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# OPTIMAL SHRINKAGE OF EIGENVALUES IN THE SPIKED COVARIANCE MODEL[1]

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*To the memory of Charles M. Stein, 1920–2016*

We show that in a common high-dimensional covariance model, the choice of loss function has a profound effect on optimal estimation.

In an asymptotic framework based on the spiked covariance model and use of orthogonally invariant estimators, we show that optimal estimation of the population covariance matrix boils down to design of an optimal shrinker $\eta$ that acts elementwise on the sample eigenvalues. Indeed, to each loss function there corresponds a unique admissible eigenvalue shrinker $\eta^*$ dominating all other shrinkers. The shape of the optimal shrinker is determined by the choice of loss function and, crucially, by inconsistency of both eigenvalues *and* eigenvectors of the sample covariance matrix.

Details of these phenomena and closed form formulas for the optimal eigenvalue shrinkers are worked out for a menagerie of 26 loss functions for covariance estimation found in the literature, including the Stein, Entropy, Divergence, Fréchet, Bhattacharya/Matusita, Frobenius Norm, Operator Norm, Nuclear Norm and Condition Number losses.

**1. Introduction.** Suppose we observe $p$-dimensional Gaussian vectors $X_i \overset{\text{i.i.d.}}{\sim} \mathcal{N}(0, \Sigma_p)$, $i = 1, \dots, n$, with $\Sigma = \Sigma_p$ the underlying $p$-by-$p$ population covariance matrix. To estimate $\Sigma$, we form the empirical (sample) covariance matrix $S = S_{n,p} = n^{-1} \sum_{i=1}^n X_i X_i'$; this is the maximum likelihood estimator. Stein [64, 65] observed that the maximum likelihood estimator $S$ ought to be improvable by eigenvalue shrinkage.

Write $S = V \Lambda V'$ for the eigendecomposition of $S$, where $V$ is orthogonal and the diagonal matrix $\Lambda = \mathrm{diag}(\lambda_1, \dots, \lambda_p)$ contains the empirical eigenvalues. Stein [65] proposed to shrink the eigenvalues by applying a specific nonlinear mapping $\varphi$ producing the estimate $\hat{\Sigma}_\varphi = V \boldsymbol{\varphi}(\Lambda) V'$, where $\varphi$ maps the space of positive diagonal matrices onto itself. In the ensuing half century, research on eigenvalue shrinkers has flourished, producing an extensive literature. We can point here only

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to a fraction, with pointers organized into early decades [7, 20, 29–31, 34], the middle decades [13, 28, 39, 40, 42, 49, 50, 57, 62, 63, 70] and the last decade [11, 12, 22, 23, 32, 44–46, 66, 69]. Such papers typically choose some loss function $L_p : S_p^+ \times S_p^+ \to [0, \infty)$, where $S_p^+$ is the space of positive semidefinite $p$-by-$p$ matrices, and develop a shrinker $\varphi$ with "favorable" risk $\mathbb{E}L_p(\Sigma, \hat{\Sigma}_\varphi(S))$.

In high-dimensional problems, $p$ and $n$ are often of comparable magnitude. There, the maximum likelihood estimator is no longer a reasonable choice for covariance estimation and the need to shrink becomes acute.

In this paper, we consider a popular large $n$, large $p$ setting with $p$ comparable to $n$, and a set of assumptions about $\Sigma$ known as the *Spiked Covariance Model* [35]. We study a variety of loss functions derived from or inspired by the literature, and *scalar* nonlinearities which act separably on the individual empirical eigenvalues. We show that to each "reasonable" nonlinearity $\eta$ there corresponds a well-defined asymptotic loss.

In the sibling problem of matrix denoising under a similar setting, it has been shown that there exists a unique asymptotically admissible shrinker [25, 61]. The same phenomenon is shown to exist here: for many different loss functions, we show that there exists a *unique optimal nonlinearity* $\eta^*$, which we explicitly provide. Perhaps surprisingly, $\eta^*$ is the only asymptotically admissible nonlinearity, namely, it offers equal or better asymptotic loss than that of any other choice of $\eta$, across all possible spiked covariance models.

1.1. *Estimation in the spiked covariance model.* Consider a sequence of covariance estimation problems, satisfying two basic assumptions.

**[ASY($\gamma$)]** The number of observations $n$ and the number of variables $p_n$ in the $n$th problem follows the proportional-growth limit $p_n/n \to \gamma$, as $n \to \infty$, for a certain $0 < \gamma \leq 1$.

Denote the population and sample covariances in the $n$th problem by $\Sigma = \Sigma_{p_n}$ and $S = S_{n,p_n}$ and assume that the eigenvalues $\ell_i$ of $\Sigma_{p_n}$ satisfy:

**[SPIKE($\ell_1, \dots, \ell_r$)]** The $r$ "spikes" $\ell_1 > \cdots > \ell_r \geq 1$ are fixed independently of $n$ and $p_n$, and $\ell_{r+1} = \cdots = \ell_{p_n} = 1$.

The spiked model exhibits three important phenomena, not seen in classical fixed-$p$ asymptotics, that play an essential role in the construction of optimal estimators. Drawing on results from [2–4, 6, 51, 59], we highlight:

(a) *Eigenvalue spreading.* Consider model [ASY($\gamma$)] in the null case $\ell_1 = \cdots = \ell_r = 1$. The empirical distribution of the sample eigenvalues $\lambda_{1n}, \dots, \lambda_{pn}$ converges as $n \to \infty$ to a nondegenerate absolutely continuous distribution, the Marchenko–Pastur or "quarter-circle" law [51]. The distribution, or "bulk", is supported on a single interval, whose limiting "bulk edges" are given by

$$\lambda_\pm(\gamma) = (1 \pm \sqrt{\gamma})^2. \tag{1.1}$$

(b) *Top eigenvalue bias.* Consider models [ASY($\gamma$)] and [SPIKE($\ell_1, \dots, \ell_r$)]. For $i = 1, \dots, r$, the leading sample eigenvalues satisfy

$$\lambda_{in} \xrightarrow{\text{a.s.}} \lambda(\ell_i), \tag{1.2}$$

where the "biasing" function

$$\lambda(\ell) = \ell + \gamma\ell/(\ell - 1), \qquad \ell \geq \ell_+(\gamma), \tag{1.3}$$

and $\lambda(\ell) \equiv (1 + \sqrt{\gamma})^2 = \lambda_+(\gamma)$ for $\ell \leq \ell_+(\gamma)$, the *Baik–Ben Arous–Péché transition point*

$$\ell_+(\gamma) = 1 + \sqrt{\gamma}. \tag{1.4}$$

Thus the empirical eigenvalues $\lambda_i$ are shifted upwards from their theoretical counterparts $\ell_i$ by an asymptotically predictable amount, of a size that exceeds $\gamma$ even for very large signal strengths $\ell_i$.

(c) *Top eigenvector inconsistency.* Again consider models [ASY($\gamma$)] and [SPIKE($\ell_1, \dots, \ell_r$)], noting that $\ell_1 > \cdots > \ell_r$ are distinct. The angles between the sample eigenvectors $v_{1n}, \dots, v_{pn}$, and the corresponding "true" population eigenvectors $u_{1n}, \dots, u_{pn}$ have nonzero limits:

$$\left|\langle u_{in}, v_{jn}\rangle\right| \xrightarrow{\text{a.s.}} \delta_{i,j} \cdot c(\ell_i), \qquad 1 \leq i, j \leq r, \tag{1.5}$$

where the cosine function is given by

$$c(\ell) = \sqrt{\frac{1 - \gamma/(\ell - 1)^2}{1 + \gamma/(\ell - 1)}}, \qquad \ell \geq \ell_+(\gamma), \tag{1.6}$$

and $c(\ell) = 0$ for $\ell \leq \ell_+(\gamma)$.

*Loss functions and optimal estimation.* Now consider a class of estimators for the population covariance $\Sigma$, based on *individual* shrinkage of the sample eigenvalues. Specifically,

$$\hat{\Sigma} = \hat{\Sigma}_\eta = \eta(\lambda_1)v_1v_1' + \cdots + \eta(\lambda_p)v_pv_p', \tag{1.7}$$

where $v_i$ is the sample eigenvector with sample eigenvalue $\lambda_i$ and $\eta(\lambda)$ is a *scalar nonlinearity*, $\eta : \mathbb{R}^+ \to [1, \infty)$, so that the *same* function acts on each sample eigenvalue. While this at first seems to be a significant limitation compared to Stein's apparently more general use of matricial functions $\varphi$ [65], the discussion in Section 8 shows that nothing is lost in our setting by the restriction to scalar shrinkers.

Consider a family of loss functions $L = \{L_p\}_{p=1}^\infty$ and a fixed nonlinearity $\eta : [0, \infty) \to \mathbb{R}$. Define the asymptotic loss relative to $L$ of the shrinkage estimator $\hat{\Sigma}_\eta$ in model [SPIKE($\ell_1, \dots, \ell_r$)] by

$$L_\infty(\ell_1, \dots, \ell_r|\eta) = \lim_{n\to\infty} L_{p_n}\bigl(\Sigma_{p_n}, \hat{\Sigma}_\eta(S_{n,p_n})\bigr), \tag{1.8}$$

assuming such limit exists. If a nonlinearity $\eta^*$ satisfies

$$L_\infty(\ell_1, \dots, \ell_r | \eta^*) \leq L_\infty(\ell_1, \dots, \ell_r | \eta) \tag{1.9}$$

for any other nonlinearity $\eta$, any $r$ and any spikes $\ell_1, \dots, \ell_r$, and if for any $\eta$ the inequality is strict at some choice of $\ell_1, \dots, \ell_r$, then we say that $\eta^*$ is the *unique asymptotically admissible* nonlinearity (nicknamed "optimal") for the loss sequence $L$.

In constructing estimators, it is natural to expect that the effect of the biasing function $\lambda(\ell)$ in (1.3) might be undone simply by applying its inverse function $\ell(\lambda)$, given by

$$\ell(\lambda) = \frac{(\lambda + 1 - \gamma) + \sqrt{(\lambda + 1 - \gamma)^2 - 4\lambda}}{2}, \qquad \lambda > \lambda_+(\gamma). \tag{1.10}$$

However, eigenvector inconsistency makes the situation more complicated (and interesting), as we illustrate using Figure 1. Focus on the plane spanned by $u_1$, the top population eigenvector, and by $v_1$, its sample counterpart. We represent $\ell_1 u_1 u_1'$, the top rank one component of $\Sigma$, by the vector $\ell_1 u_1$. The corresponding top rank one component of $S$ is $\lambda_1 v_1 v_1'$, represented by $\lambda_1 v_1$. If we apply the inverse function (1.10) to $\lambda_1$, we obtain $\ell(\lambda_1) v_1 v_1'$. Since $v_1$ is not collinear with $u_1$, there is a nonvanishing error $\ell(\lambda_1) v_1 v_1' - \ell_1 u_1 u_1'$ that remains, even though $\ell(\lambda_1) - \ell_1 = O_p(n^{-1/2})$. As the picture suggests, it is quite possible that a different amount of shrinkage, $\eta(\lambda_1) v_1 v_1'$ will lead to smaller error. However, we will see that *the optimal choice of $\eta$ depends greatly on the particular error measure $L_p(\Sigma, \hat{\Sigma})$ that is chosen.*

To give the flavor of results to be developed systematically later, we now look at four error measures in common use. The first three, based on the operator, Frobe-

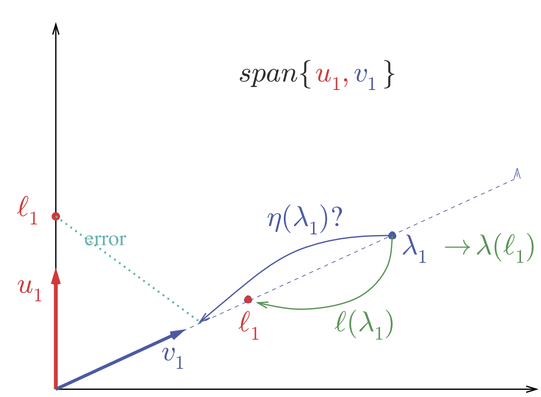


FIG. 1. *Shrinking empirical eigenvalue $\lambda_1$ to a value $\eta(\lambda_1)$ that is smaller than the inverse function $\ell(\lambda_1)$ may reduce the error of estimation.*

nius and nuclear norms, use the singular values $\sigma_j$ of $\hat{\Sigma} - \Sigma$:

$$
\begin{aligned}
L^O(\Sigma, \hat{\Sigma}) &= \|\hat{\Sigma} - \Sigma\|_\infty = \max_i \sigma_i, \\
L^F(\Sigma, \hat{\Sigma}) &= \|\hat{\Sigma} - \Sigma\|_2 = \Big(\sum_i \sigma_i^2\Big)^{1/2}, \\
L^N(\Sigma, \hat{\Sigma}) &= \|\hat{\Sigma} - \Sigma\|_1 = \sum_i \sigma_i, \\
L^{\mathrm{st}}(\Sigma, \hat{\Sigma}) &= \operatorname{tr}(\Sigma^{-1}\hat{\Sigma} - I) - \log\det(\Sigma^{-1}\hat{\Sigma}).
\end{aligned}
\tag{1.11}
$$

The fourth is Stein's loss, widely studied in covariance estimation [13, 38, 64].

For convenience, we begin with the single spike model SPIKE($\ell$), so that $\Sigma = \Sigma_\ell = I + (\ell - 1)u_1 u_1'$. When $\eta$ is continuous, the losses have a deterministic asymptotic limit $L_\infty(\ell|\eta)$ defined in (1.8).

For many losses, including (1.11), this deterministic limiting loss has a simple form, and we can evaluate, often analytically, the optimal shrinkage function, namely the shrinkage function satisfying (1.9). For example, writing $\eta^*(\lambda) = \eta_*(\ell(\lambda))$, for the four popular loss functions (1.11) we find that on $\ell > 1 + \sqrt{\gamma}$ the corresponding four optimal shrinkers are

$$
\begin{aligned}
&\eta_*^O(\ell) = \ell, \qquad \eta_*^F(\ell) = \ell c^2 + s^2, \\
&\eta_*^N(\ell) = \max\big(1 + (\ell - 1)(1 - 2s^2), 1\big), \qquad \eta_*^{\mathrm{St}}(\ell) = \ell/\big(c^2 + \ell s^2\big),
\end{aligned}
\tag{1.12}
$$

where $s^2 = 1 - c^2$. Figure 2 shows these four optimal shrinkers as a function of the sample eigenvalue $\lambda$. These are just four examples; The full list of optimal shrinkers we discover in this paper appears in Table 2. In all cases, $\eta_*(\ell) \equiv 1$ for $\ell \le 1 + \sqrt{\gamma}$. Figure 3 in Section 6 below shows all the full list of optimal shrinkers when $\gamma = 1$.

The main conclusion is that the *optimal shrinkage function depends strongly on the loss function* chosen. The operator norm shrinker $\eta_*^O$ simply inverts the biasing function $\lambda(\ell)$, while the other functions shrink by much larger, and very different, amounts, with $\eta_*^{\mathrm{St}}$ typically shrinking most. There are also important qualitative differences in the optimal shrinkers: $\eta_*^O$ is discontinuous at the bulk edge $\lambda = \lambda_+(\gamma)$. The others are continuous, but $\eta_*^N$ has the additional feature that it shrinks a *neighborhood* of the bulk to 1.

REMARK. The optimal shrinker also depends on $\gamma$, so we might write $\eta^*(\lambda, \gamma)$. In model [ASY($\gamma$)], one can use the same $\gamma$ for each problem size $n$. Alternatively, in the $n$th problem, one might use $\gamma_n = p_n/n$. The former choice is simpler, as $\eta^*$ can be regarded as a univariate function of $\lambda$, and so we make it in Sections 1–6. The latter choice is preferable technically, and perhaps also in practice, when one has $p$ and $n$, but not $\gamma$. It does, however, require us to treat $\eta(\lambda, c)$ as a bivariate function; see Section 7.

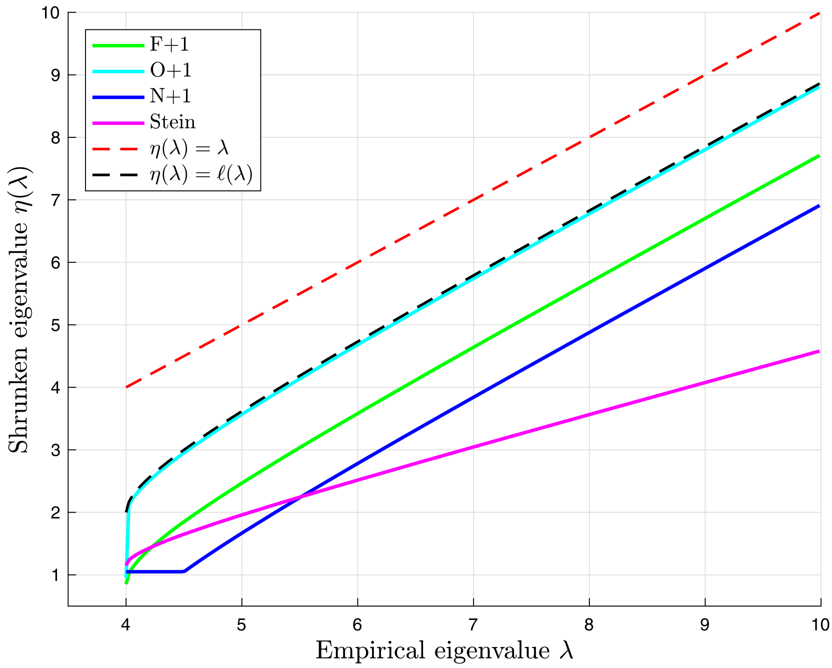


FIG. 2. *Vertical axis: optimal shrinkers $\eta_*$ from* (1.12), *shown as functions $\eta_*(\ell(\lambda))$ of the empirical eigenvalue $\lambda$, horizontal axis. Here, $\gamma = \lim p_n/n = 1$, so $\lambda_+(\gamma) = 4$. (Color online.) The $+1$ in the legend* F + 1 *etc. refers to a naming convention*, *Table* 1.

1.2. *Some key observations*. The sections to follow construct a framework for evaluating and optimizing the asymptotic loss (1.8). We highlight here some observations that will play an important role. Beforehand, let us introduce a useful modification of (1.7) to a *rank-aware* shrinkage rule:

$$\hat{\Sigma}_{\eta,r} = \sum_{i=1}^{r} \eta(\lambda_i) v_i v_i' + \sum_{i=r+1}^{p} v_i v_i', \tag{1.13}$$

where the dimension $r$ of the spiked model is taken as known. While our main results concern estimators $\hat{\Sigma}_\eta$ that naturally do not require $r$ to be known in advance, it will be easier conceptually and technically to analyze rank-aware shrinkage rules as a preliminary step.

[OBS. 1] *Simultaneous block diagonalization.* (Lemmas 1 and 5). There exists a (random) basis $W$ such that

$$W' \Sigma W = \left( \bigoplus_i A_i \right) \oplus I_{p-2r},$$

$$W' \hat{\Sigma}_{\eta,r} W = \left( \bigoplus_i B_i \right) \oplus I_{p-2r},$$

where $A_i$ and $B_i$ are square blocks of equal size $d_i$, and $\sum d_i = 2r$. (Here, and below, $A \oplus B$ denotes a block-diagonal matrix with blocks $A$ and $B$).

[OBS. 2] *Decomposable loss functions.* The loss functions (1.11) and many others studied below satisfy either

$$L_p(\Sigma, \hat{\Sigma}_{\eta,r}) = \sum_i L_{d_i}(A_i, B_i)$$

or the corresponding equality with *sum* replaced by *max*.

[OBS. 3] *Asymptotic deterministic loss.* (Lemmas 3 and 7). For rank-aware estimators, when $\eta$ and $L$ are suitably continuous, almost surely

$$L_\infty(\ell_1, \dots, \ell_r|\eta) = \lim_{p\to\infty} L_p(\Sigma, \hat{\Sigma}_{\eta,r}).$$

[OBS. 4] *Asymptotic equivalence of losses.* (Proposition 2). Conclusions derived for rank-aware estimators (1.13) carry over to the original estimators (1.7) because, under suitable conditions

$$L_p(\Sigma, \hat{\Sigma}_\eta) - L_p(\Sigma, \hat{\Sigma}_{\eta,r}) \xrightarrow{P} 0.$$

This relies on the fact that in the [SPIKE($\ell_1, \dots, \ell_r$)] model, the sample noise eigenvalues $\lambda_{in}$, $i \geq r+1$ "stick to the bulk" in an appropriate sense.

1.3. *Organization of the paper.* For simplicity of exposition, we assume a single spike, $r = 1$, in the first half of the paper. [OBS. 1], [OBS. 2] and [OBS. 3] are developed respectively in Sections 2, 3 and 4, arriving at an explicit formula for the asymptotic loss of a shrinker. Section 5 illustrates the assumptions with our list of 26 decomposable matrix loss functions. In Section 6, we use the formula to characterize the asymptotically unique admissible nonlinearity for any decomposable loss, provide an algorithm for computing the optimal nonlinearity and provide analytical formulas for many of the 26 losses. Section 7 extends the results to the general case where $r > 1$ spikes are present. We develop [OBS. 4], remove the rank-aware assumption and explore some new phenomena that arise in cases where the optimal shrinker turns out to be discontinuous. In Section 8, we show, at least for Frobenius and Stein losses, that our optimal univariate shrinkage estimator, which applies the same scalar function to each sample eigenvalue, in fact asymptotically matches the performance of the best *orthogonally-equivariant* covariance estimator under assumption [SPIKE($\ell_1, \dots, \ell_r$)]. Section 9 extends to the more general spiked model with $\Sigma_p = \mathrm{diag}(\ell_1, \dots, \ell_r, \sigma^2, \dots, \sigma^2)$ for $\sigma > 0$ known or unknown. Section 10 discusses our results in light of the high-dimensional covariance estimation work of El Karoui [22] and Ledoit and Wolf [46]. Some proofs and calculations are deferred to the supplementary article [15], where we also evaluate and document the strong signal (large-$\ell$) asymptotics of the optimal shrinkage estimators, and the asymptotic percent improvement over naive hard thresholding of the sample covariance eigenvalues. Additional technical details and software are provided in the Code Supplement available online as a permanent URL from the Stanford Digital Repository [16].

**2. Simultaneous block-diagonalization.** We first develop [OBS. 1] in the simplest case, $r = 1$, assuming a rank-aware shrinker. In general, the estimator $\hat{\Sigma}_\eta$ and estimand $\Sigma$ are not simultaneously diagonalizable. However, in the particular case that both are rank-one perturbations of the identity, we will see that simultaneous block diagonalization is possible.

Some notation is needed. We denote the eigenvalues and eigenvectors of the spectral decompostion $S_{n,p_n} = V \Lambda V'$ by

$$\operatorname{spec}(S_{n,p_n}) = \big[(\lambda_{1n}, \dots, \lambda_{pn}), (v_{1n}, \dots, v_{pn})\big].$$

Whenever possible, we suppress the index $n$ and write, for example, $S$, $\lambda_i$ and $v_i$ instead. Similarly, we often write $\Sigma_p$ or even $\Sigma$ for $\Sigma_{p_n}$.

LEMMA 1. *Let $\Sigma$ and $\hat{\Sigma}$ be (fixed, nonrandom) $p$-by-$p$ symmetric positive definite matrices with*

$$\operatorname{spec}(\Sigma) = \big[(\ell, 1, \dots, 1), (u_1, \dots, u_p)\big], \tag{2.1}$$

$$\operatorname{spec}(\hat{\Sigma}) = \big[(\eta, 1, \dots, 1), (v_1, \dots, v_p)\big]. \tag{2.2}$$

*Let $c = \langle u_1, v_1 \rangle$ and $s = \sqrt{1 - c^2}$. Then there exists an orthogonal matrix $W$, which depends on $\Sigma$ and $\hat{\Sigma}$, such that*

$$W' \Sigma W = A(\ell) \oplus I_{p-2}, \tag{2.3}$$

$$W' \hat{\Sigma} W = B(\eta, c) \oplus I_{p-2}, \tag{2.4}$$

*where the fundamental $2 \times 2$ matrices $A$ and $B$ are given by*

$$A(\ell) = \begin{bmatrix} \ell & 0 \\ 0 & 1 \end{bmatrix}, \qquad B(\eta, c) = I_2 + (\eta - 1) \begin{bmatrix} c \\ s \end{bmatrix} \begin{bmatrix} c & s \end{bmatrix}. \tag{2.5}$$

PROOF. Let $\Delta = \operatorname{diag}(\eta, 1, \dots, 1) = I + (\eta - 1) e_1 e_1'$, where $e_1$ denotes the unit vector in the first co-ordinate direction. It is evident that

$$\Sigma = I + (\ell - 1) u_1 u_1', \qquad \hat{\Sigma} = I + (\eta - 1) v_1 v_1'. \tag{2.6}$$

It is natural then to work in the "common" basis of $u_1$ and $v_1$. We apply one step of Gram–Schmidt if we can, setting

$$z = \begin{cases} (v_1 - c u_1)/s & \text{if } s \neq 0, \\ u_p & \text{if } s = 0. \end{cases}$$

In the second exceptional case, $v_1 = \pm u_1$, so we pick a convenient vector orthogonal to $u_1$. In either case, the columns of the $p \times 2$ matrix $W_2 = [u_1 \; z]$ are orthonormal and their span contains both $u_1$ and $v_1$. Now fill out $W_2$ to an orthogonal matrix $W = [W_2 \; W_2^{\perp}]$. Observe now that if $y$ lies in the column span of $W_2$ and $\alpha$ is a scalar, then necessarily

$$W'(I_p + \alpha y y')W = (I_2 + \alpha \check{y}\check{y}) \oplus I_{p-2}, \qquad \check{y} = W_2' y.$$

The expressions (2.3)–(2.5) now follow from the rank one perturbation forms (2.6) along with

$$W_2' u_1 = \begin{bmatrix} u_1' u_1 \\ z' u_1 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \text{and} \quad W_2' v_1 = \begin{bmatrix} u_1' v_1 \\ z' v_1 \end{bmatrix} = \begin{bmatrix} c \\ s \end{bmatrix}. \qquad \square$$

**3. Decomposable loss functions.** Here and below, by *loss function* $L_p$ we mean a function of two $p$-by-$p$ positive semidefinite matrix arguments obeying $L_p \geq 0$, with $L_p(A, B) = 0$ if and only if $A = B$. A *loss family* is a sequence $L = \{L_p\}_{p=1}^{\infty}$, one for each matrix size $p$. We often write loss function and refer to the entire family. [OBS. 2] calls out a large class of loss functions which naturally exploit the simultaneously block-diagonalizability property of Lemma 1; we now develop this observation.

DEFINITION 1 (Orthogonal invariance). We say the loss function $L_p(A, B)$ is *orthogonally invariant* if for each orthogonal $p$-by-$p$ matrix $O$,

$$L_p(A, B) = L_p(OAO', OBO').$$

For given $p$ and a given sequence of block sizes $\{d_i\}$ such that $\sum_i d_i = p$, consider block-diagonal matrix decompositions of $p$ by $p$ matrices $A$ and $B$ into blocks $A^i$ and $B^i$ of size $d_i$:

$$A = \bigoplus_i A^i, \qquad B = \bigoplus_i B^i. \tag{3.1}$$

DEFINITION 2 (Sum-decomposability and max-decomposability). We say the loss function $L_p(A, B)$ is *sum-decomposable* if for all decompositions (3.1),

$$L_p(A, B) = \sum_i L_{d_i}(A^i, B^i).$$

We say that it is *max-decomposable* if if for all decompositions (3.1),

$$L_p(A, B) = \max_i L_{d_i}(A^i, B^i).$$

Clearly, such loss functions can exploit the simultaneous block diagonalization of Lemma 1. Indeed, we have the following.

LEMMA 2 (Reduction to two-dimensional problem). *Consider an orthogonally invariant loss function, $L_p$, which is sum- or max-decomposable. Suppose that $\Sigma$ and $\hat{\Sigma}$ satisfy (2.1) and (2.2), respectively. Then*

$$L_p(\Sigma, \hat{\Sigma}) = L_2(A(\ell), B(\eta, c)).$$

PROOF. Lemma 1 provides a change of basis $W$ yielding decompositions (2.3) and (2.4). From the invariance and decomposability hypotheses,

$$\begin{aligned} L_p(\Sigma, \hat{\Sigma}) &= L_p\big(W'\Sigma W, W'\hat{\Sigma} W\big) \\ &= L_p\big(A(\ell) \oplus I_{p-2}, B(\eta, c) \oplus I_{p-2}\big) \\ &= L_2\big(A(\ell), B(\eta, c)\big). \end{aligned}$$ □

**4. Asymptotic loss in the spiked covariance model.** Consider the spiked model with a single spike, $r = 1$, namely, make assumptions [ASY($\gamma$)] and [SPIKE($\ell$)]. The principal $2 \times 2$ block estimator occurring in Lemmas 1 and 2 is $B(\eta(\lambda_{1n}), c_{1n})$ where $\lambda_{1n}$ is the largest eigenvalue of $S_n$ and $c_{1n} = \langle u_{1n}, v_{1n}\rangle$.

If $\eta$ is continuous, then the convergence results (1.2) and (1.5) imply that the principal block converges as $n \to \infty$. Specifically,

$$B\big(\eta(\lambda_{1n}), c_{1n}\big) \xrightarrow{\text{a.s.}} B\big(\eta\big(\lambda(\ell)\big), c(\ell)\big) =: B(\ell, \eta), \tag{4.1}$$

say, with the convergence occurring in all norms on $2 \times 2$ matrices.

In accord with [OBS. 3], we now show that the asymptotic loss (1.8) is a deterministic, explicit function of the population spike $\ell$. For now, we will continue to assume that the shrinker $\eta$ is rank-aware. Alternatively, we can make a different simplifying assumption on $\eta$, which will be useful in what follows.

DEFINITION 3. We say that a scalar function $\eta : [0, \infty) \to [1, \infty)$ is a *bulk shrinker* if $\eta(\lambda) = 1$ when $\lambda \le \lambda_+(\gamma)$, and a *neighborhood bulk shrinker* if for some $\varepsilon > 0$, $\eta(\lambda) = 1$ whenever $\lambda \le \lambda_+(\gamma) + \varepsilon$.

The neighborhood bulk shrinker condition on $\eta$ is rather strong, but does hold for $\eta_*^N$ in (1.12), for example. [Note that our definitions ignore the lower bulk edge $\lambda_-(\gamma)$, which is of less interest in the spiked model.]

LEMMA 3 (A formula for the asymptotic loss). *Adopt models* [ASY($\gamma$)] *and* [SPIKE($\ell$)] *with* $\ell > \ell_+(\gamma)$. *Suppose* (a) *that the family* $L = \{L_p\}$ *of loss functions is orthogonally invariant and sum- or max-decomposable, and that* $B \mapsto L_2(A, B)$ *is continuous. Let* $\hat{\Sigma}_\eta = \hat{\Sigma}_\eta(S_{n,p_n})$ *be given by* (1.7), *and let* $\hat{\Sigma}_{\eta,1}$ *be the corresponding rank-aware shrinkage rule* (1.13) *for* $r = 1$. *Suppose the scalar nonlinearity* $\eta$ *is continuous on* $(\lambda_+(\gamma), \infty)$. *Then*

$$L_{p_n}(\Sigma_{p_n}, \hat{\Sigma}_{\eta,1}) \xrightarrow{\text{a.s.}} L_2\big(A(\ell), B(\ell, \eta)\big). \tag{4.2}$$

*Furthermore, if* (b) $\eta$ *is a neighborhood bulk shrinker, then* $L_{p_n}(\Sigma_{p_n}, \hat{\Sigma}_\eta)$ *also has this limit a.s.*

Each of the 26 losses considered in this paper satisfies conditions (a).

PROOF. In the rank-aware case, $\hat{\Sigma}_\eta = \hat{\Sigma}_{\eta,1}$ satisfies

$$\mathrm{spec}(\hat{\Sigma}_\eta) = \big[\big(\eta(\lambda_{1n}), 1, \dots, 1\big), (v_{1n}, \dots, v_{pn})\big],$$

Lemma 2 implies that

$$L_p(\Sigma, \hat{\Sigma}_\eta) = L_2\big(A(\ell), B\big(\eta(\lambda_{1n}), c_{1n}\big)\big) \xrightarrow{\text{a.s.}} L_2\big(A(\ell), B(\ell, \eta)\big),$$

where the limit on the right-hand side follows from convergence (4.1) and the assumed continuity of $L_2$.

Now assume that $\eta$ is a neighborhood bulk shrinker. From (1.2), we know that $\lambda_{1n} \xrightarrow{\text{a.s.}} \lambda(\ell)$ From eigenvalue interlacing [see (7.11) below], we have $\lambda_{2n} \le \mu_{1n}$, where $\mu_{1n}$ is the largest eigenvalue of a white Wishart matrix $W_{p_n-1}(n, I)$, and satisfies $\mu_{1n} \xrightarrow{\text{a.s.}} \lambda_+$, from [27]. Let $\varepsilon > 0$ be small enough that $\lambda_+ + \varepsilon < \lambda(\ell)$ and also lies in the neighborhood shrunk to 1 by $\eta$. Hence, there exists a random variable $\hat{n}$ such that almost surely, $\lambda_{2n} < \lambda_+ + \varepsilon < \lambda_{1n}$ for all $n > \hat{n}$. For such $n$, the first display above of this proof applies and we then obtain the second display as before. $\square$

**5. Examples of decomposable loss functions.** Many of the loss functions that appear in the literature are *Pivot-Losses*. They can be obtained via the following common recipe.

DEFINITION 4 (Pivots). A *matrix pivot* is a matrix-valued function $\Delta(A, B)$ of two real positive definite matrices $A, B$ such that: (i) $\Delta(A, B) = 0$ if and only if $A = B$, (ii) $\Delta$ is orthogonally equivariant and (iii) $\Delta$ respects block structure in the sense that

$$\Delta\big(OAO', OBO'\big) = O\Delta(A, B)O', \tag{5.1}$$

$$\Delta\Big(\bigoplus A^i, \bigoplus B^i\Big) = \bigoplus \Delta(A^i, B^i) \tag{5.2}$$

for any orthogonal matrix $O$ of the appropriate dimension.

Matrix pivots can be symmetric-matrix valued, for example, $\Delta(A, B) = A - B$, but need not be, for example, $\Delta(A, B) = A^{-1}B - I$.

DEFINITION 5 (Pivot-losses). Let $g$ be a nonnegative function of a symmetric matrix variable that is definite: $g(A) = 0$ if and only if $A = 0$, and orthogonally invariant: $g(O\Delta O') = g(\Delta)$ for any orthogonal matrix $O$. A symmetric-matrix valued pivot $\Delta$ induces an orthgonally-invariant *pivot loss*

$$L(A, B) = g\big(\Delta(A, B)\big). \tag{5.3}$$

More generally, for any matrix pivot $\Delta$, set $|\Delta| = (\Delta'\Delta)^{1/2}$ and define

$$L(A, B) = g\big(|\Delta|(A, B)\big). \tag{5.4}$$

An orthogonally invariant function $g$ depends on its matrix argument $\Delta$ or $|\Delta|$ only through its eigenvalues or singular values $\delta_1, \dots, \delta_p$. We abuse notation to write $g(\Delta) = g(\delta_1, \dots, \delta_p)$. Observe that if $g$ has either of the forms

$$g(\delta_1, \dots, \delta_p) = \sum_j g_1(\delta_j) \quad \text{or} \quad g(\delta_1, \dots, \delta_p) = \max_j g_1(\delta_j),$$

for some univariate $g_1$, then the pivot loss $L(A, B) = g(\Delta(A, B))$ (symmetric pivot) or $L(A, B) = g(|\Delta|(A, B))$ (general pivot) is respectively sum- or max-decomposable. In case $\Delta$ is symmetric, the two definitions agree so long as $g_1$ is an even function of $\delta$.

5.1. *Examples of sum-decomposable losses*. There are different strategies to derive sum-decomposable pivot-losses. First, we can use statistical discrepancies between the Normal distributions $\mathcal{N}(0, A)$ and $\mathcal{N}(0, B)$:

1. *Stein loss* [13, 38, 64]: Stein's loss is defined as

$$L^{\mathrm{st}}(A, B) = \mathrm{tr}\big(A^{-1}B - I\big) - \log\big(\det(B)/\det(A)\big).$$

This is just twice the Kullback distance $D_{\mathrm{KL}}(\mathcal{N}(0, B)||\mathcal{N}(0, A))$. Stein's loss is a pivot-loss with respect to $\Delta(A, B) = A^{-1/2}BA^{-1/2}$ and $g(\Delta) = \mathrm{tr}(\Delta - I) - \log\det(\Delta) = \sum_i g_1(\delta_i)$, where $g_1(\delta) = \delta - 1 - \log\delta$.

2. *Entropy/divergence losses*: Because the Kullback discrepancy is not symmetric in its arguments, we may consider two other losses: reversing the arguments we get *Entropy* loss $L^{\mathrm{ent}}(A, B) = L^{\mathrm{st}}(B, A)$ [40, 63] and summing the Stein and Entropy losses gives *divergence* loss:

$$L^{\mathrm{div}}(A, B) = L^{\mathrm{st}}(A, B) + L^{\mathrm{st}}(B, A) = \mathrm{tr}\big(A^{-1}B - I\big) + \mathrm{tr}\big(B^{-1}A - I\big);$$

see [28, 43]. Each can be shown to be sum-decomposable, following the same argument as above.

3. *Bhattarcharya/Matusita affinity* [37, 52]: Let

$$L^{\mathrm{aff}}(A, B) = \frac{1}{2}\log\frac{|A + B|/2}{|A|^{1/2}|B|^{1/2}}.$$

This measures the statistical distinguishability of $\mathcal{N}(0, A)$ and $\mathcal{N}(0, B)$ based on independent observations, since $L^{\mathrm{aff}} = \frac{1}{2}\log(\int\sqrt{\phi_A}\sqrt{\phi_B})$ with $\phi_A$ and $\phi_B$ the densities of $\mathcal{N}(0, A)$ and $\mathcal{N}(0, B)$. Hence convergence of affinity loss to zero is equivalent to convergence of the underlying densities in Hellinger or Variation distance. This is a pivot-loss w.r.t. $\Delta(A, B) = A^{-1/2}BA^{-1/2}$ and

$$g(\Delta) = \frac{1}{4}\log\big(\det(2I + \Delta + \Delta^{-1})/4\big) = \sum_i g_1(\delta_i),$$

as is seen by setting $C = A^{-1/2}(A + B)B^{-1/2}$ and noting that $C'C = (2I + \Delta + \Delta^{-1})$. Here, $g_1(\delta) = \frac{1}{4}\log(2 + \delta + \delta^{-1})/4$.

4. *Fréchet discrepancy* [18, 55]: Let $L^{\mathrm{fre}}(A, B) = \mathrm{tr}(A + B - 2A^{1/2}B^{1/2})$. This measures the minimum possible mean-squared difference between zero-mean random vectors with covariances $A$ and $B$, respectively. This is a pivot-loss w.r.t. $\Delta(A, B) = A^{1/2} - B^{1/2}$, and $g(\Delta) = \mathrm{tr}(\Delta^2) = \sum_i g_1(\delta_i)$ with $g_1(\delta) = \delta^2$.

Second, we may obtain sum-decomposable pivot-losses $L(A, B) = g(\Delta(A, B))$ by simply taking $g$ to be one of the standard matrix norms:

1. *Squared error loss* [11, 34, 44, 46]: Let $L^{F,1}(A, B) = \|A - B\|_F^2$. This is a pivot-loss w.r.t. $\Delta(A, B) = A - B$ and $g(\Delta) = \mathrm{tr}\,\Delta'\Delta = \sum_i g_1(\delta_i)$ with $g_1(\delta) = \delta^2$.
2. *Squared error loss on precision* [29]: Let $L^{F,2}(A, B) = \|A^{-1} - B^{-1}\|_F^2$. This is a pivot-loss w.r.t. $\Delta(A, B) = A^{-1} - B^{-1}$ and $g(\Delta) = \mathrm{tr}\,\Delta'\Delta$.
3. *Nuclear norm loss.* Let $L^{N,1}(A, B) = \|A - B\|_*$ where $\|\Delta\|_*$ denotes the nuclear norm of the matrix $\Delta$, that is, the sum of its singular values. This is a pivot-loss w.r.t. $\Delta(A, B) = A - B$ and $g(\Delta) = \sum_i |\delta_i|$.
4. Let $L^{F,3}(A, B) = \|A^{-1}B - I\|_F^2$. This is a pivot-loss w.r.t. $\Delta(A, B) = A^{-1}B - I$. It was studied in [31, 60, 62] and later work.
5. Let $L^{F,7}(A, B) = \|\log(A^{-1/2}BA^{-1/2})\|_F^2$, where $\log(\cdot)$ denotes the matrix logarithm[3] [24, 48]. This is a pivot-loss w.r.t.

$$\Delta(A, B) = \log\bigl(A^{-1/2}BA^{-1/2}\bigr).$$

5.2. *Examples of max-decomposable losses*. Max-decomposable losses arise by applying the operator norm (the maximal singular value or eigenvalue of a matrix) to a suitable pivot. Here are a few examples:

1. *Operator norm loss* [21]: Let $L^{O,1}(A, B) = \|A - B\|_{\mathrm{op}}$. This is a pivot-loss w.r.t. $\Delta(A, B) = A - B$ and $g(\Delta) = \|\Delta\|_{\mathrm{op}} = \max_i \delta_i$.
2. *Operator norm loss on precision*: Let $L^{O,2}(A, B) = \|A^{-1} - B^{-1}\|_{\mathrm{op}}$. This is a pivot-loss w.r.t. $\Delta(A, B) = A^{-1} - B^{-1}$.
3. *Condition number loss*: Let $L^{O,7}(A, B) = \|\log(A^{-1/2}BA^{-1/2})\|_{\mathrm{op}}$. This is a pivot-loss w.r.t. $\Delta(A, B) = \log(A^{-1/2}BA^{-1/2})$, related to [69]. In the spiked model discussed below, $L^{O,7}$ effectively measures the condition number of $A^{-1/2}BA^{-1/2}$.

We adopt the systematic naming scheme $L^{\mathrm{norm},\mathrm{pivot}}$ where norm $\in \{F, O, N\}$, and pivot $\in \{1, \dots, 7\}$. This set of 21 combinations covers the previous matrix norm examples and adds some more. Together with Stein's loss and the others based on statistical discrepancy mentioned above, we arrive at a set of 26 loss functions, Table 1, to be studied in this paper.

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[3]The matrix logarithm transfers the matrices from the Riemannian manifold of symmetric positive semidefinite matrices to its tangent space at $A$. It can be shown that $L^{F,7}$ is the squared geodesic distance in this manifold. This metric between covariances has attracted attention, for example, in diffusion tensor MRI [19, 48].

TABLE 1
*Systematic notation for the 26 loss functions considered in this paper*

| **Pivot** | **MatrixNorm** Frobenius | Operator | Nuclear |
|---|---|---|---|
| $A-B$ | $L^{F,1}$ | $L^{O,1}$ | $L^{N,1}$ |
| $A^{-1}-B^{-1}$ | $L^{F,2}$ | $L^{O,2}$ | $L^{N,2}$ |
| $A^{-1}B-I$ | $L^{F,3}$ | $L^{O,3}$ | $L^{N,3}$ |
| $B^{-1}A-I$ | $L^{F,4}$ | $L^{O,4}$ | $L^{N,4}$ |
| $A^{-1}B+B^{-1}A-2I$ | $L^{F,5}$ | $L^{O,5}$ | $L^{N,5}$ |
| $A^{-1/2}BA^{-1/2}-I$ | $L^{F,6}$ | $L^{O,6}$ | $L^{N,6}$ |
| $\log(A^{-1/2}BA^{-1/2})$ | $L^{F,7}$ | $L^{O,7}$ | $L^{N,7}$ |
| | **Statistical measures** | | |
| | **St** | **Ent** | **Div** |
| Stein | $L^{\mathrm{st}}$ | $L^{\mathrm{ent}}$ | $L^{\mathrm{div}}$ |
| Affinity | | $L^{\mathrm{aff}}$ | |
| Fréchet | | $L^{\mathrm{fre}}$ | |

## 6. Optimal shrinkage for decomposable losses.

6.1. *Formally optimal shrinker.* Formula (4.2) for the asymptotic loss has only been shown to hold in the single spike model and only for a certain class of nonlinearities $\eta$. In fact, the same is true in the $r$-spike model and for a much broader class of nonlinearities $\eta$. To preserve the narrative flow of the paper, we defer the proof, which is more technical, to Section 7. Instead, we proceed under the single spike model, and simply assume that $L_\infty(\ell|\eta)$ from (4.2) is the correct limiting loss, and draw conclusions on the optimal shape of the shrinker $\eta$.

DEFINITION 6 (Optimal shrinker). Let $L = \{L_p\}_{p=1}^{\infty}$ be a given loss family and let $L_\infty(\ell|\eta)$ be the asymptotic loss corresponding to a nonlinearity $\eta$, as defined in (4.2), under assumption [ASY($\gamma$)]. If $\eta^*$ satisfies

$$L_\infty(\ell|\eta^*) = \min_\eta L_\infty(\ell|\eta), \qquad \forall \ell \geq 1, \tag{6.1}$$

and for any $\eta \neq \eta^*$ there exists $\ell \geq 1$ with $L_\infty(\ell, \eta^*) < L_\infty(\ell, \eta)$, then we say that $\eta^*$ is the *formally optimal* shrinker for the loss family $L$ and shape factor $\gamma$, and denote the corresponding shrinkage rule by $\lambda \mapsto \eta^*(\lambda; \gamma, L)$.

Below, we call formally optimal shrinkers simply "optimal". By definition, the optimal shrinkage rule $\eta^*(\lambda; \gamma, L)$ is the unique admissible rule, in the asymptotic sense, among rules of the form $\hat{\Sigma}_\eta(S_{n,p}) = V\eta(\Lambda)V'$ in the single-spike model.

In the single spiked model (and as we show later, generally in the spiked model), one never regrets using the optimal shrinker over any other (reasonably regular) univariate shrinker. In light of our results so far, an obvious characterization of an optimal shrinker is as follows.

THEOREM 1 (Characterization of optimal shrinker). *Let $L = \{L_p\}_{p=1}^{\infty}$ be a loss family. Define*

$$F(\ell, \eta) = L_2\left(\begin{bmatrix} \ell & 0 \\ 0 & 1 \end{bmatrix}, \begin{bmatrix} 1 + (\eta - 1)c^2 & (\eta - 1)cs \\ (\eta - 1)cs & 1 + (\eta - 1)s^2 \end{bmatrix}\right). \tag{6.2}$$

*Here*, $c = c(\ell)$ *and* $s = s(\ell)$ *satisfy* $c^2(\ell) = \frac{1-\gamma/(\ell-1)^2}{1+\gamma/(\ell-1)}$ *and* $s^2(\ell) = 1 - c^2(\ell)$. *Suppose that for any* $\ell > \ell_+(\gamma)$, *there exists a unique minimizer*:

$$\eta^*(\ell) := \operatorname*{arg\,min}_{\eta \geq 1} F(\ell, \eta). \tag{6.3}$$

*Further suppose that for every* $1 \leq \ell \leq \ell_+(\gamma)$ *we have* $\arg\min_{\eta \geq 1} G(\eta) = 1$, *where*

$$G(\ell, \eta) = L_2\left(\begin{bmatrix} \ell & 0 \\ 0 & 1 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & \eta \end{bmatrix}\right). \tag{6.4}$$

*Then the shrinker*

$$\eta^*(\lambda) = \begin{cases} \eta^*(\ell(\lambda)), & \ell > \lambda_+(\gamma), \\ 1, & 1 \leq \ell \leq \lambda_+(\gamma), \end{cases}$$

*where* $\ell(\lambda)$ *is given by* (1.10), *is the optimal shrinker of the loss family* $L$.

Many of the 26 loss families discussed in Section 3 admit a closed form expression for the optimal shrinker; see Table 2. For others, we computed the optimal shrinker numerically, by implementing in software a solver for the simple scalar optimization problem (6.3). Figure 3 portrays the optimal shrinkers for our 26 loss functions. We refer readers interested in computing specific individual shrinkers to our reproducibility advisory at the bottom of this paper, and invite the reader to explore the code supplement [16], consisting of online resources and code we offer.

6.2. *Optimal shrinkers collapse the bulk.* We first observe that, for any of the 26 losses considered, the optimal shrinker collapses the bulk to 1. The following lemma is proved in the supplemental article [15]:

LEMMA 4. *Let* $L$ *be any of the* 26 *losses mentioned in Table* 1. *Then the rule* $\eta^{**}(\ell) = 1$ *is unique asymptotically admissible on* $[1, \ell_+(\gamma)]$, *namely, for every* $\ell \in [1, \ell_+(\gamma)]$ *we have* $\mathbb{E}L(\ell, \eta) \geq L(\ell, \eta^{**})$, *with strict inequality for at least one point in* $[1, \ell_+(\gamma)]$.

TABLE 2

*Optimal shrinkers $\eta^*(\lambda)$ for 18 of the loss families $L$ discussed. Values shown are shrinkers for $\lambda > \lambda_+(\gamma)$. All shrinkers obey $\eta^*(\lambda) = 1$ for $\lambda \le \lambda_+(\gamma)$. Here, $\ell$, $c$ and $s$ depend on $\lambda$ (and implicitly on $\gamma$) according to (1.10), (1.6) and $s = \sqrt{1-c^2}$. In cases marked "N/A", the optimal shrinker does not seem to admit a simple closed form, but can be easily calculated numerically*

| | **Matrix Norm** | | |
|---|---|---|---|
| **Pivot** | **Frobenius** | **Operator** | **Nuclear** |
| $A - B$ | $\ell c^2 + s^2$ | $\ell$ | $\max(1 + (\ell - 1)(1 - 2s^2), 1)$ |
| $A^{-1} - B^{-1}$ | $\frac{\ell}{c^2+\ell s^2}$ | $\ell$ | $\max(\frac{\ell}{c^2+(2\ell-1)s^2}, 1)$ |
| $A^{-1}B - I$ | $\frac{\ell c^2+\ell^2 s^2}{c^2+\ell^2 s^2}$ | N/A | $\max(\frac{\ell}{c^2+\ell^2 s^2}, 1)$ |
| $B^{-1}A - I$ | $\frac{\ell^2 c^2+s^2}{\ell c^2+s^2}$ | N/A | $\max(\frac{\ell^2 c^2+s^2}{\ell}, 1)$ |
| $A^{-1/2}BA^{-1/2} - I$ | $1 + \frac{(\ell-1)c^2}{(c^2+\ell s^2)^2}$ | $1 + \frac{\ell-1}{c^2+\ell s^2}$ | $\max(\frac{\ell-(\ell-1)^2 c^2 s^2}{(c^2+\ell s^2)^2}, 1)$ |
| | **Statistical measures** | | |
| | **St** | **Ent** | **Div** |
| Stein | $\frac{\ell}{c^2+\ell s^2}$ | $\ell c^2 + s^2$ | $\sqrt{\frac{\ell^2 c^2+\ell s^2}{c^2+\ell s^2}}$ |
| Fréchet | | $(\sqrt{\ell}c^2 + s^2)^2$ | |
| Affine | | $\frac{(1+c^2)\ell+s^2}{1+c^2+\ell s^2}$ | |

As part of the proof of Lemma 4, in Table 6 in the supplemental article [15], we explicitly calculate the fundamental loss function $G(\ell, \eta)$ of (6.4) for many of the loss families discussed in this paper.

To determine the optimal shrinker $\eta^*(\lambda; \gamma, L)$ for each of our loss functions $L$, it therefore remains to determine the map $\lambda \mapsto \eta^*(\lambda)$ or equivalently $\ell \mapsto \eta^*(\lambda(\ell))$ only for $\ell > \ell_+(\gamma)$. This is our next task.

6.3. *Optimal shrinkers by computer.* The scalar optimization problem (6.3) is easy to solve numerically, so that one can always compute the optimal shrinker at any desired value $\lambda$. In the code supplement [16], we provide the Matlab code to compute the optimal nonlinearity for each of the 26 loss families discussed. In the sibling problem of singular value shrinkage for matrix denoising, [26] demonstrates numerical evaluation of optimal shrinkers for the Schatten-$p$ norm, where analytical derivation of optimal shrinkers appears to be impossible.

6.4. *Optimal shrinkers in closed form.* We were able to obtain simple analytic formulas for the optimal shrinker $\eta^*$ in each of 18 loss families from Section 3. While the optimal shrinkers are of course functions of the empirical eigenvalue $\lambda$, in the interest of space, we state the lemmas and provide the formulas in terms of

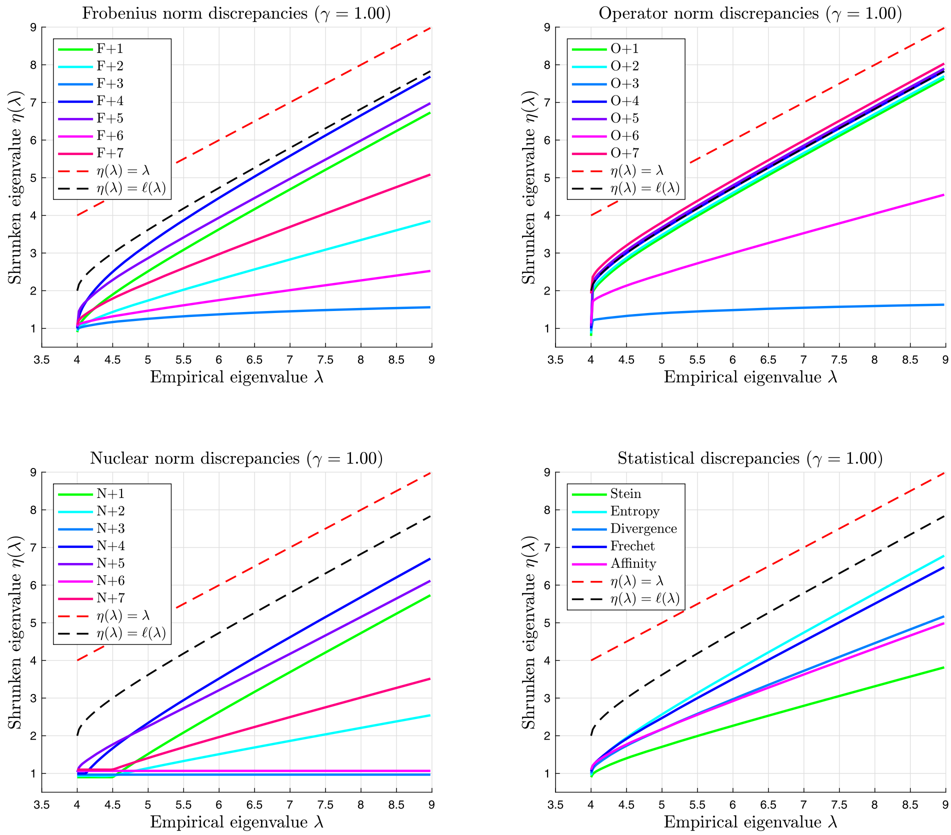


FIG. 3. *Optimal Shrinkers for* 26 *Component Loss Functions for* $\gamma = 1$ *and* $4 \le \lambda \le 10$. *Upper Left*: *Frobenius-norm-based losses*; *Lower Left*: *Nuclear-Norm based losses*; *Upper Right*: *Operator-norm-based losses*; *Lower Right*: *Statistical Discrepancies*. (*Color online*; *curves jittered in vertical axis to avoid overlap*.) *The supplemental article* [15] *contains a larger version of these plots*. *Reproducibility advisory*: *The code supplement* [16] *includes a script that reproduces any one of these individual curves*.

the quantities $\ell$, $c$ and $s$. To calculate any of the nonlinearities below for a specific empirical eigenvalue $\lambda$, use the following procedure:

1. If $\lambda \le \lambda_+(\gamma)$ set $\eta^*(\lambda) = 1$. Otherwise:
2. Calculate $\ell(\lambda)$ using (1.10).
3. Calculate $c(\lambda) = c(\ell(\lambda))$ using (1.6) and (1.10).
4. Calculate $s(\lambda) = s(\ell(\lambda))$ using $s(\ell) = \sqrt{1 - c^2(\ell)}$.
5. Substitute $\ell(\lambda)$, $c(\lambda)$ and $s(\lambda)$ into the formula provided to get $\eta^*(\lambda)$.

The closed forms we provide are summarized in Table 2. Note that $\ell$, $c$ and $s$ refer to the functions $\ell(\lambda)$, $c(\ell(\lambda))$ and $s(\ell(\lambda))$. These formulae are formally derived in a sequence of lemmas that are stated and proved in the supplemental article [15]. The proofs also show that these optimal shrinkers are unique, as in each case the optimal shrinker is shown to be the unique minimizer, as in (6.3), of (6.2). We make some remarks on these optimal shrinkers by focusing first on operator norm loss for covariance and precision matrices:

$$\eta^*(\lambda;\gamma,L^{O,1}) = \eta^*(\lambda;\gamma,L^{O,2}) = \begin{cases} \ell, & \ell > \ell_+(\gamma), \\ 1, & \ell \le \ell_+(\gamma). \end{cases} \tag{6.5}$$

This asymptotic relationship reflects the classical fact that in finite samples, the top empirical eigenvalue is always biased upwards of the underlying population eigenvalue [10, 68]. Formally defining the (asymptotic) bias as

$$\mathrm{bias}(\eta,\ell) = \eta\big(\lambda(\ell)\big) - \ell,$$

we have $\mathrm{bias}(\lambda(\ell),\ell) > 0$. The formula $\eta^*(\lambda) = \ell$ shows that the optimal nonlinearity for operator norm loss is what we might simply call a *debiasing* transformation, mapping each empirical eigenvalue back to the value of its "original" population eigenvalue, and the corresponding shrinkage estimator $\hat{\Sigma}_\eta$ uses each *sample* eigenvectors with its corresponding *population* eigenvalue. In words, within the top branch of (6.5), the effect of *operator-norm optimal shrinkage is to debias the top eigenvalue*:

$$\mathrm{bias}\big(\eta^*(\cdot;\gamma,L^{O,1}),\ell\big) = \mathrm{bias}\big(\eta^*(\cdot;\gamma,L^{O,2}),\ell\big) = 0, \qquad \forall \ell > \ell_+(\gamma).$$

On the other hand, within the bottom branch, the effect is to *shrink the bulk to 1*. In terms of Definition 3, we see that $\eta^*$ is a bulk shrinker, but not a neighborhood bulk shrinker.

One might expect asymptotic debiasing from *every* loss function, but, perhaps surprisingly, precise asymptotic debiasing is exceptional. In fact, none of the other optimal nonlinearities in Table 2 is precisely debiasing.

In the supplemental article [15], we also provide a detailed investigation of the large-$\lambda$ asymptotics of the optimal shrinkers, including their asymptotic slopes, asymptotic shifts and asymptotic percent improvement.

**7. Beyond formal optimality.** The shrinkers we have derived and analyzed above are formally optimal, as in Definition 6, in the sense that they minimize the formal expression $L_\infty(\ell|\eta)$. So far we have only shown that formally optimal shrinkers actually minimize the asymptotic loss (namely, are asymptotically unique admissible) in the single-spike case, under assumptions [$\mathrm{ASY}(\gamma)$] and [$\mathrm{SPIKE}(\ell)$], and only over neighborhood bulk shrinkers.

In this section, we show that formally optimal shrinkers in fact minimize the asymptotic loss in the general Spiked Covariance Model, namely under assumptions [$\mathrm{ASY}(\gamma)$] and [$\mathrm{SPIKE}(\ell_1,\dots,\ell_r)$], and over a large class of bulk shrinkers, which are possibly not neighborhood bulk shrinkers.

We start by establishing the rank $r$ analog of Lemma 1. For a vector $\ell \in \mathbb{R}^r$, let $\Delta_r(\ell) = \mathrm{diag}(\ell_1,\dots,\ell_r)$.

LEMMA 5. *Assume that $\Sigma$ and $\hat{\Sigma}$ are fixed matrices with*

$$\operatorname{spec}(\Sigma) = \big[(\ell_1, \dots, \ell_r, 1, \dots, 1), (u_1, \dots, u_p)\big],$$
$$\operatorname{spec}(\hat{\Sigma}) = \big[(\eta_1, \dots, \eta_r, 1, \dots, 1), (v_1, \dots, v_p)\big].$$

*Let $U_r$ and $V_r$ denote the $p$-by-$r$ matrices consisting of the top $r$ eigenvectors of $\Sigma$ and $\hat{\Sigma}$, respectively. Suppose that $[U_r \; V_r]$ has full rank $2r$, and consider the $QR$ decomposition*

$$\begin{bmatrix} U_r & V_r \end{bmatrix} = QR,$$

*where $Q$ has $2r$ orthonormal columns and the $2r \times 2r$ matrix $R$ is upper triangular. Let $R_2$ denote the $2r \times r$ submatrix formed by the last $r$ columns of $R$. Fill out $Q$ to an orthogonal matrix $W = [Q \; Q^{\perp}]$. Then in the transformed basis we have the simultaneous block decompositions*:

$$W' \Sigma W = \Sigma_{2r}^{\circ} \oplus I_{p-2r}, \qquad \Sigma_{2r}^{\circ} = \Delta_r(\ell) \oplus I_r, \tag{7.1}$$

$$W' \hat{\Sigma} W = \hat{\Sigma}_{2r}^{\circ} \oplus I_{p-2r}, \qquad \hat{\Sigma}_{2r}^{\circ} = I_{2r} + R_2 \Delta_r(\eta - 1) R_2'. \tag{7.2}$$

PROOF. We start with observations about the structure of $Q$ and $R$. Since the first $r$ columns of $Q$ are identically those of $U_r$, we let $Z_r$ be the $n$-by-$r$ matrix such that $Q = [U_r \; Z_r]$. For the same reason, $R$ has the block structure

$$R = \begin{bmatrix} I_{r \times r} & R_{12} \\ 0_{r \times r} & R_{22} \end{bmatrix},$$

where the matrices $R_{12}$ and $R_{22}$ satisfy $V_r = U_r R_{12} + Z_r R_{22}$, so that

$$R_{12} = U_r' V_r, \qquad R_{22} = Z_r' V_r. \tag{7.3}$$

Since $V_r$ has orthogonal columns, we have

$$\begin{aligned} I_r = V_r' V_r = R_{12}' R_{12} + R_{22}' R_{22}, \\ R_{22}' R_{22} = I - R_{12}' R_{12}. \end{aligned} \tag{7.4}$$

Let $H$ be a $p \times r$ matrix whose columns lie in the column span of $Q$ and let $\Delta$ be an $r \times r$ diagonal matrix. Observe that

$$\begin{aligned} W'(I + H \Delta H')W &= I + W' H \Delta H' W \\ &= (I_{2r} + Q' H \Delta H' Q) \oplus I_{p-2r} = C_{2r} \oplus I_{p-2r}, \end{aligned}$$

say, since the columns of $Q^{\perp}$ are orthogonal to those of $H$.

By analogy to (2.6), we may write

$$\Sigma = I + U_r(\Delta_r(\ell) - I_r) U_r', \qquad \hat{\Sigma} = I + V_r(\Delta_r(\eta) - I_r) V_r' \tag{7.5}$$

and so both of the form $I + H\Delta H'$, with $H = U_r$ and $V_r$, respectively. We find that

$$Q'U_r = \begin{bmatrix} I_r \\ 0 \end{bmatrix}, \qquad Q'V_r = \begin{bmatrix} R_{12} \\ R_{22} \end{bmatrix} = R_2.$$

We can then compute the value of $C_{2r}$ in the two cases to be given by $\Sigma_{2r}^{\circ}$ and $\hat{\Sigma}_{2r}^{\circ}$ respectively, which establishes (7.1) and (7.2), and hence the lemma. □

We intend to apply Lemma 5 to $\Sigma$ and $\hat{\Sigma} = \hat{\Sigma}_{\eta,r}$, the "rank-aware" modification (1.13) of the estimator $\hat{\Sigma}_\eta$ in (1.7). Assume now that $\hat{\Sigma}$ and the $p \times r$ matrix $V_{r,n}$ formed by the top eigenvectors of $V$ are random.

LEMMA 6. *The rank of* $[U_r \ V_{r,n}]$ *equals* $2r$ *almost surely.*

PROOF. Let $\Pi_r(V)$ be the projection that picks out the first $r$ columns of an orthogonal matrix $V$. For a fixed $r$-frame $U_r$, we consider the event

$$A = \{V \in O_p : \operatorname{rank}([U_r \ \Pi_r(V)]) < 2r\},$$

where $O_p$ is the group of orthogonal $p$-by-$p$ matrices. Let $P_\Sigma(d\Lambda, dV)$ denote the joint distribution of eigenvalues $\Lambda = \operatorname{diag}(\lambda_1, \dots, \lambda_p)$ and eigenvectors $V$ when $S \sim W_p(n, \Sigma)$. As shown by [33], $P_\Sigma$ is absolutely continuous with respect to $\nu_p \times \mu_p$, the product of Lebesgue measure on $\mathbb{R}^p$ and Haar measure on $O(p)$. Since $\mu_p(A) = 0$, it follows that $P_\Sigma(A) = 0$. □

LEMMA 7. *Adopt models* [ASY($\gamma$)] *and* [SPIKE($\ell_1, \dots, \ell_r$)] *with* $\ell_1, \dots, \ell_r > \ell_+(\gamma)$. *Suppose the scalar nonlinearity* $\eta$ *is continuous on* $(\lambda_+(\gamma), \infty)$. *For each* $p$, *there exists w.p.* 1 *an orthogonal change of basis* $W$ *such that*

$$W'\Sigma W = \Sigma_{2r} \oplus I_{p-2r}, \qquad W'\hat{\Sigma}_{\eta,r} W = \hat{\Sigma}_{2r} \oplus I_{p-2r}, \tag{7.6}$$

*where the* $2r \times 2r$ *matrices* $\Sigma_{2r}$, $\hat{\Sigma}_{2r}$ *satisfy*

$$\Sigma_{2r} = \bigoplus_{i=1}^{r} A(\ell_i), \qquad \hat{\Sigma}_{2r} \xrightarrow{\text{a.s.}} \bigoplus_{i=1}^{p} B(\ell_i, \eta), \tag{7.7}$$

*and the* $2 \times 2$ *matrices* $A(\ell)$, $B(\ell, \eta)$ *are defined at* (2.5).

*Suppose also that the family* $L = \{L_p\}$ *of loss functions is orthogonally invariant and sum- or max-decomposable, and that* $B \to L_{2r}(A, B)$ *is continuous. Then*

$$L_p(\Sigma, \hat{\Sigma}_{\eta,r}) \xrightarrow{\text{a.s.}} \Big(\sum / \max\Big)_{i=1,\dots,r} L_2\big(A(\ell_i), B(\ell_i, \eta)\big). \tag{7.8}$$

*If* $\eta$ *is a neighborhood bulk shrinker, then* $L_p(\Sigma, \hat{\Sigma}_\eta)$ *also has this limit a.s.*

This is the rank $r$ analog of Lemma 3. The optimal nonlinearity $\eta^*$ is continuous on $[0, \infty)$ for all losses except the operator norm ones, for which $\eta^*$ is continuous except at $\lambda = \lambda_+(\gamma)$. Our result (7.7) requires only continuity on $(\lambda_+(\gamma), \infty)$ and so is valid for all 26 loss functions, as is the deterministic limit (7.8) for the rank-aware $\hat{\Sigma}_{\eta,r}$. However, as we saw earlier, only the nuclear norm based loss functions yield optimal functions that are neighborhood bulk shrinkers. To show that (7.8) holds for $L_p(\Sigma, \hat{\Sigma}_\eta)$ for most other important shrinkage functions, some further work is needed; see Section 7.1 below.

PROOF. We apply Lemma 5 to $\Sigma$ and $\hat{\Sigma}_{\eta,r}$ on the set of probability 1 provided by Lemma 6. First, we rewrite (7.2) to show the subblocks of $R$:

$$\hat{\Sigma}^\circ_{2r} = I_{2r} + \begin{bmatrix} R_{12} \\ R_{22} \end{bmatrix} \Delta_r\big(\eta^{(n)} - 1\big) \begin{bmatrix} R'_{12} & R'_{22} \end{bmatrix},$$

where we write $\eta^{(n)} = (\eta(\lambda_{1,n}), \dots, \eta(\lambda_{r,n}))$ to show explicitly the dependence on $n$. The limiting behavior of $R$ may be derived from (7.3) and (7.4) along with spiked model properties (1.2) and (1.5), so we have,[4] as $n \to \infty$,

$$\begin{aligned} R_{12} = U'_r V_{r,n} &\overset{\text{a.s.}}{\to} \Delta_r(c), \\ R_{22}R'_{22} = I - R_{12}R'_{12} &\overset{\text{a.s.}}{\to} \Delta_r\big(s^2\big), \\ R_{22} &\overset{\text{a.s.}}{\to} \Delta_r(s). \end{aligned} \tag{7.9}$$

Here, $c = (c(\ell_1), \dots, c(\ell_r))$ and $s = (s(\ell_1), \dots, s(\ell_r))$.

Again by (1.2) $\lambda_{i,n} \overset{\text{a.s.}}{\to} \lambda(\ell_i) > \lambda_+(\gamma)$ and so continuity of $\eta$ above $\lambda_+(\gamma)$ assures that $\Delta_r(\eta^{(n)} - 1) \to \Delta_r(\eta - 1)$, where $\eta = (\eta_i)$ and $\eta_i = \eta(\lambda(\ell_i))$. Together with (1.5), we obtain simplified structure in the limit,

$$\hat{\Sigma}^\circ_{2r} \overset{\text{a.s.}}{\to} I_{2r} + \begin{bmatrix} \Delta_r\big((\eta-1)c^2\big) & \Delta_r\big((\eta-1)cs\big) \\ \Delta_r\big((\eta-1)cs\big) & \Delta_r\big((\eta-1)s^2\big) \end{bmatrix}. \tag{7.10}$$

To rewrite the limit in block diagonal form, let $\Pi_{2r}$ be the permutation matrix corresponding to the permutation defined by

$$(1, \dots, 2r) \mapsto (1, r+1, 2, r+2, 3, \dots, 2r).$$

Permuting rows and columns in (7.1) and (7.10) using $\Pi_{2r}$ to obtain

$$\Sigma_{2r} := \Pi'_{2r} \Sigma^\circ_{2r} \Pi_{2r} = \bigoplus_{i=1}^{r} A(\ell_i),$$

$$\hat{\Sigma}_{2r} := \Pi'_{2r} \hat{\Sigma}^\circ_{2r} \Pi_{2r} \overset{\text{a.s.}}{\to} \bigoplus_{i=1}^{p} B(\ell_i, \eta),$$

[4]For simplicity, we chose the $QR$ decomposition to make the sign of $s(\ell_i)$ positive.

we obtain (7.7). Using (7.6), the orthogonal invariance and sum/max decomposability, along with the continuity of $L_{2r}(A, \cdot)$, we have

$$\begin{aligned}
L_p(\Sigma_p, \hat{\Sigma}_{\eta,r}) &= L_p(\Sigma_{2r} \oplus I_{p-2r}, \hat{\Sigma}_{2r} \oplus I_{p-2r}) \\
&= L_{2r}(\Sigma_{2r}, \hat{\Sigma}_{2r}) \\
&= L_{2r}\big(\Pi_{2r}' \Sigma_{2r} \Pi_{2r}, \Pi_{2r}' \hat{\Sigma}_{2r} \Pi_{2r}\big) \\
&\stackrel{\text{a.s.}}{\to} L_{2r}\left(\bigoplus_{i=1}^{r} A(\ell_i), \bigoplus_{i=1}^{p} B(\ell_i, \eta)\right) \\
&= \Big(\sum / \max\Big)_{i=1,\dots r} L_2\big(A(\ell_i), B(\ell_i, \eta)\big),
\end{aligned}$$

which completes the proof of Lemma 7. $\square$

7.1. *Removing the rank-aware condition.* In this section, we prove Proposition 2 below, whereby the asymptotic losses coincide for a given estimator sequence $\hat{\Sigma}_\eta$ and the rank-aware versions $\hat{\Sigma}_{\eta,r}$. This result is plausible because of two observations:

1. Null eigenvalues *stick to the bulk*, that is, for $i \geq r+1$, most eigenvalues $\lambda_{in} \leq \lambda_+(\gamma)$ and the few exceptions are not much larger. Hence, if $\eta$ is a continuous bulk shrinker, we expect $\hat{\Sigma}_\eta$ to be close to $\hat{\Sigma}_{\eta,r}$,
2. under a suitable continuity assumption on the loss functions $L_p$, $L(\Sigma, \hat{\Sigma}_\eta)$ should then be close to $L(\Sigma, \hat{\Sigma}_{\eta,r})$.

Observation 1 is fleshed out in two steps. The first step is eigenvalue comparison: The sample eigenvalue $\lambda_{in}$ arise as eigenvalues of $XX'/n$ when $X$ is a $p_n$-by-$n$ matrix whose rows are i.i.d. draws from $\mathcal{N}(0, \Sigma_{p_n})$. Let $\Pi : \mathbb{R}^{p_n} \to \mathbb{R}^{p_n - r}$ denote the projection on the last $p_n - r$ coordinates in $\mathbb{R}^{p_n}$ and let $\mu_{1n} \geq \cdots \geq \mu_{p_n-r,n}$ denote the eigenvalues of $\Pi X(\Pi X)'/n$. By the Cauchy interlacing theorem (e.g., [8], page 59), we have

$$\lambda_{in} \leq \mu_{i-r,n} \qquad \text{for } r+1 \leq i \leq p_n, \tag{7.11}$$

where the $(\mu_{in})$ are the eigenvalues of a white Wishart matrix $W_{p_n-r}(n, I)$.

The second step is a bound on eigenvalues of a white Wishart that exit the bulk. Before stating it, we return to an important detail introduced in the Remark concluding Section 1.1.

Definition 3 of a bulk shrinker depends on the parameter $\gamma = \lim p/n$ through $\lambda_+(\gamma)$. Making that dependence explicit, we obtain a bivariate function $\eta(\lambda, c)$. In model $[\textsc{Asy}(\gamma)]$ and in the $n$th problem, we might use $\eta(\lambda, c_n)$ either with $c_n = \gamma$ or $c_n = p/n$. For Proposition 1 below, it will be more natural to use the latter choice. We also modify Definition 3 as follows.

DEFINITION 7. We call $\eta : [0, \infty) \times (0, 1] \to [1, \infty)$ a *jointly continuous bulk shrinker* if $\eta(\lambda, c)$ is jointly continuous in $\lambda$ and $c$, satisfies $\eta(\lambda, c) = 1$ for $\lambda \leq \lambda_+(c)$ and is dominated: $\eta(\lambda, c) \leq M\lambda$ for some $M$ and all $\lambda$.

The following result is proved in [36], Theorem 2(a).

PROPOSITION 1. *Let $(\mu_{in})_{i=1}^N$ denote the sample eigenvalues of a matrix distributed as $W_N(n, I)$, with $N/n \to \gamma > 0$. Suppose that $\eta(\lambda, c)$ is a jointly continuous bulk shrinker and that $c_n - N/n = O(n^{-2/3})$. Then for $q > 0$,*

$$\|\eta(\mu_{in}, c_n) - 1\|_{\ell_q(\mathbb{R}^N)} \xrightarrow{P} 0. \tag{7.12}$$

The continuity assumption on the loss functions may be formulated as follows. Suppose that $A, B_1, B_2$ are $p$-by-$p$ positive definite matrices, with $A$ satisfying assumption [SPIKE$(\ell_1, \ldots, \ell_r)$] and $\operatorname{spec}(B_k) = [(\eta_{ki}), (v_i)]$, thus $B_1$ and $B_2$ have the same eigenvectors. Set $\eta_1 = \max\{\eta_{11}, \eta_{21}\}$. We assume that for some $q \in [1, \infty]$ and some continuous function $C(\ell_1, \eta_1)$ not depending on $p$, we have

$$\left|L_p(A, B_1) - L_p(A, B_2)\right| \leq C(\ell_1, \eta_1)\|\eta_1 - \eta_2\|_{\ell_q(\mathbb{R}^p)} \tag{7.13}$$

whenever $\|\eta_1 - \eta_2\|_{\ell_q(\mathbb{R}^p)} \leq 1$. Condition (7.13) is satisfied for all 26 of the loss functions of Section 3, as is verified in Proposition 1 in SI.

In the next proposition, we adopt the convention that estimators $\hat{\Sigma}_\eta$ of (1.7) and $\hat{\Sigma}_{\eta,r}$ of (1.13) are constructed with a jointly continuous bulk shrinker, which we denote $\eta(\lambda, c_n)$.

PROPOSITION 2. *Adopt models* [ASY$(\gamma)$] *and* [SPIKE$(\ell_1, \ldots, \ell_r)$]. *Suppose also that the family $L = \{L_p\}$ of loss functions is orthogonally invariant and sum- or max-decomposable, and satisfies continuity condition* (7.13). *If $\eta(\lambda, c_n)$ is a jointly continuous bulk shrinker with $c_n = p_n/n$, then*

$$L_p(\Sigma, \hat{\Sigma}_\eta) - L_p(\Sigma, \hat{\Sigma}_{\eta,r}) \xrightarrow{P} 0,$$

*and so $L_p(\Sigma, \hat{\Sigma}_\eta)$ converges in probability to the deterministic asymptotic loss* (7.8).

PROOF. In the left-hand side of (7.13), substitute $A = \Sigma$, $B_1 = \hat{\Sigma}_\eta$ and $B_2 = \hat{\Sigma}_{\eta,r}$. By definition, $\hat{\Sigma}_\eta$ and $\hat{\Sigma}_{\eta,r}$ share the same eigenvectors. The components of $\eta_1 - \eta_2$ then satisfy

$$\eta_{1i} - \eta_{2i} = \begin{cases} \eta(\lambda_{in}, c_n) - 1, & i \geq r + 1, \\ 0, & 1 \leq i \leq r. \end{cases}$$

We now use (7.11) to compare the eigenvalues $\lambda_{in}$ of the spiked model to those of a suitable white Wishart matrix to which Proposition 1 applies. The function

$\eta^{\uparrow}(\mu, c) = \max\{\eta(\lambda, c), 1 \le \lambda \le \mu\}$ and is nondecreasing and jointly continuous. Hence $\eta(\lambda_{in}, c_n) \le \eta^{\uparrow}(\lambda_{in}, c_n) \le \eta^{\uparrow}(\mu_{i-r,n}, c_n)$, and so

$$\sum_{i=r+1}^{p} [\eta(\lambda_{in}, c_n) - 1]^q \le \sum_{j=1}^{p-r} [\eta^{\uparrow}(\mu_{jn}, c_n) - 1]^q,$$

with a corresponding bound for $q = \infty$. From continuity condition (7.13),

$$\left| L_p(\Sigma, \hat{\Sigma}_\eta) - L_p(\Sigma, \hat{\Sigma}_{\eta,r}) \right| \le C\big(\ell_1, \eta(\lambda_{1n}, c_n)\big) \|\eta^{\uparrow}(\mu_{jn}, c_n) - 1\|_{\ell_q(\mathbb{R}^{p-r})}.$$

The constant $C(\ell_1, \eta(\lambda_{1n}, c_n))$ remains bounded by (1.2). The $\ell_q$ norm converges to 0 in probability, applying Proposition 1 to the eigenvalues of $W_{p_n - r}(n, I)$, with $N = p_n - r$, noting that $c_n - N/n = r/n = O(n^{-2/3})$. $\square$

7.2. *Asymptotic loss for discontinuous optimal shrinkers*. Formula (6.5) showed that the optimal shrinker $\eta^*(\lambda, \gamma)$ for operator norm losses $L^{O,1}$, $L^{O,2}$ is *discontinuous* at $\ell = \ell_+(\gamma) = 1 + \sqrt{\gamma}$. In this section, we show that when $\eta^*$ is used, a deterministic asymptotic loss exists for $L^{O,1}$, but *not* for $L^{O,2}$. The reason will be seen to lie in the behavior of the optimal component loss $F_*(\ell) = L_2[A(\ell), B(\ell, \eta^*)]$. Indeed, calculation based on (6.2), (6.5) shows that for $\ell \ge \ell_+$,

$$F_*(\ell) = \left[\frac{\ell^a \gamma(\ell - 1)}{\ell - 1 + \gamma}\right]^{1/2} \to F_*(\ell_+) = \begin{cases} \sqrt{\gamma}, & a = 1, \\ \dfrac{\sqrt{\gamma}}{1 + \sqrt{\gamma}}, & a = -1 \end{cases}$$

as $\ell \downarrow \ell_+$, where indices $a = 1$ and $-1$ correspond to $F_*^{O,1}$ and $F_*^{O,2}$ respectively. Importantly, $F_*^{O,1}$ is strictly increasing on $[\ell_+, \infty)$ while $F_*^{O,2}$ is strictly decreasing there.

PROPOSITION 3. *Adopt models* $[\mathrm{ASY}(\gamma)]$ *and* $[\mathrm{SPIKE}(\ell_1, \dots, \ell_r)]$ *with* $\ell_r > \ell_+(\gamma)$. *Consider the optimal shrinker* $\eta^*(\lambda, \gamma_n)$ *with* $\gamma_n = p_n/n$ *given by* (6.5) *for both* $L^{O,1}$ *and* $L^{O,2}$. *For* $L^{O,1}$, *the asymptotic loss is well-defined*:

$$\|\hat{\Sigma}_\eta - \Sigma\|_\infty - \|\hat{\Sigma}_{\eta,r} - \Sigma\|_\infty \xrightarrow{P} 0. \tag{7.14}$$

*However, for* $L^{O,2}$,

$$\|\hat{\Sigma}_\eta^{-1} - \Sigma^{-1}\|_\infty - \|\hat{\Sigma}_{\eta,r}^{-1} - \Sigma^{-1}\|_\infty \xrightarrow{\mathcal{D}} W, \tag{7.15}$$

*where* $W$ *has a two point distribution in which*

$$W = \begin{cases} F_*^{O,2}(\ell_+) - F_*^{O,2}(\ell_r) & \text{with prob } 1 - F_1(0), \\ 0 & \text{otherwise}, \end{cases}$$

*and* $F_1(0) = \mathbb{P}\{TW_1 \le 0\}$ *for a real Tracy–Widom variate* $TW_1$ [67].

Roughly speaking, there is positive limiting probability that the largest noise eigenvalue will exit the bulk distribution, and in such cases the corresponding component loss $F_*(\ell_+)$—which is due to noise alone—exceeds the largest component loss due to any of the $r$ spikes, namely $F_*(\ell_r)$. Essentially, this occurs because precision losses $L^{\{O,F,N\},2}(a\Sigma, a\hat{\Sigma})$ *decrease* as signal strength $a$ increases. The effect is not seen for $L^{\{F,N\},2}$ because the optimal shrinkers in those cases are continuous at $\ell_+$.

PROOF. For the proof, write $\|\cdot\|$ for $\|\cdot\|_\infty$. Let $W = [W_1\ W_2]$ be the orthogonal change of basis matrix constructed in Lemma 7, with $W_1$ containing the first $2r$ columns. We treat the two losses $L^{O,1}$ and $L^{O,2}$ at once using an exponent $a = \pm 1$, and write $\eta^a(\lambda)$ for $\eta^a(\lambda, \gamma_n)$. Thus, let

$$\Delta = \Delta_n = \hat{\Sigma}_\eta^a - \hat{\Sigma}_{\eta,r}^a = \sum_{i=r+1}^{p} [\eta^a(\lambda_i) - 1] v_i v_i',$$

and observe that the loss of the rank-aware estimator

$$\Psi = \Psi_n = \hat{\Sigma}_{\eta,r}^a - \hat{\Sigma}^a = \sum_{i=1}^{r} [\eta^a(\lambda_i) - 1] v_i v_i' - \sum_{i=1}^{r} (\ell_i^a - 1) u_i u_i'$$

lies in the column span of $W_1$. We have $\hat{\Sigma}_\eta^a - \Sigma^a = \Psi_n + \Delta_n$, and the main task will be to show that for $a = \pm 1$,

$$\|\Psi_n + \Delta_n\| = \max(\|\Psi_n\|, \|\Delta_n\|) + o_P(1). \tag{7.16}$$

Assuming the truth of this for now, let us derive the proposition. The quantities of interest in (7.14), (7.15) become

$$\begin{aligned} \|\hat{\Sigma}_\eta^a - \hat{\Sigma}^a\| - \|\hat{\Sigma}_{\eta,r}^a - \hat{\Sigma}^a\| &= \|\Psi_n + \Delta_n\| - \|\Psi_n\| \\ &= \max(\|\Delta_n\| - \|\Psi_n\|, 0) + o_P(1). \end{aligned}$$

First, note from Lemma 7 that

$$\|\Psi_n\| \xrightarrow{\text{a.s.}} \max_{1 \le i \le r} F_*(\ell_i). \tag{7.17}$$

Observe that for *both* $a = 1$ and $-1$,

$$\|\Delta_n\| = \max_{i \ge r+1} |\eta^{*a}(\lambda_{in}) - 1| = |\eta^a(\lambda_{r+1,n}) - 1|.$$

The rescaled noise eigenvalue $p^{2/3}(\lambda_{r+1,n} - \lambda_+(\gamma_n)) \xrightarrow{\mathcal{D}} \sigma(\gamma) W$ has a limiting real Tracy–Widom distribution with scale factor $\sigma(\gamma) > 0$ [5], Proposition 5.8. Hence, using the discontinuity of the optimal shrinker $\eta^*$, and the square root singularity from above

$$\eta^*(\lambda_{r+1,n}, \gamma_n) = \begin{cases} \ell_+(\gamma_n) + O_P(p^{-1/3}), & \lambda_{r+1,n} > \lambda_+(\gamma_n), \\ 1, & \lambda_{r+1,n} \le \lambda_+(\gamma_n). \end{cases}$$

Consequently, recalling that $F_*(\ell_+) = |(1+\sqrt{\gamma})^a - 1|$, we have

$$\|\Delta_n\| \to_P F_*(\ell_+) I(TW > 0). \tag{7.18}$$

For $L^{O,1}$, with $a = 1$, $F_*(\ell)$ is strictly increasing and so from (7.17) and (7.18), we obtain $\|\Psi_n\| \geq \|\Delta_n\| + o_P(1)$, and hence (7.14). For $L^{O,2}$, with $a = -1$, $F_*(\ell)$ is strictly decreasing and so on the event $TW > 0$,

$$\|\Delta_n\| - \|\Psi_n\| \xrightarrow{\mathcal{D}} F_*(\ell_+) - F_*(\ell_r) > 0,$$

which leads to (7.15), and hence the main result.

It remains to prove (7.16). For a symmetric block matrix,

$$\max(\|A\|, \|C\|) \leq \left\| \begin{pmatrix} A & B \\ B' & C \end{pmatrix} \right\| \leq \max(\|A\|, \|C\|) + \|B\|. \tag{7.19}$$

Apply this to $W'(\Psi + \Delta)W$ with

$$\begin{aligned} A_n &= W_1'(\Psi + \Delta)W_1, \\ B_n &= W_1'(\Psi + \Delta)W_2 = W_1'\Delta W_2, \\ C_n &= W_2'(\Psi + \Delta)W_2 = W_2'\Delta W_2, \end{aligned}$$

since $\Psi W_2 = 0$. Hence

$$\|\Psi_n + \Delta_n\| = \max(\|A_n\|, \|C_n\|) + O_P(\|B_n\|). \tag{7.20}$$

We now show that $\|\Delta W_1\| \xrightarrow{P} 0$. Using notation from Lemma 5,

$$W_1 = [U_r \quad V_r] R^{-1} = \left[U_r \quad (V_r - U_r R_{12}) R_{22}^{-1}\right].$$

Since $\Delta v_k = 0$ for $k = 1, \ldots, r$,

$$\|\Delta W_1\| \leq \|\Delta U_r\| (1 + \|R_{12} R_{22}^{-1}\|).$$

From (7.9), we have $\|R_{12} R_{22}^{-1}\| \to \|\Delta_r(c/s)\| = c(\ell_1)/s(\ell_1)$, and hence is bounded. Observe that $\Delta u_k = \sum_{i=r+1}^{p} \delta_{in}^a (v_i' u_k) v_i$, where we have set $\delta_{in} = \eta(\lambda_i, \gamma_n) - 1$. Note from (6.5) that $\delta_{in} = 0$ unless $\lambda_i > \lambda_+(\gamma_n)$. With $N_n = \#\{i \geq r+1 : \lambda_{in} > \lambda_+(\gamma_n)\}$, we then have

$$\|\Delta U_r\| \leq \sqrt{r} \max_{k=1,\ldots,r} \|\Delta u_k\|_2 \leq \sqrt{r} \|\Delta\| N_n \max_{k \leq r; i > r} |v_i' u_k|. \tag{7.21}$$

From (7.18), we have $\|\Delta_n\| = O_P(1)$. Since each $v_i, i > r$ is uniformly distributed on $S^{p-1}$, a simple union bound based on (7.23) below yields

$$\max_{i > r, k \leq r} (v_i' u_k)^2 = O_P\left(\frac{\log p}{p}\right). \tag{7.22}$$

It remains to bound $N_n$. From the interlacing inequality (7.11),

$$N_n \leq \tilde{N}_n = \#\{j \geq 1 : \mu_{jn} > \lambda_+(\gamma_n)\},$$

where $\{\mu_{jn}\}$ are the eigenvalues of a white Wishart matrix $W_{p_n-r}(n, I)$. This quantity is bounded in [36], Theorem 2(c), which says that $\tilde{N}_n = O_p(1)$. In more detail, we make the correspondences $N \leftarrow p_n - r$, $\gamma_N \leftarrow (p_n - r)/n$ and $c_N \leftarrow p_n/n$ so that $c_N - \gamma_N = r/n = o(n^{-2/3})$ and obtain $E\tilde{N}_n \to c_0 \doteq 0.17$.

From (7.21) and the preceding two paragraphs, we conclude that $\|\Delta U_r\| = O_P(p^{-1/2}\sqrt{\log p})$ and so $\|\Delta W_1\| \xrightarrow{P} 0$.

Returning to (7.20), we deduce now that $\|B_n\| \le \|\Delta W_1\| \xrightarrow{P} 0$. From the definition of $W_1$, we have $\|W_1' \Psi W_1\| = \|\Psi\|$, and hence the inequalities:

$$\big|\|A_n\| - \|\Psi_n\|\big| \le \|W_1' \Delta W_1\| \xrightarrow{P} 0.$$

Now observe that $\|C_n\| \le \|\Delta_n\|$. Apply (7.19) to $W'\Delta W$ to get

$$\|\Delta_n\| \le \|C_n\| + \|W_1' \Delta W_1\| + \|W_2' \Delta W_1\|,$$

and hence that $\|C_n\| \ge \|\Delta_n\| - o_P(1)$. Thus $\|C_n\| = \|\Delta_n\| + o_P(1)$. Inserting these results into (7.20), we obtain

$$\|\Psi_n + \Delta_n\| = \max(\|A_n\|, \|C_n\|) + o_P(1) = \max(\|\Psi_n\|, \|\Delta_n\|) + o_P(1),$$

which completes the proof of (7.16), and hence of Proposition 3. □

Finally, we record a concentration bound for the uniform distribution on spheres. While more sophisticated results are known [47], an elementary bound suffices for us.

LEMMA 8. *If $U$ is uniformly distributed on $S^{n-1}$ and $u \in S^{n-1}$ is fixed, then for $M > 0$ and $n \ge 4$,*

$$P\big(|\langle U, u\rangle| \ge 2\sqrt{Mn^{-1}\log n}\big) < \sqrt{\pi/2} \cdot n^{1/2-M}. \tag{7.23}$$

PROOF. Since $U_1^2 := \langle U, u\rangle^2$ has the Beta$(\frac{1}{2}, \frac{n-1}{2})$ distribution,

$$P(U_1^2 \ge a) \le B\left(\frac{1}{2}, \frac{n-1}{2}\right)^{-1} \int_a^1 t^{-\frac{1}{2}}(1-t)^{\frac{n-3}{2}}\, dt \le \gamma_n (1-a)^{\frac{n}{2}-1},$$

where by Gautschi's inequality [54, 56], (5.6.4),

$$\gamma_n = B\left(\frac{1}{2}, \frac{1}{2}\right) \Big/ B\left(\frac{1}{2}, \frac{n-1}{2}\right) = \sqrt{\pi}\,\Gamma\left(\frac{n}{2}\right) \Big/ \Gamma\left(\frac{n-1}{2}\right) < \sqrt{\pi n/2}.$$

Since $(1 - x/m)^m < e^{-x}$ for $x, m > 0$, and $4/n \ge 2/(n-2)$ for $n \ge 4$,

$$P(U_1^2 \ge 4Mn^{-1}\log n) < \sqrt{\pi n/2}\left(1 - \frac{M\log n}{n/2 - 1}\right)^{n/2-1} < \sqrt{\pi/2} \cdot n^{1/2-M}. \qquad \square$$

**8. Optimality among equivariant procedures.** The notion of optimality in asymptotic loss, with which we have been concerned so far, is relatively weak. Also, the class of covariance estimators we have considered, namely procedures that apply the *same* univariate shrinker to all empirical eigenvalues, is fairly restricted.

Consider the much broader class of orthogonally-equivariant procedures for covariance estimation [49, 53, 65], in which estimates take the form $\hat{\Sigma} = V \Delta V'$. Here, $\Delta = \Delta(\Lambda)$ is *any* diagonal matrix that depends on the empirical eigenvalues $\Lambda$ in possibly a more complex way than the simple scalar element-wise shrinkage $\eta(\Lambda)$ we have considered so far. One might imagine that the extra freedom available with more general shrinkage rules would lead to improvements in loss, relative to our optimal scalar nonlinearity; certainly the proposals of [46, 49, 65] are of this more general type.

The smallest achievable loss by any orthogonally equivariant procedure is obtained with the "oracle" procedure $\hat{\Sigma}^{\text{oracle}} = V \Delta^{\text{oracle}} V'$, where

$$\Delta^{\text{oracle}} = \arg\min_{\Delta} L\bigl(\Sigma, V \Delta V'\bigr), \tag{8.1}$$

the minimum being taken over diagonal matrices with diagonal entries $\geq 1$. Clearly, this optimal performance is not attainable, since the minimization problem explicitly demands perfect knowledge of $\Sigma$, precisely the object that we aim to recover. This knowledge is never available to us in practice, hence the label *oracle*.[5] Nevertheless, this optimal performance is a legitimate benchmark.

Interestingly, at least for the popular Frobenius and Stein losses, our optimal nonlinearities $\eta^*$ deliver oracle-level performance—asymptotically. To state the result, recall expression (6.2) for these losses: $F(\ell, \Delta) = L_2(A(\ell), B(\ell, \Delta))$.

THEOREM 2 (Asymptotic optimality among all equivariant procedures). *Let $L$ denote either the direct Frobenius loss $L^{F,1}$ or the Stein loss $L^{\text{st}}$. Consider a problem sequence satisfying assumptions* [ASY($\gamma$)] *and* [SPIKE($\ell_1, \dots, \ell_r$)]. *We have*

$$\lim_{n\to\infty} L_{p_n}\bigl(\Sigma, \hat{\Sigma}^{\text{oracle}}\bigr) =_P L_\infty(\ell_1 \dots, \ell_r | \eta^*) = \sum_{i=1}^{r} F\bigl(\ell_i, \eta^*\bigr),$$

*where $\eta^*$ is the optimal shrinker for the losses $L^{F,1}$ or $L^{\text{st}}$ in Table 2.*

In short, the shrinker $\eta^*(\cdot)$, which has been designed to minimize the *limiting* loss, asymptotically delivers the same performance as the oracle procedure, which

[5] The oracle procedure does not attain zero loss since it is "doomed" to use the eigenbasis of the empirical covariance, which is a random basis corrupted by noise, to estimate the population covariance.

has the lowest possible loss, in finite-$n$, over the entire class of covariance estimators by arbitrary high-dimensional shrinkage rules. On the other hand, by definition, the oracle procedure outperforms every orthogonally-equivariant statistical estimator. We conclude that $\eta^*$—as one such orthogonally-invariant estimator—is indeed optimal (in the sense of having the lowest limiting loss) among all orthogonally invariant procedures. While we only discuss the cases $L^{F,1}$ and $L^{\mathrm{st}}$, we suspect that this theorem holds true for many of the 26 loss functions considered.

PROOF. We first outline the approach. We can write $\Sigma$ and $\Sigma^{-1}$ in the form $I + F$, and $\hat{\Sigma}_\Delta = I + \tilde{\Delta}$ with

$$F = \sum_{k=1}^{r} \beta_k u_k u_k', \qquad \tilde{\Delta} = \sum_{i=1}^{p} \tilde{\Delta}_i v_i v_i',$$

where $\beta_k = \ell_k - 1$ for $L^{F,1}$ and $\ell_k^{-1} - 1$ for $L^{\mathrm{st}}$ and $\tilde{\Delta}_i = \Delta_i - 1$. Write

$$\operatorname{tr} F\tilde{\Delta} = \sum_{i=1}^{p} \tilde{\Delta}_i b_i, \qquad b_i := \sum_{k=1}^{r} \beta_k (u_k' v_i)^2. \tag{8.2}$$

For both $L = L^{F,1}$ and $L^{\mathrm{st}}$, we establish a decomposition

$$L_p(\Sigma, \hat{\Sigma}_\Delta) = \sum_{i=1}^{r} F(\ell_i, \Delta_i) + a(\Delta_i - 1)\varepsilon_i + \sum_{i=r+1}^{p} H(b_i, \Delta_i). \tag{8.3}$$

Here, $a$ is a constant depending only on the loss function,

$$\varepsilon_i = b_i - \beta_i c(\ell_i)^2, \tag{8.4}$$

and

$$H(b, \Delta) = \begin{cases} (\Delta - 1)^2 - 2(\Delta - 1)b & \text{for } L^{F,1}, \\ (\Delta - 1)(1 + b) - \log \Delta & \text{for } L^{\mathrm{st}}. \end{cases} \tag{8.5}$$

Decomposition (8.3) shows that the oracle estimator (8.1) may be found term by term, using just univariate minimization over each $\Delta_i$. Consider the first sum in (8.3), and let $\tilde{F}(\ell_i, \Delta_i)$ denote the summand. We will show that

$$\min_{\Delta_i} \tilde{F}(\ell_i, \Delta_i) \xrightarrow{P} \min_{\Delta_i} F(\ell_i, \Delta_i), \tag{8.6}$$

and that

$$\sum_{i=r+1}^{p} \min_{\Delta_i} H(b_i, \Delta_i) = O_P\left(\frac{\log^2 p}{p}\right). \tag{8.7}$$

Together (8.6) and (8.7) establish the theorem.

Turning to the details, we begin by showing (8.3). For Frobenius loss, we have from our definitions and (8.2) that

$$\|\hat{\Sigma}_\Delta - \Sigma\|_F^2 = \operatorname{tr}(\tilde{\Delta} - F)(\tilde{\Delta} - F)' = \sum_{i=1}^{p}(\Delta_i - 1)^2 - 2(\Delta_i - 1)b_i + \sum_{i=1}^{r}(\ell_i - 1)^2.$$

For $i \geq r+1$, each summand in the first sum equals $H(b_i, \Delta_i)$ and for $i \leq r$, we use the decomposition $b_i = (\ell_i - 1)c(\ell_i)^2 + \varepsilon_i$. We obtain decomposition (8.3) with $a = -2$ and

$$F(\ell, \Delta) = (\ell - 1)^2 - 2(\ell - 1)(\Delta - 1)c^2 + (\Delta - 1)^2.$$

For Stein's loss, our definitions yield

$$\begin{aligned} L^{\mathrm{st}}(\Sigma, \hat{\Sigma}_\Delta) &= \operatorname{tr}\tilde{\Delta} + \operatorname{tr} F + \operatorname{tr} F\tilde{\Delta} - \log(|\hat{\Sigma}_\Delta|/|\Sigma|) \\ &= \sum_{i=1}^{p} \tilde{\Delta}_i(1 + b_i) - \log \Delta_i + \sum_{k=1}^{r} \beta_k + \log \ell_k. \end{aligned}$$

Again, for each $i \geq r+1$, each summand in the first sum equals $H(b_i, \Delta_i)$ and with $b_i = (\ell_i - 1)c(\ell_i)^2 + \varepsilon_i$ we obtain (8.3) with $a = 1$ and

$$F(\ell, \Delta) = (\ell^{-1} - 1) + (\Delta - 1)(c^2/\ell + s^2) - \log(\Delta/\ell).$$

It remains to verify (8.6) and (8.7). Theorem 1 says that for $1 \leq i \leq r$,

$$\varepsilon_i = \sum_{k=1}^{r} \beta_k\big[(u_k' v_i)^2 - \delta_{k,i} c(\ell_i)^2\big] \xrightarrow{P} 0,$$

which yields (8.6). From (8.5), we observe that in our two cases

$$h(b) := \min_{\Delta} H(b, \Delta) = \begin{cases} -b^2 \\ -b + \log(1 + b) \end{cases} = O(b^2). \tag{8.8}$$

Now, using (8.2) and (7.22), we get

$$\max_{r+1 \leq i \leq p} |b_i| \leq r \max_{1 \leq k \leq r} |\beta_k| \cdot \max_{i > r, k \leq r} (u_k' v_i)^2 = O_P\left(\frac{\log p}{p}\right).$$

From the previous two displays, we conclude

$$\sum_{i=r+1}^{p} \min_{\Delta_i} H(b_i, \Delta_i) = \sum_{i=r+1}^{p} h(b_i) = O_P\left(\frac{\log^2 p}{p}\right),$$

which is (8.7), and so completes the full proof. □

**9. Optimal shrinkage with common variance $\sigma^2 \neq 1$.** Simply put, the spiked covariance model is a proportional growth independent-variable Gaussian model, where all variables, except the first $r$, have common variance $\sigma$. Literature on the spiked model often simplifies the situation by assuming $\sigma^2 = 1$, as we have done in our assumption [SPIKE($\ell_1, \dots, \ell_r$)] above. To consider optimal shrinkage in the case of general common variance $\sigma^2 > 0$, assumption [SPIKE($\ell_1, \dots, \ell_r$)] has to be replaced by

[SPIKE($\ell_1, \dots, \ell_r | \sigma^2$)] The population eigenvalues in the $n$th problem, namely the eigenvalues of $\Sigma_{p_n}$, are given by $(\ell_1, \dots, \ell_r, \sigma^2, \dots, \sigma^2)$, where the number of "spikes" $r$ and their amplitudes $\ell_1 > \cdots > \ell_r \geq 1$ are fixed independently of $n$ and $p_n$.

In this section, we show how to use an optimal shrinker, designed for the spiked model with common variance $\sigma^2 = 1$, in order to construct an optimal shrinker for a general common variance $\sigma^2$, namely, under assumptions [ASY($\gamma$)] and [SPIKE($\ell_1, \dots, \ell_r | \sigma^2$)].

9.1. *$\sigma^2$ known.* Let $\Sigma_p$ and $S_{n,p}$ be population and sample covariance matrices, respectively, under assumption [SPIKE($\ell_1, \dots, \ell_r | \sigma^2$)]. When the value of $\sigma$ is known, the matrices $\tilde{\Sigma}_p = \Sigma_p / \sigma^2$ and the sample covariance matrix $\tilde{S}_{n,p} = S_{n,p} / \sigma^2$ constitute population and sample covariance matrices, respectively, under assumption [SPIKE($\ell_1, \dots, \ell_r$)]. Let $L$ be any of the loss families considered above and let $\eta$ be a shrinker. Define the shrinker $\tilde{\eta}$ corresponding to $\eta$ by

$$\tilde{\eta} : \lambda \mapsto \sigma^2 \cdot \eta\big(\lambda / \sigma^2\big). \tag{9.1}$$

Observe that for each of the loss families we consider, $L_p(\sigma^2 A, \sigma^2 B) = \sigma^{2\kappa} L_p(A, B)$, where $\kappa \in \{-2, -1, 0, 1, 2\}$ depends on the family $\{L_p\}$ alone. Hence

$$L_p\big(\Sigma_p, \hat{\Sigma}_{\tilde{\eta}}(S_{n,p})\big) = \sigma^{2\kappa} L_p\big(\tilde{\Sigma}_p, \hat{\Sigma}_\eta(\tilde{S}_{n,p})\big).$$

It follows that if $\eta^*$ is the optimal shrinker for the loss family $L$, in the sense of Definition 6, under Assumption [SPIKE($\ell_1, \dots, \ell_r$)], then $\tilde{\eta}^*$ is the optimal shrinker for $L$ under Assumption [SPIKE($\ell_1, \dots, \ell_r | \sigma^2$)]. Formula (9.1) therefore allows us to translate each of the optimal shrinkers given above to a corresponding optimal shrinker in the case of a general common variance $\sigma^2 > 0$.

9.2. *$\sigma^2$ unknown.* In practice, even if one is willing to assume a common variance $\sigma^2$ and subscribe to the spiked model, the value of $\sigma^2$ is usually unknown. Assume however that we have a sequence of estimators $\{\hat{\sigma}_n\}_{n=1,2,\dots}$, where for each $n$, $\hat{\sigma}_n$ is a real function of a $p_n$-by-$p_n$ positive definite symmetric matrix argument. Assume further that under the spiked model with general common variance $\sigma^2$, namely under assumptions [ASY($\gamma$)] and [SPIKE($\ell_1, \dots, \ell_r | \sigma^2$)], the sequence of estimators is consistent in the sense that $\hat{\sigma}_n(S_{n,p_n}) \to \sigma$, almost surely. For a continuous shrinker $\eta$, define a sequence of shrinkers $\{\tilde{\eta}_n\}_{n=1,2,\dots}$ by

$$\tilde{\eta}_n : \lambda \mapsto \hat{\sigma}_n^2 \cdot \eta(\lambda/\hat{\sigma}_n^2). \tag{9.2}$$

Again for each of the loss families we consider, almost surely,

$$\lim_{n\to\infty} L_{p_n}(\Sigma_{p_n}, \hat{\Sigma}_{\tilde{\eta}_n}(S_{n,p_n})) = \sigma^{2\kappa} \lim_{n\to\infty} L_{p_n}(\tilde{\Sigma}_{p_n}, \hat{\Sigma}_{\eta}(\tilde{S}_{n,p_n})).$$

We conclude that, using (9.2), any consistent sequence of estimators $\hat{\sigma}_n$ yields a sequence of shrinkers with the same asymptotic loss as the optimal shrinker for known $\sigma^2$. In other words, at least inasmuch as the asymptotic loss is concerned, under the spiked model, there is no penalty for not knowing $\sigma^2$.

Estimation of $\sigma^2$ under Assumption [SPIKE($\ell_1, \dots, \ell_r | \sigma^2$)] has been considered in [41, 58, 61] where several approaches have been proposed. As an simple example of a consistent sequence of estimators $\hat{\sigma}_n$, we consider the following simple and robust approach based on matching of medians [25]. The underlying idea is that for a given value of $n$ the sample eignevalues $\lambda_{r+1}, \dots, \lambda_{p_n}$ form an approximate Marčenko–Paster bulk inflated by $\sigma^2$, and that a median sample eigenvalue is well suited to detect this inflation as it is unaffected by the sample spikes $\lambda_1, \dots, \lambda_r$.

Define, for a symmetric $p$-by-$p$ positive definite matrix $S$ with eigenvalues $\lambda_1, \dots, \lambda_p$ the quantity

$$\mu(S) = \frac{\lambda_{\mathrm{med}}}{\mu_\gamma}, \tag{9.3}$$

where $\lambda_{\mathrm{med}}$ is a median of $\lambda_1, \dots, \lambda_p$ and $\mu_\gamma$ is the median of the Marčenko–Pastur distribution, namely, the unique solution in $\lambda_-(\gamma) \le x \le \lambda_+(\gamma)$ to the equation

$$\int_{\lambda_-(\gamma)}^{x} \frac{\sqrt{(\lambda_+(\gamma) - t)(t - \lambda_-(\gamma))}}{2\pi\gamma t}\, dt = \frac{1}{2}, \tag{9.4}$$

where as before $\lambda_\pm(\gamma) = (1 \pm \sqrt{\gamma})^2$. Note that the median $\mu_\gamma$ is not available analytically but can easily be obtained numerically, for example, using remarks on the Marčenko–Pastur cumulative distribution function included in SI. Now for a sequence $\{S_{n,p_n}\}$ of sample covariance matrices, define the sequence of estimators:

$$\hat{\sigma}_n : S_{n,p_n} \mapsto \sqrt{\mu(S_{n,p_n})}. \tag{9.5}$$

LEMMA 9. *Let $\sigma^2 > 0$, and assume* [ASY($\gamma$)] *and* [SPIKE($\ell_1, \dots, \ell_r | \sigma^2$)]. *Then almost surely*

$$\lim_{n\to\infty} \hat{\sigma}_n(S_{n,p_n}) = \sigma.$$

In summary, using (9.1) (for $\sigma^2$ known) or (9.2) with (9.5) (for $\sigma^2$ unknown) one can use the optimal shrinkers for each of the loss families discussed above, designed for the case $\sigma = 1$, to construct a shrinker that is optimal, for the same loss family, under the spiked model with common variance $\sigma^2 \neq 1$.

**10. Discussion.** In this paper, we considered covariance estimation in high dimensions, where the dimension $p$ is comparable to the number of observations $n$. We chose a fixed-rank principal subspace, and let the dimension of the problem grow large. A different asymptotic framework for covariance estimation would choose a principal subspace whose rank is a fixed *fraction* of the problem dimension; that is, the rank of the principal subspace is growing rather than fixed. (In the sibling problem of matrix denoising, compare the "spiked" setup [25, 26, 61] with the "fixed fraction" setup of [14].)

In the fixed fraction framework, some of underlying phenomena remain qualitatively similar to those governing the spiked model, while new effects appear. Importantly, the relationships used in this paper, predicting the location of the top empirical eigenvalues, as well as the displacement of empirical eigenvectors, in terms of the top theoretical eigenvalues, no longer hold. Instead, a complex nonlinear relation exists between the limiting distribution of the empirical eigenvalues and the limiting distribution of the theoretical eigenvalues, as expressed by the Marčenko–Pastur (MP) relation between their Stieltjes transforms [1, 51].

Covariance shrinkage in the proportional rank model should then, naturally, make use of the so-called *MP Equation*. Noureddine El Karoui [22] proposed a method for debiasing the empirical eigenvalues, namely, for estimating (in a certain specific sense) their corresponding population eigenvalues; Olivier Ledoit and Sandrine Peché [44] developed analytic tools to also account for the inaccuracy of empirical eigenvectors, and Ledoit and Michael Wolf [46] have implemented such tools and applied them in this setting.

The proportional rank case is indeed subtle and beautiful. Yet, the fixed-rank case deserves to be worked out carefully. In particular, the shrinkers we have obtained here in the fixed-rank case are extremely simple to implement, requiring just a few code lines in any scientific computing language. In comparison, the covariance estimation ideas of [22, 46], based on powerful and deep insights from MP theory, require a delicate, nontrivial effort to implement in software, and call for expertise in numerical analysis and optimization. As a result, the simple shrinkage rules we propose here may be more likely to be applied correctly in practice, and to work as expected, even in relatively small sample sizes.

An analogy can be made to shrinkage in the normal means problem, for example [17]. In that problem, often a full Bayesian model applies, and in principle a Bayesian shrinkage would provide an optimal result [9]. Yet, in applications one often wants a simple method which is easy to implement correctly, and which is able to deliver much of the benefit of the full Bayesian approach. In literally thousands of cases, simple methods of shrinkage—such as thresholding—have been chosen over the full Bayesian method for precisely that reason.

**Reproducible research.** In the code supplement [16], we offer a Matlab software library that includes:

1. A function to compute the value of each of the 26 optimal shrinkers discussed to high precision.
2. A function to test the correctness of each of the 18 analytic shrinker formulas provided.
3. Scripts that generate each of the figures in this paper, or subsets of them for specified loss functions.

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## SUPPLEMENTARY MATERIAL

**Proofs and additional results** (DOI: 10.1214/17-AOS1601SUPP; .pdf). In the supplementary material, we provide proofs omitted from the main text for space considerations and auxiliary lemmas used in various proofs. Notably, we prove Lemma 4, and provide detailed derivations of the 17 explicit formulas for optimal shrinkers, as summarized in Table 2. In addition, in the supplementary material we offer a detailed study of the large-$\lambda$ asymptotics (asymptotic slope and asymptotic shift) of the optimal shrinkers discovered in this paper, and tabulate the asymptotic behavior of each optimal shrinker. We also study the asymptotic percent improvement of the optimal shrinkers over naive hard thresholding of the sample covariance eigenvalues.

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