Fig. 1. Comparison of the eigenvalues of the true covariance matrix for an exponential correlation and the sample covariance matrix versus invcov estimate. The conventional eigenvalue estimate gives 50 eigenvalues that are precisely zero, which is not correct. Our invcov estimate is much closer to the actual eigenvalue distribution.

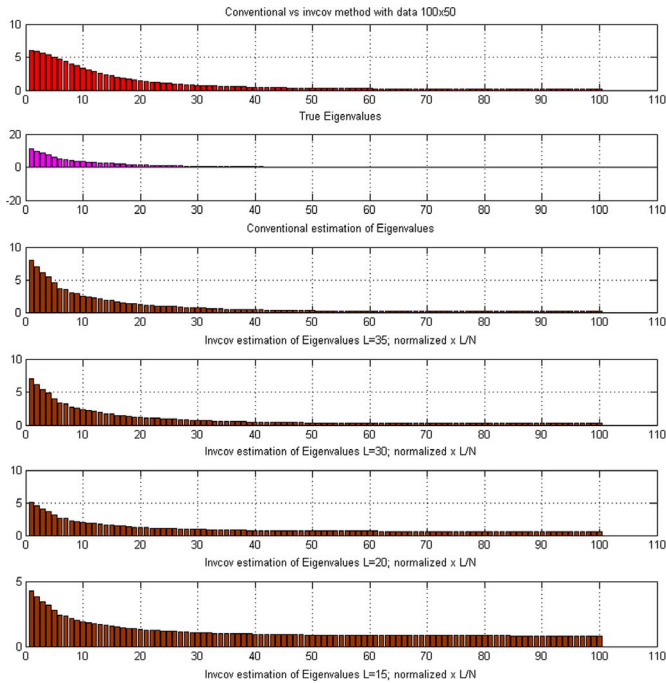


Fig. 2. Comparison of the eigenvalues of the true covariance matrix (the identity matrix) and sample covariance matrix versus invcov estimate.

$\|\Sigma - \text{invcov}_L(K_x)^{-1}\|_2$  for the different values of  $L$  and we compare it with  $\|\Sigma - K_{LW}\|_2$ . We use  $\beta = 10, 50$  and  $100$ . We can see that our method outperform Ledoit and Wolf for a big

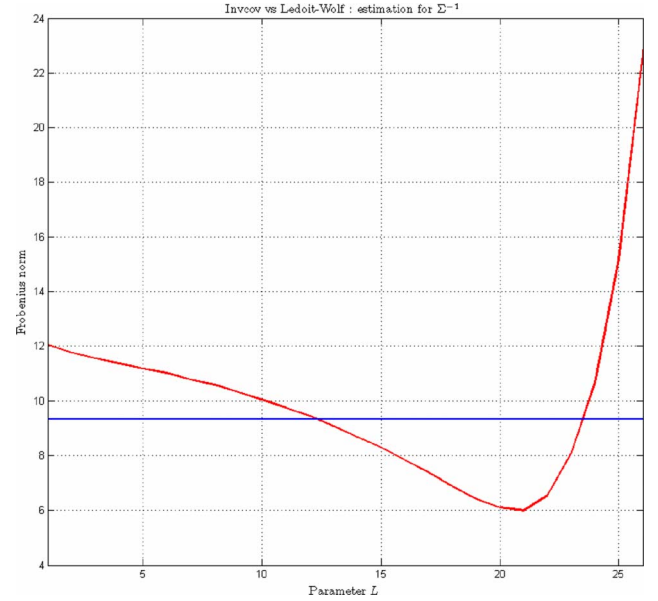


Fig. 3. Performance comparison with respect to Ledoit and Wolf for  $\beta = 10$ . The horizontal blue line is the performance of the LW estimate, our invcov estimate outperforms LW for  $L$  between 15 and 22.

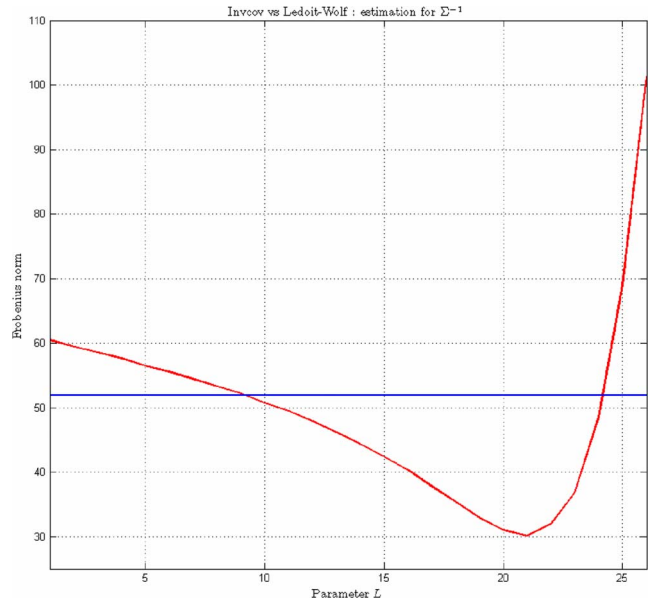


Fig. 4. Performance comparison with respect to Ledoit and Wolf for  $\beta = 50$ .

range of the parameter  $L$ . We also note that in the three cases  $L = 21$  is the optimum.

## X. COMMENTS

Our investigation indicates that the new method presented in this article is interesting and promising from the mathematical point of view, as well as the practical one. Even though we were able to find the asymptotic formulas as well as closed form expressions for  $\text{invcov}_L$ , and more generally for  $\text{fcov}_L$ , both estimates for  $\Sigma^{-1}$  and  $f(\Sigma)$ , there is a natural question still unanswered. How to find the optimum  $L$ ?

In many respects the problem of choosing  $L$  is analogous to the problem of choosing optimal diagonal loading parameters.

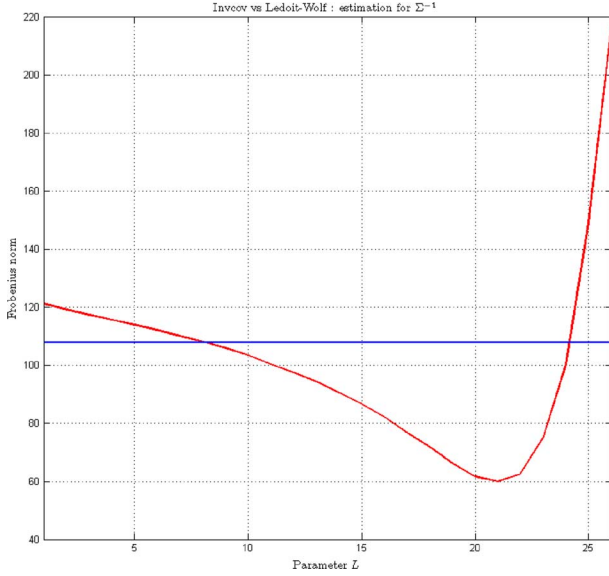


Fig. 5. Performance comparison with respect to Ledoit and Wolf for  $\beta = 100$ .

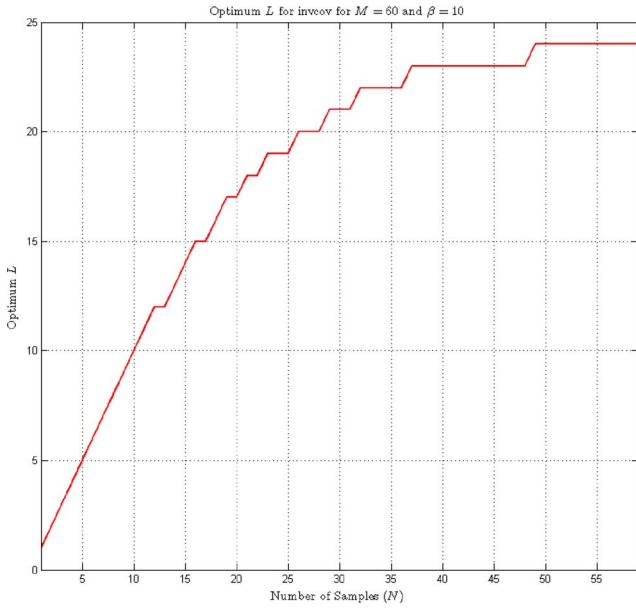


Fig. 6. Optimum  $L$  for  $\Sigma$  a Toeplitz matrix with  $\beta = 10$  and  $M = 60$ .

It is fair to say that, after many attempts by many researchers their is still no universally best way to choose the diagonally loading parameters. Nevertheless, our limited experience with using invcov does point towards some promising directions for selecting  $L$ . For instance, assume we know that the matrix  $\Sigma$  is an  $M \times M$  Toeplitz distributed with entries  $\Sigma_{i,j} = \exp(-\frac{1}{\beta}|i-j|)$  with unknown  $\beta$ . In the simulations presented in Section IX we see that for  $M = 60$ ,  $N = 30$  the optimum  $L$  is equal to 21 and it seems to be independent of the value of  $\beta$ . In Fig. 6 we computed for fixed  $M = 60$  and  $\beta = 10$  the optimum  $L$  as a function of the number of samples  $N$  (training data). As we can see the behavior of the optimum  $L$  is nontrivial.

In the application of invcov to the linear estimation problem it was noted that the error covariance expression for the estimator based on a single dimensionality-reducing matrix (18) is

a product of a term which decreases with increasing  $L$  and a term which increases with increasing  $L$ . Further investigations are needed to quantify this trade-off. A similar trade-off for the Capon spectral estimator was noted [2]. At present, however, we have no comprehensive algorithm for selecting  $L$ , and we believe that the problem merits further research.

## APPENDIX I

### AVERAGE OVER THE PERMUTATION MATRICES

In this Appendix we study what happen if we substitute the average over the isotropically random unitary matrices by the set of permutation matrices. Let  $D$  be an  $N \times N$  diagonal matrix with  $D = \text{diag}(d_1, \dots, d_N)$  and  $L \leq N$ . We will denote  $e_p$  the orthonormal vector  $1 \times N$  in  $\mathbb{C}^N$  whose entries are zero except at the  $p$ th-coordinate that is 1. A permutation matrix is a  $L \times N$  matrix of the form

$$\Phi = \begin{pmatrix} e_{p_1} \\ e_{p_2} \\ \vdots \\ e_{p_L} \end{pmatrix} \quad \text{where } p_i \neq p_j \text{ for } i \neq j.$$

*Theorem 2:* Let  $D$  be a diagonal matrix as before. Then

$$\mathbb{E}[\Phi^*(\Phi D \Phi^*)^{-1} \Phi : \Phi \text{ } L \times N \text{ permutation}] = \frac{L}{N} D^{-1}.$$

*Proof:* We will first show that

$$\Phi D \Phi^* = \text{diag}(d_{p_1}, d_{p_2}, \dots, d_{p_L}).$$

Given  $1 \leq p \leq N$  then  $e_p \cdot D = d_p e_p$ . Therefore

$$\begin{aligned} \Phi D \Phi^* &= \begin{pmatrix} d_{p_1} e_{p_1} \\ d_{p_2} e_{p_2} \\ \vdots \\ d_{p_L} e_{p_L} \end{pmatrix} (e_{p_1}^T \quad e_{p_2}^T \quad \dots \quad e_{p_L}^T) \\ &= \text{diag}(d_{p_1}, d_{p_2}, \dots, d_{p_L}). \end{aligned}$$

Hence

$$(\Phi D \Phi^*)^{-1} = \text{diag}(d_{p_1}^{-1}, d_{p_2}^{-1}, \dots, d_{p_L}^{-1}).$$

Thus

$$\Phi^*(\Phi D \Phi^*)^{-1} \Phi = \sum_{i=1}^L d_{p_i}^{-1} e_{p_i}^T e_{p_i}. \quad (134)$$

Note that  $E_p := e_p^T e_p$  is the matrix that has all entries zero except at the  $(p, p)$  entry which is 1. The total number of different permutation matrices is  $\frac{N!}{(N-L)!}$ . Therefore

$$\mathbb{E}[\Phi^*(\Phi D \Phi^*)^{-1} \Phi] = \frac{(N-L)!}{N!} \cdot \sum_{(p_1, \dots, p_L)} \left[ \sum_{i=1}^L d_{p_i}^{-1} E_{p_i} \right]$$

where the first sum is running over all the possible permutation matrices. The number of permutation matrices that have  $e_p$  as one of their rows is  $\frac{(N-1)!L!}{(L-1)!(N-L)!}$ . Hence

$$\begin{aligned} \mathbb{E}[\Phi^*(\Phi D \Phi^*)^{-1} \Phi] &= \frac{(N-L)!}{N!} \frac{(N-1)!L!}{(L-1)!(N-L)!} \cdot D^{-1} \\ &= \frac{L}{N} D^{-1}. \end{aligned}$$

■

#### ACKNOWLEDGMENT

The authors would like to thank T. Bengtsson and Y. Baryshnikov for many helpful discussions and comments.

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