ScreeNOT: EXACT MSE-OPTIMAL SINGULAR VALUE THRESHOLDING IN CORRELATED NOISE

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**ScreeNOT**: Exact MSE-Optimal Singular Value Thresholding in Correlated Noise

David L. Donoho † Matan Gavish † Elad Romanov †

Abstract

We derive a formula for optimal hard thresholding of the singular value decomposition in the presence of correlated additive noise; although it nominally involves unobservables, we show how to apply it even where the noise covariance structure is not a-priori known or is not independently estimable.

The proposed method, which we call **ScreeNOT**, is a mathematically solid alternative to Cattell’s ever-popular but vague Scree Plot heuristic from 1966.

ScreeNOT has a surprising oracle property: it typically achieves exactly, in large finite samples, the lowest possible MSE for matrix recovery, on each given problem instance – i.e. the specific threshold it selects gives exactly the smallest achievable MSE loss among all possible threshold choices for that noisy dataset and that unknown underlying true low rank model. The method is computationally efficient and robust against perturbations of the underlying covariance structure.

Our results depend on the assumption that the singular values of the noise have a limiting empirical distribution of compact support; this model, which is standard in random matrix theory, is satisfied by many models exhibiting either cross-row correlation structure or cross-column correlation structure, and also by many situations where there is inter-element correlation structure. Simulations demonstrate the effectiveness of the method even at moderate matrix sizes. The paper is supplemented by ready-to-use software packages implementing the proposed algorithm.

**Key Words.** Singular value thresholding, Optimal threshold, Scree Plot, Low-rank matrix denoising

**Code Supplement.** Implementation of the proposed algorithm, scripts generating all figures in this paper, and many additional simulations are available at the code supplement [Donoho et al., 2020] and permanently deposited at the Stanford Digital Repository. Note that Python, R and Matlab packages implementing the ScreeNOT algorithm have been published, see the code supplement for more information.

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[1] https://purl.stanford.edu/py196rk3919
1 Introduction

Across a wide variety of scientific and technical fields, practitioners have found many valuable applications of singular value thresholding (SVT). This procedure starts from the singular value decomposition (SVD), which represents the data matrix $Y$ as

$$Y = \sum_{i=1}^{\min(n,p)} y_i \cdot u_i v_i^\top,$$  \hspace{1cm} (1)

using the empirical singular values $\{y_i\}_{i=1}^{\min(n,p)}$, and the empirical left- and right- singular vectors of $Y$, denoted here $u_i$ and $v_i$.

In such applications, it is generally claimed that the small singular values represent ‘noise’ and the large singular values ‘signal’; practitioners attempt to separate signal from noise by setting a threshold $\theta$ (say), and using, in place of $Y$, the partial reconstruction containing only would-be signal components:

$$\hat{X}_\theta = \sum_{i} y_i \mathbb{1}_{\{y_i > \theta\}} \cdot u_i v_i^\top.$$  \hspace{1cm} (2)

How do practitioners determine the threshold $\theta$? Often, by eye. They plot the ordered singular values and spot ‘elbows’. Sometimes, they give this a scholarly veneer by saying they are using the ‘scree-plot method’; they might even formally cite the originator of this folk-tradition, [Cattell, 1966] which still gets more than 1000 citations yearly. According to the method prescribed in that paper, the practitioner plots the values $\{y_i\}$ and uses her eyes to distinguish between ‘signal’ and ‘noise’ singular values of $Y$.

How should they determine the threshold? Relevant theory and methodology literature spans multiple disciplines over multiple decades; we mention only a few entry points, including: [Wold, 1978, Jackson, 1993, Lagerlund et al., 1997, Edfors and Sandell, 1998, Alter et al., 2000, Achlioptas and McSherry, 2001, Azar et al., 2001, Jolliffe, 2005, Price et al., 2006, Hoff, 2006, Bickel and Levina, 2008, Owen and Perry, 2009, Perry, 2009, Chatterjee, 2015, Gavish and Donoho, 2014]. Progress has been made in our understanding of the underlying problem, and many valuable quantitative approaches have been developed - to which we here add one more. Our contribution relies on recent advances in random matrix theory which point, we think convincingly, to the method introduced here. This method typically offers the exact optimal loss available on each specific, finite dataset $Y$.

Our task formalization supposes that: (a) there is an underlying matrix $X$ of fixed rank $r$ - though $X$ and even its rank $r$ are unknown to us; (b) only a potentially loose upper bound on the signal rank $r$ is known; (c) the data matrix $Y$ has the signal+noise form $Y = X + Z$, where $Z$ is a noise matrix with a general covariance structure – also unknown to us; (d) we use hard thresholding of singular values, exactly as in (2) above; (e) we adopt squared error loss:

$$\text{SE}[X|\theta] = ||\hat{X}_\theta - X||_F^2.$$  \hspace{1cm} (3)

As goal, we literally aim to choose a loss-minimizing value $\theta_{\text{opt}} = \theta_{\text{opt}}(Y|X)$ solving:

$$\text{SE}[X|\theta_{\text{opt}}] = \min_\theta \text{SE}[X|\theta].$$  \hspace{1cm} (4)

\footnote{And not some variant, such as soft thresholding or a more general shrinkage.}

\footnote{$||X||_F^2 = \sum_{i,j} X_{ij}^2$ denotes the squared Frobenius norm.}
Aiming for $\theta_{\text{opt}}(Y|X)$ may seem overambitious, as we know only the data matrix $Y$, and not $X$. Wait and see.

Essentially this problem was studied previously by two of the authors in the special case of white noise. [Gavish and Donoho, 2014] supposed that the underlying noise $Z$ matrix has i.i.d Gaussian zero-mean entries and the problem is scaled so that the columns of $Z$ have unit Euclidean squared norm in expectation, and considered a sequence of increasingly large problems. In the square case, when $Y$ has as many rows as columns: the authors found results which, in light of our results below, say that, with eventually overwhelming probability, we have $\theta_{\text{opt}} = 4/\sqrt{3}$. Their analysis relied on then-recent advances in the ‘Johnstone spiked model’ of random matrix theory [Johnstone, 2001]; they proposed a method for white noise with unknown variance, where the threshold formula became $\theta_{\text{opt}} \approx 4/\sqrt{3} \cdot \frac{y_{\text{med}}}{\sqrt{n} \cdot .6528}$, where $y_{\text{med}}$ denotes the median empirical singular value of $Y$.

Understanding the white noise case cannot be the end of the story. Practitioners ordinarily don’t know that their noise is white, and in fact realistic noise models can include correlations between columns, rows, or even general row-column combinations. Fortunately, a broad range of noise models can be studied using appropriate advances that have been made in random matrix theory. In this broader context, as we show, a more general formula for the optimal threshold can be given, which of course reduces to $4/\sqrt{3}$ in the above ‘square-matrix in white noise’ case, but which is inevitably quite a bit more sophisticated in general.

Section 2 below describes ScreeNOT, our proposed deployment of this formula on actual data. The acronym NOT stands for Noise-adaptive Optimal Thresholding; ‘adaptive’ refers to the algorithm’s optimality across a wide range of unknown noise covariances. The prefix ‘Scree’ reminds us that, still today, in many cases, the alternative would simply be ‘eyeballing’ the Scree Plot [Cattell, 1966]. Cattell and his many followers clearly believed that something, some visible feature, in the scree plot – namely, in the collection of data singular values $\{y_i\}$ – could tell us where the noise stopped and the signal began. But what exactly? In a very concrete sense, the ScreeNOT algorithm shows that the information needed to separate signal from noise truly been there in the distribution of empirical singular values, where Cattell and followers all hoped it was - the information now being clearly identified as a specific functional of the CDF of singular values.

The method, once implemented, surprised us by the finite-sample optimality it exhibited; in simulations at reasonable problem sizes it typically achieves the exact minimal loss (4) for the given dataset, even though the method is not entitled to know the underlying low-rank model $X$ or specifics of the noise model on $Z$; we initially expected a weaker and more ‘asymptotic’ optimality property, perhaps similar to the one shown in [Gavish and Donoho, 2014]. Our analysis below proves typicality of such exact optimality in finite samples. This strong optimality is partly due to the penetrating nature of random matrix theory; but also to the very specific task: minimizing squared error loss (3) of singular value thresholding (2).

**Underlying Analysis.** Hoping to make the paper helpful to prospective users of the proposed method, we have made the Introduction and also Section 2 mostly independent of the analysis to come; however, we now very briefly offer mathematically-oriented readers some.

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$\frac{4}{\sqrt{3}}$ is approximately the median of the standard quarter-circle law; see the original paper.

[^4]: That is, the authors of [Gavish and Donoho, 2014] adopted a slightly different viewpoint involving asymptotic MSE, and showed that $4/\sqrt{3}$ is optimal, whereas we consider here exact finite sample MSE loss, and show that with eventually overwhelming probability, $4/\sqrt{3}$ is exactly optimal on each typical realization.

[^5]: $\sqrt{.6528}$ is approximately the median of the standard quarter-circle law; see the original paper.
insight about the approach being followed in later sections and the tools being developed there.

At heart, this paper concerns the asymptotic analysis of a sequence of matrix recovery problems where the problem sizes \( n \) and \( p \) grow to \( \infty \) in a proportional fashion. We assume that the matrix \( X \) has \( r \) nonzero singular values \( x_1, \ldots, x_r \) which are fixed independently of \( n \) and \( p \). About the sequence of random noise matrices \( Z = Z_{n,p} \), we assume that the sequence of empirical cumulative distribution functions (CDF’s) of noise singular values converges to a compactly supported distribution \( F_Z \) with certain qualitative restrictions at boundary of the support.

Using results of Benaych-Georges and Nadakuditi [Benaych-Georges and Nadakuditi, 2012a], we obtain an expression for an asymptotically optimal hard threshold, as a functional \( T(\cdot) \) of the limiting CDF of noise singular values \( F_Z \). The functional is continuous and even differentiable in certain senses.

Admittedly, the limiting CDF of noise singular values \( F_Z \) is not observable to the statistician, as we only observe a sample of the signal+noise singular values mixed together. Performing a kind of amputation and prosthetic extension on the CDF \( F_Y \) of singular values of \( Y \), which we do observe, we construct a modified empirical CDF \( \hat{F}_n \) which consistently estimates the limiting CDF of noise-only singular values. Applying the hard threshold selection functional to this modified empirical CDF \( \hat{F}_n \) gives our proposed method, in the form \( \hat{\theta} = T(\hat{F}_n) \). As we show in Section 2, there is a quite explicit and computationally tractable algorithm for computing \( T(\hat{F}_n) \), which we label \textbf{ScreeNOT}.

Owing to the continuity of the hard threshold functional \( T(\cdot) \), and the consistency of the constructed CDF, the resulting method is a consistent estimator of the underlying asymptotically optimal threshold \( T(F_Z) \). We also prove a finite-sample optimality of the method. Specifically, the ScreeNOT algorithm is shown to be exactly optimal for squared error loss with high probability, in large-enough finite samples, under very general model assumptions. For generic configurations of signal singular values \( (x_i)_{i=1}^r \), there is, in large finite samples, an optimal interval of thresholds, all achieving the optimal MSE at that realization; the consistency of the optimal threshold estimator implies that eventually for large-enough \( n \), with overwhelming probability, the proposed method achieves the exact optimal MSE loss.

**Outline.** This paper is organized as follows. In Section 2 we offer a practical, succinct description of the ScreeNOT algorithm, for the convenience of prospective users. In Section 3 we introduce the signal+noise model used and survey relevant results from random matrix theory. In Section 4 we state our main results regarding the optimality and stability properties of ScreeNOT, both in finite matrix size and asymptotically as the matrix size grows to infinity. In Section 5 we demonstrate the mathematical results in various simulations and numerical examples; for space considerations only a handful of figures are shown, with most simulation results deferred to Appendix C and available in the code supplement [Donoho et al., 2020]. The results are proved in Section 6, with some proofs referred to Appendix A and Appendix B.

**Reproducibility advisory.** Implementation of the proposed algorithm, scripts generating all figures in this paper, and many additional simulations have been permanently deposited and are available at the code supplement [Donoho et al., 2020].
The ScreeNOT Procedure: User-level description

In this section we give a brief self-contained description of our proposed procedure. Note that Python, R and Matlab packages implementing the ScreeNOT algorithm have been published, see the code supplement [Donoho et al., 2020] for more information.

2.1 Procedure API

ScreeNOT selects a hard threshold for singular values, which can in finite samples give the optimal MSE approximation of a low rank matrix from a noisy version; the noise may be correlated, and the threshold will adapt to that appropriately.

2.1.1 Inputs

The user provides these inputs to ScreeNOT:

- $y$: the singular values $y_1, \ldots, y_{\min(n,p)}$ of the data matrix $Y$;
- $n, p$: size parameters of the data matrix $Y$.
- $k$: upper bound on the rank $r$ of the underlying unknown signal matrix $X$ which is to be recovered. This upper bound may be very loose.

2.1.2 Outputs

ScreeNOT returns $\hat{\theta} = \hat{\theta}(Y)$, the value to be used in singular value thresholding.

To use the threshold, the user should reconstruct an approximation to the underlying signal matrix $X$ using the empirical singular values $y_i$ and the empirical singular vectors $u_i$ and $v_i$ as follows:

$$\hat{X}_n = \sum_{i} y_i \mathbb{I}_{\{y_i > \hat{\theta}\}} \cdot u_i v_i^T.$$

In this reconstruction, the singular values smaller than $\hat{\theta}$ are judged to be noise and the corresponding singular decomposition components are ignored.

2.2 Example in a stylized application

We next construct a synthetic-data example, in which we know ground truth for demonstration purposes. The synthetic data $Y = X + Z$ and the invocation of ScreeNOT are based on these ingredients.

**Signal $X$:** The underlying signal matrix, unbeknownst to the hypothetical user, has rank 4, with singular values $(x_1, \ldots, x_4) = (4, 3, 2, 1)$.

**Noise $Z$:** The underlying noise, unbeknownst to the hypothetical user, follows an AR(1) process in the row index, within each column. The AR(1) process has parameter $\rho = .2$, and additionally each entry is divided by $\sqrt{n}$, so to have variance $1/n$.

**Problem Size:** $n = p = 500$

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That is, the columns of $Z$ are independent and distributed as $z_i \sim \mathcal{N}(\mu, \sigma^2)$, where the random vector $z$ has entries:

$$z_i = \epsilon_1, \quad z_i = \rho \cdot z_{i-1} + (1 - \rho) \cdot \epsilon_i \quad \text{for} \ 2 \leq i \leq p,$$

where $\epsilon_1, \ldots, \epsilon_p \sim \mathcal{N}(0,1)$. 

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6
Rank bound: \( k = 12 \). The user specifies a bound of \( k = 12 \) on the possible rank of the signal. Figure 1 shows a so-called scree plot [Cattell, 1966] of the first 30 empirical singular values \( y_i \). For this particular instance, it is verified (by exhaustive search) that the minimal loss is attained by retaining the first three principal components of \( Y \); in other words, thresholding at any point \( \theta \in (y_3, y_4) \) is optimal. The threshold \( \hat{\theta} \) returned by the ScreeNOT procedure is indicated by the green horizontal line, and, indeed, it falls inside the optimal interval.

2.3 Internals of the Procedure

We briefly describe the computational task performed by ScreeNOT.

Step 1. Sort the singular values in non-increasing order: \( y_1 \geq \ldots \geq y_p \).

Step 2. Compute the “pseudo singular values”:

\[
\tilde{y}_i = y_{k+1} + \frac{1 - \left(\frac{i - 1}{k+1}\right)^{2/3}}{2^{2/3} - 1} (y_{k+1} - y_{2k+1}) \quad \text{for } i = 1, \ldots, k,
\]

and set \( \tilde{y}_i = y_i \) for \( i = k + 1, \ldots, p \).

Step 3. Define the four scalar functions \( \varphi, \tilde{\varphi}, \varphi', \tilde{\varphi}' \) by

\[
\varphi(y) = \frac{1}{p} \sum_{i=1}^{p} \frac{y}{y^2 - \tilde{y}_i^2}, \quad \varphi'(y) = -\frac{1}{p} \sum_{i=1}^{p} \frac{y^2 + \tilde{y}_i^2}{(y^2 - \tilde{y}_i^2)^2},
\]

and

\[
\tilde{\varphi}(y) = \gamma \varphi(y) + \frac{1 - \gamma}{y}, \quad \tilde{\varphi}'(y) = \gamma \varphi'(y) - \frac{1 - \gamma}{y^2}.
\]

\(^7\)We assume that \( 2k + 1 < p \). Our proposed estimator is expected to perform poorly when \( k \) is large compared to \( p \).
Now define

$$\Psi(y) = y \cdot \left( \frac{\phi'(y)}{\phi(y)} + \frac{\tilde{\phi}'(y)}{\tilde{\phi}(y)} \right).$$

**Step 4.** Assuming that $\tilde{y}_1, \ldots, \tilde{y}_p$ are not all zero, the function $y \mapsto \Psi(y)$ can be shown to be continuous and strictly increasing for $y > \tilde{y}_1$. Moreover, $\lim_{y \searrow \tilde{y}} \Psi = -\infty$ and $\Psi(\infty) = -2$. The computed hard threshold is the unique value $\hat{\theta}$ satisfying

$$\Psi(\hat{\theta}) = -4. \quad (5)$$

This equation is then solved numerically (by binary search, say).

**Step 5.** The algorithm returns the value $\hat{\theta}$.

Evidently, the procedure as stated costs $O(n \log(n))$ flops; the dominant cost is sorting the singular values; ordinarily of course, sorting is performed anyway as part of a standard SVD. In that situation, the additional computational effort is $O(n)$, which is unimportant compared to the cost of the underlying SVD.

### 2.4 How the procedure works on the stylized application

Figure 2(a) shows a plot of $\Psi(\theta)$ as a function of $\theta$. The horizontal blue line indicates the desired level $-4$. The vertical green line indicates the crossing point, $\hat{\theta}$, which is the value returned by ScreeNOT.

Figure 2(b) shows a plot of the loss $SE[\theta | X]$ versus $\theta$. The red horizontal line shows the optimum achievable loss. The green vertical line shows the threshold selected by the procedure. It intersects the loss curve within the optimal level and the achieved loss is therefore optimal.

![Figure 2](image_url)

(a) Solving the master equation (5)  
(b) MSE loss $SE[\theta | X]$ over $\theta$

Figure 2: Calculation of the optimal threshold $\hat{\theta}$ on the stylized example of Section 2.2. (a) Left panel: Horizontal axis: candidate thresholds $\theta$. Vertical axis: The function $\Psi(\theta)$. The ScreeNOT algorithm solves the equation $\Psi(\theta) = -4$ for $\theta$. Vertical green line shows the solution, denoted by $\hat{\theta}$. This is the value returned by ScreeNOT. (b) Right panel: The MSE loss function $SE[\theta | X]$ for the stylized example of Section 2.2, plotted over candidate thresholds $\theta$. There is an interval of values $\theta$ all achieving the lowest possible loss; The threshold $\hat{\theta}$ returned by ScreeNOT (shown by the vertical green line) is located inside this optimal interval.
3 Setup and background from random matrix theory

The rest of this paper is dedicated to formal analysis of the ScreeNOT algorithm. To that end, we now define a precise signal+noise model and set up the necessary notation.

An asymptotic model for low-rank matrices observed in additive noise. To recap, let $X_n$ be an unknown $n$-by-$p$ matrix, to be estimated. We observe a noisy measurement of $X_n$, $Y_n = X_n + Z_n$, where $Z_n$ is a noise matrix, which is statistically independent of $X_n$. Our analysis employs an asymptotic framework originating in Random Matrix Theory, and considers a sequence of such problems $n, p \to \infty$, with the following generative assumptions.

1. Limiting shape: the dimensions $n, p$ tend to infinity together at a fixed ratio $p/n \to \gamma$. More concretely, fix $\gamma \in (0, 1]$ and set $p = p_n = \lceil \gamma n \rceil$. Denoting $\gamma_n = p_n/n$, of course, $\gamma \leq \gamma_n < \gamma + \frac{1}{n}$ and $\gamma_n \to \gamma$ as $n \to \infty$.

2. Fixed signal rank and singular values: The matrix $X_n$ has fixed rank $r = \text{rank}(X_n)$ and fixed singular values. Specifically, let $r$ be constant, and fix $r$ positive and distinct numbers $x_1 > \ldots > x_r > 0$. $X_n$ is the matrix

$$X_n = \sum_{i=1}^{r} x_i a_{i,n} b_{i,n}^\top,$$

where $a_{i,n} \in \mathbb{R}^n$ (resp. $b_{i,n} \in \mathbb{R}^p$) for $i = 1, \ldots, r$ are sequences of left (resp. right) singular vectors of $X_n$, obeying a generative assumption as described next. We let $x = (x_1, \ldots, x_r)$ denote the vector of singular values and we refer to either the matrix $X$ or just $x$ as the signal. We refer to the vector of singular values $x = (x_1, \ldots, x_r)$ as the signal.

3. Incoherent signal singular vectors. The vectors $a_{1,n}, \ldots, a_{r,n}$ (resp. $b_{1,n}$) constitute a random, uniformly distributed orthonormal $r$-frame in $\mathbb{R}^n$ (resp. in $\mathbb{R}^p$).\(^8\)

4. Compactly supported, limiting bulk distribution of noise singular values. Each matrix $Z_n$ is statistically independent of $X_n$. Let $z_{1,n}, \ldots, z_{p,n}$ denote its singular values, with empirical CDF $F_{Z_n}$, $F_{Z_n}(z) = p^{-1} \sum_{i=1}^{p} 1_{\{z_{i,n} \leq z\}}$. There is a limiting empirical CDF (LECDF) $F_Z$ such that $F_{Z_n} \to F_Z$ a.s. at continuity points.

Moreover, we assume that $F_Z$ is compactly supported\(^9\) and denote the upper edge of the support (sometimes called the noise bulk edge) by

$$Z_+ \equiv Z_+(F_Z) = \sup \{ z : F_Z(z) < 1 \}.$$

We also assume that $F_Z$ is nontrivial ($dF_Z$ is not a single atom at $z = 0$), in other words, $Z_+(F_Z) > 0$. Note that neither the distribution $F_Z$ nor its bulk edge $Z_+(F_Z)$ are assumed to be known to the statistician.

5. No outliers straying from the bulk. Asymptotically, no singular values of $Z_n$ can be found above the bulk edge:

$$z_{1,n} = \|Z_n\| \xrightarrow{a.s.} Z_+(F_Z).$$

---

\(^8\)In other words, $a_{1,n}, \ldots, a_{r,n}$ are sampled from the $O(n)$-invariant distribution on the Stiefel manifold $V_r(\mathbb{R}^n)$. Equivalently, one can assume that $a_{i,n}$ and $b_{i,n}$ are any arbitrary sequences of orthonormal $r$-frames, and the distribution of $Z_n$ is invariant to multiplication by $O(n)$ to the left and by $O(p)$ to the right.

\(^9\)This will seem strange to many statisticians when they first encounter it; but note that if $Z_n$ is a standard Gaussian white noise, then even though the distribution of matrix entries is not compactly supported, the limiting bulk distribution of singular values is compactly supported, in $[(1 - \sqrt{2}), (1 + \sqrt{2})]$.
6. Thickness of the bulk edge. The following condition holds:

\[
\lim_{y \to Z_n(F_Z)} \int (y - z)^{-2} \, dF_Z(z) = \infty,
\]

where the limit is taken from the right. That is, \( F_Z \) puts “sufficient” mass near the upper edge of its support. Under this condition, when the signal singular values \( x_i \) are sufficiently small, the amount of “information” one can obtain about the corresponding singular vectors \( \mathbf{a}_{i,n} \mathbf{b}_{i,n}^\top \) from the leading singular vectors of \( Y_n \) also vanishes.

This assumption is by no means esoteric. For example, suppose that \( F_Z \) has a continuous density \( f_Z \) in a neighborhood of \( z_+ = Z_+(F_Z) \), where it behaves like \( f_Z(z) \sim C(z - z_+)^{\alpha} \) as \( z \to z_+ \); here \( \alpha > 0 \) is some exponent. Then this condition holds whenever \( \alpha \leq 1 \). In Section 3.2, we mention a broad class of noise matrices \( Z_n \) for which this property holds with \( \alpha = 1/2 \).

Class of estimators and performance measure. Our goal is to estimate \( X_n \). We consider the family of singular value hard-thresholding estimators: \( \hat{X}_\theta = \hat{X}_\theta(Y_n) \), where

\[
\hat{X}_\theta = \sum_{i=1}^p y_{i,n} \mathbb{1}_{y_{i,n} > \theta} \cdot \mathbf{u}_{i,n} \mathbf{v}_{i,n}^\top,
\]

where \( Y_n = \sum_{i=1}^p y_{i,n} \mathbf{u}_{i,n} \mathbf{v}_{i,n}^\top \) is an SVD. We measure the error with respect to Frobenius norm (squared error)\(^{10}\), where we denote:

\[
\text{SE}_n[\theta] = \|X_n - \hat{X}_\theta(Y_n)\|_F^2.
\]

Our task is to choose \( \theta \), so as to make \( \text{SE}_n[\theta] \) as small as possible, in an appropriate sense (note that \( \text{SE}_n[\theta] \) is a random variable - we do not take the expectation of \( X_n \) and \( Y_n \)). The best possible performance is given by the Oracle Loss

\[
\text{SE}_n^*[\theta] = \min_{\theta \geq 0} \text{SE}_n[\theta],
\]

which is the best loss one can achieve over the family of singular value hard-threshold estimators, even knowing the true signal \( X_n \). Our goal in this paper is to develop a threshold selector that, “typically for large \( n \)”, attains the oracle loss \( \text{SE}_n^*[\theta] \). Note that the oracle loss \( \text{SE}_n^*[\theta] \) is also a random variable, and it is not a priori clear how to estimate it. An important observation is that the (random) function \( \theta \mapsto \text{SE}_n[\theta] \) is piecewise constant, with finitely many jumps (specifically, these are at the singular values of \( Y_n, y_{1,n}, \ldots, y_{p,n} \)). In particular, the minimum of \( \text{SE}_n[\theta] \) is attained not strictly at a point, but on an interval (or a union of intervals).

3.1 Background from random matrix theory

The Spiked Model. Our perspective on the matrix denoising problem extends the one proposed by Perry [Perry, 2009] and Shabalin and Nobel [Shabalin and Nobel, 2013]. In the model they proposed, which was inspired by Johnstone’s Spiked Covariance model [Johnstone, 2001], one works under the same model \( Y_n = X_n + Z_n \) as described above, but specifically assumes that the noise matrix \( Z_n \) is column-normalized and white, namely, that its entries are properly scaled \( i.i.d \) random variables. This model’s close sibling, the Spiked Model for high-dimensional covariance, has been extensively studied in the probability and statistics literature, to such an extent that we cannot point to all of the existing literature here. Seminal works

\(^{10}\)Recall that for a matrix \( A \), \( \|A\|_F^2 = \sum_{i,j} |A_{i,j}|^2 \).
such as [Bai and Yao, 2008, Baik and Silverstein, 2006, Paul, 2007] and others have shown that the randomness in the Spiked Model can be neatly described in terms of the so-called BBP phase transition, similar to the one discovered in [Baik et al., 2005]; and of the displacement of the sample eigenvectors relative to the population eigenvectors; and of the rotation of the sample eigenvectors relative to the populations eigenvectors.

In the matrix denoising setup we consider here, the model described by our assumptions above has been studied in [Benaych-Georges and Nadakuditi, 2012b], and the same three underlying phenomena were identified and quantified:

1. **BBP phase transition:** Let $z_+ = Z_+(F_Z)$ denote the noise bulk edge. There is a functional $X_+(F_Z, \gamma)$ that depends on the LECDF $F_Z$ and the asymptotic shape $\gamma$ that defines an important threshold phenomenon in the behavior of limiting empirical singular values. Setting $x_+ = X_+(F_Z, \gamma)$, then for any $i = 1, \ldots, r$ where $x_i \leq x_+$,

$$y_{i,n} \overset{d.s.}\rightarrow z_+, \quad n \to \infty.$$  

In short, sufficiently small signal singular values $x_i$ do not produce outliers beyond the noise bulk edge. As we are about to see, the situation for $x_i > x_+$ is quite different. The split between $x_i \geq x_+$ is sometimes called the Baik-Ben Arous-Péché (BBP) phase transition, after the original example of this type [Baik et al., 2005].

2. **Limiting location of outlier singular values:** The limiting value of $y_{n,i}$ is not its underlying population counterpart $x_i$. There is instead a functional $\mathcal{Y}(x; F_Z, \gamma)$, depending on $F_Z$ and $\gamma$, describing this limiting behavior. The function of $x$ obtained by fixing $F_Z$, and $\gamma$ - $\mathcal{Y}(x) = \mathcal{Y}(x; F_Z, \gamma)$ - explains how the asymptotic limit varies with theoretical singular value $x$. For any $i = 1, \ldots, r$ where $x_i \geq x_+ \in X_+$,

$$y_{i,n} \overset{d.s.}\rightarrow y_{i,\infty} = \mathcal{Y}(x_i), \quad n \to \infty.$$  

The function $x \mapsto \mathcal{Y}(x)$ is strictly increasing and one-to-one between $[x_+, \infty)$ and $[z_+, \infty)$.

3. **No limiting cross-correlation of non-corresponding principal subspaces:** For $i \neq j$, empirical dyad $u_{n,i}v_{n,i}^T$ ultimately decorrelates from each of the non-corresponding population dyads $a_{n,j}b_{n,j}^T$. For any $i, j = 1, \ldots, r$ such that $i \neq j$,

$$\langle a_{n,i}, u_{n,i} \rangle \cdot \langle b_{n,j}, v_{n,j} \rangle \overset{d.s.}\rightarrow 0, \quad n \to \infty.$$  

4. **Limiting cross-correlation of corresponding principal subspaces:** Suppose the signal singular values $(x_i)_{i=1}^r$ are distinct. The empirical dyad $u_{n,i}v_{n,i}^T$ does correlate with its theoretical counterpart $a_{n,i}b_{n,i}^T$, but not perfectly. The limit is described by a functional $C(x; F_Z, \gamma)$ depending on $x, F_Z$ and $\gamma$. Fixing once again $F_Z$ and $\gamma$, we get a function of $x$, $C(x) = C(x; F_Z, \gamma)$, such that, with $x_+ = X_+(F_Z, \gamma)$,

$$\langle a_{n,i}, u_{n,i} \rangle \cdot \langle b_{n,i}, v_{n,i} \rangle \overset{d.s.}\rightarrow \begin{cases} C(x_i) & x_i > x_+ \\ 0 & x_i \leq x_+ \end{cases}.$$  

We now give formulas for $X_+$ and the mappings $\mathcal{Y}(\cdot)$ and $C(\cdot)$, as computed in [Benaych-Georges and Nadakuditi, 2012b]. For a CDF $H$, let

$$\varphi(y; H) = \int \frac{y}{y^2 - z^2} dH(z),$$  

(13)
which defines a smooth function on \( y > Z_+(H) \). Its derivative is

\[
\phi'(y; H) = -\int \frac{y^2 + z^2}{(y^2 - z^2)^2} dH(z). \tag{14}
\]

Also define

\[
\tilde{\phi}_\gamma(y; H) = \gamma \phi(y; H) + \frac{(1 - \gamma)}{y}, \quad \tilde{\phi}'_\gamma(y; H) = \gamma \phi'(y) - \frac{1 - \gamma}{y^2}. \tag{15}
\]

Note that \( \tilde{\phi}_\gamma(y; H) \) is simply \( \phi(y; \tilde{H}_\gamma) \), where \( \tilde{H}_\gamma(z) = \gamma H(z) + (1 - \gamma)1_{\{z \geq 0\}} \). This so-called companion CDF \( \tilde{H}_\gamma \) describes the same distribution of nonzero singular values as \( H \), diluted by ‘zero padding’ and has the following interpretation: if \( Z_n \) is a sequence of \( n \)-by-\( p \) matrices with a limiting singular value distribution \( H \), then \( Z_n^\gamma \) has a limiting singular value distribution \( \tilde{H}_\gamma \)\(^{11}\). Let

\[
\begin{align*}
\mathcal{D}_\gamma(y; H) &\equiv \phi(y; H) \cdot \tilde{\phi}_\gamma(y; H), \\
\mathcal{D}'_\gamma(y; H) &\equiv \phi'(y; H) \cdot \tilde{\phi}_\gamma(y; H) + \phi(y; H) \cdot \tilde{\phi}'_\gamma(y; H).
\end{align*} \tag{16}
\]

To ease the notation in coming paragraphs, we put for short \( \mathcal{D}_\gamma(y) = \mathcal{D}_\gamma(y; \gamma, F_Z) \), and similarly for \( \phi(y), \tilde{\phi}_\gamma(y) \). Let \( z_+ = Z_+(F_Z) \) denote the bulk edge. The BBP phase transition location \( x_+ = \mathcal{X}_+(F_Z, \gamma) \) is given by

\[
x_+ = \lim_{y \rightarrow z_+} (\mathcal{D}_\gamma(y))^{-1/2}, \tag{17}
\]

equivalently, \( 1/x_+^2 = \lim_{y \rightarrow z_+} \mathcal{D}_\gamma(y) \). It is easy to verify that \( \phi(y), \tilde{\phi}_\gamma(y) \) and \( \mathcal{D}_\gamma(y) \) are non-negative, strictly decreasing functions of \( y > z_+ \), each tending to \( 0 \) as \( y \rightarrow \infty \). Thus, \( \mathcal{D}_\gamma(\cdot) \) maps the interval \( (z_+, \infty) \) bijectively into \( (x_+, 0) \); denote by \( \mathcal{D}_\gamma^{-1}(\cdot) \equiv \mathcal{D}_\gamma^{-1}(\cdot; F_Z) \) the inverse mapping.

We finally can give formulas for the fundamental phenomenological limits described earlier. The limiting empirical signal singular value \( y_{i,\infty} = \mathcal{Y}(x_i) = \mathcal{Y}(x_i; F_Z, \gamma) \) obeys

\[
\mathcal{Y}(x) = \mathcal{D}_\gamma^{-1}\left(\frac{1}{x^2}\right), \quad \text{for } x > x_+, \tag{18}
\]

equivalently, \( \mathcal{D}_\gamma(\mathcal{Y}(x)) = 1/x^2 \). The asymptotic cosine \( C(x) \equiv C(x; F_Z, \gamma) \) is given by

\[
C(x) = -\frac{2}{x^3} \cdot \frac{1}{\mathcal{D}_\gamma(\mathcal{Y}(x))}, \quad \text{for } x > x_+. \tag{19}
\]

We sometimes adopt the implicit parameterization of \( C(x) \) in terms of \( y = \mathcal{Y}(x) \):

\[
C(x) = -2 \cdot \left(\frac{\mathcal{D}_\gamma(y)}{\mathcal{D}'_\gamma(y)}\right)^{3/2}, \quad \text{where } y = \mathcal{Y}(x) \text{ and } x > x_+. \tag{20}
\]

\(^{11}\)Practitioners will recognize that computer software often offers two options for SVD outputs, a ‘fat’ output with zero padding and a ‘thin’ output with those superfluous zeros stripped away. If \( H \) denotes the LECDF of the ‘thin’ output singular values, then \( \tilde{H} \) is the corresponding LECDF of the fat outputs.
Existence of a BBP phase transition. Recall that \( x_+ = X_+(F_Z, \gamma) \) gives the threshold such that whenever \( x_i \leq x_+ \), one does not observe an outlier singular value away from the bulk of \( Y \). Not all noise distributions display this phase transition phenomenon, i.e. they may not exhibit \( x_+ > 0 \); indeed, by Eq. (17), \( X_+ > 0 \) if and only if \( \lim_{y \to z_+(F_Z)} D_x(y; F_Z) < \infty \), equivalently, \( \lim_{y \to z_+(F_Z)} \int (y - z)^{-1} dF_Z(z) < \infty \). This condition entails that near its own bulk edge, \( F_Z \) is not “thick”. For example, when \( F_Z \) has a density in a neighborhood of \( z_+ = Z_+(F_Z) \) that behaves as \( f_Z(z) \sim C(z - z_+)^{\alpha} \), this condition is satisfied whenever \( \alpha > 0 \). For example, the family of noise distributions described in Section 3.2 is of this type (with \( \alpha = 1/2 \)); they all display a BBP phase transition. Moreover, Assumption 6 gives \( \lim_{x \to y} D_x(y; F_Z) = -\infty \). From Eq. (20), this means that if \( x_+ \equiv X_+(F_Z, \gamma) > 0 \), then \( C(x_+) = 0 \) as \( x \to x_+ \) from the right. Curiously, when \( x_+ = 0 \), this does not have to be the case. For instance, when \( dF_Z = \delta_1 \) and \( \gamma = 1 \), an easy computation shows \( x_+ = 0 \) and \( C(x) = \frac{\theta^3}{x^{\gamma + 1}} \), where \( \gamma = \gamma(x) = 1 \) and \( Z_+(F_Z) = 1 \). We see that \( \lim_{x \to x_+} C(x) = 1/2 \); this means that an arbitrarily small signal already creates a very strong bias in the direction of the principal singular vectors of \( Y_n \).

**Notation.** We use throughout the paper the notation

\[
y_i,\omega = \begin{cases} \mathcal{Y}(x_i) & \text{when } x_i > X_+, \\ Z_+(F_Z) & \text{when } x_i \leq X_+. \end{cases}
\]

By the results of [Benaych-Georges and Nadakuditi, 2012b], the singular values of \( Y_n, y_{1,n} \geq \ldots \geq y_{p,n} \), satisfy \( y_{i,n} \xrightarrow{d_{x,i}} y_{i,\omega} \) for any fixed index \( i \) (for \( i > r \) this is an easy consequence of the interlacing inequality for singular values).

### 3.2 Noise matrices with correlated columns

We conclude this section by mentioning an important family of noise matrices satisfying our assumptions, namely, noise matrices with independent rows, having cross-column correlations. We consider noise matrices of the form \( Z_n = W_n S_n^{1/2} \), where \((W_n)\) and \((S_n)\) are sequences of matrices obeying:

- \( W_n \) is an \( n \)-by-\( p \) matrix with i.i.d elements. Specifically, let \( W \) denote a random variable with moments

\[
\mathbb{E}(W) = 0, \quad \mathbb{E}(W^2) = 1, \quad \mathbb{E}(W^4) < \infty.
\]

The entries of \( W_n \) are i.i.d, and has the law \((W_n)_{ij} \xrightarrow{d} n^{-1/2} W \), that is, scaled so to have variance \( 1/n \). Finiteness of the fourth moment of \( W \) is essential; see [Bai et al., 1998].

- \( (S_n) \) is a sequence of non-random \( p \)-by-\( p \) matrices. Let \( \lambda_1(S_n) \geq \ldots \geq \lambda_p(S_n) \) be the eigenvalues of \( S_n \), and denote by \( F_{S_n}(\lambda) = \int_{\lambda(S_n) \leq \lambda} \mathbb{I} \lambda(S_n) \leq \lambda \) the empirical CDF of its eigenvalues. We assume that the sequence \((F_{S_n})\) converges to a compactly supported LECDF \( F_S \). Moreover, the denoting the upper and lower edges of the support by

\[
\lambda_+(F_S) = \sup \{ \lambda : F_S(\lambda) < 1 \}, \quad \lambda_-(F_S) = \inf \{ \lambda : F_S(\lambda) > 0 \},
\]

we assume that \( \lambda_1(S_n) \to \lambda_+(F_S) \) and \( \lambda_p(S_n) \to \lambda_-(F_S) \).

We refer to a random matrix ensemble of the form above as a **noise matrix with correlated columns**. They appear, for example, in the following scenario: We observe \( n \) i.i.d \( p \)-dimensional samples \( y_i = x_i + z_i \), where \( x_i \) are instances of a signal vector, assumed to be supported in an \( r \)-dimensional subspace, and \( z_i = S_n^{1/2} w_i \) is a vector of correlated noise, with covariance
Cov(w_i) = S_n. Let Y_n be the n-by-p matrix, whose rows are n^{-1/2}y^\top_i (define X_n, W_n and S_n similarly). Then Y_n = X_n + Z_n = X_n + W_nS_n^{1/2}, where observe that rank(X_n) ≤ r, by assumption. For any estimator \( \hat{X} = \hat{X}(Y_n) \), let \( \hat{x}_1, \ldots, \hat{x}_n \) be the rows of the matrix \( n \cdot \hat{X} \). Then the Frobenius loss is just the average loss in estimating the signal samples \( \mathbf{x} \) by the vectors \( \hat{x}_i : \|X_n - \hat{X}(Y_n)\|_F^2 = n^{-1} \sum_{i=1}^n \|x_i - \hat{x}_i\|_2^2 \).

Much is known about the singular values of \( Z_n \):

1. **Limiting singular value distribution:** \( F_{Z_n} \) converges weakly almost surely to a compactly supported law \( F_Z \). This limiting law is defined in terms of its Stieltjes transform\(^{12}\), \( m(y) = \int (z^2 - y)^{-1}dF_Z(z) \); \( m(y) \) is the unique Stieltjes transform satisfying the equation
   \[
m(y) = \int \frac{1}{t(1 - \gamma - \gamma y m(y)) - y} dF_S(t), \quad \text{for all } y \in \mathbb{C} \setminus \mathbb{R} .
   \]

2. **Extreme singular values:** The largest and smallest singular values of \( Z_n \) converge almost surely to the upper and lower edges of the support of the limiting law \( F_Z \):
   \[
   Z_+(F_{Z_n}) \xrightarrow{a.s.} Z_+(F_Z), \quad y_-(F_{Z_n}) \xrightarrow{a.s.} y_-(F_Z).
   \]

3. **Behavior at the edge of the bulk:** On \( \mathbb{R} \setminus \{0\} \), the limiting law \( F_Z \) is absolutely continuous with respect to Lebesgue measure. Denoting by \( f_Z \) the corresponding density, it behaves like \( f_Z(z) \sim C (z - Z_+(F_Z))^{1/2} \) as \( z \to Z_+(F_Z) \). This is the same behavior as a Marcenko-Pastur law, corresponding to \( S_n = I \). This edge behavior will motivate one of our strategies for estimating \( F_{Z_n} \) from the observed singular values \( F_{Y_n} \) (imputation, see Section 4.2); this is an important step in the ScreeNOT algorithm. Also, note that in particular, the limiting noise CDF \( F_Z \) satisfies Assumption 6.

4. **CLT for linear spectral statistics:** Denote
   \[
   \underline{y} = (1 - \sqrt{\gamma})^2 \cdot \liminf_{n \to \infty} \lambda_p(S_n), \quad \overline{y} = (1 + \sqrt{\gamma})^2 \cdot \limsup_{n \to \infty} \lambda_1(S_n).
   \]

   Note that \( \overline{y}^{1/2} \leq y_-(F_Z) \leq Z_+(F_Z) \leq \overline{y}^{1/2} \). Let \( g \) be analytic on an open domain in \( \mathbb{C} \) containing the closed interval \( [\underline{y}, \overline{y}] \). Set
   \[
   \Phi_n[g] = \int g(z^2) (dF_Z - dF_{Z_n})(z),
   \]
   which is a random variable.\(^{13}\) Then the sequence \( p \cdot \Phi_n[g] \) is tight. If, moreover, \( E(W^4) = 3 \), then \( p \cdot \Phi_n[g] \) converges in law to a Gaussian random variable.

For properties (1) and (2), we refer to [Bai et al., 1998] and the references therein (see also the book [Bai and Silverstein, 2010]). Property (3) is proved in [Silverstein and Choi, 1995]. Property (4) is proved in [Bai and Silverstein, 2004].

\(^{12}\) \( m(y) \) is in fact the Stieltjes transform of the limiting eigenvalue distribution of \( Z^\top Z \):

\[
m(y) = \int (z - y)^{-1}dF_{Z^\top Z}(z) = \int (z^2 - y)dF_Z(z).
\]

\(^{13}\) A random variable of the form \( \int h(z)F_{Z_n}(z) = p^{-1} \sum_{i=1}^n h(z_{i,n}) \) is called a linear spectral statistic.
We do this by applying the optimal threshold functional $T_\gamma(F_Z)$, which is given as a certain functional $T_\gamma$ of the asymptotic aspect ratio $\gamma$ and the limiting noise CDF $F_Z$. Relying on the fact that SE$_n$[$x|\theta$] can only take a finite number of values as $\theta$ varies, we show that thresholding at $T_\gamma(F_Z)$ has rather strong optimality properties: it in fact attains oracle loss, at finite $n$, with probability increasing to 1 as $n \to \infty$. We then move on to the practical setting of interest, in which $F_Z$ is unknown. We propose a method for consistently estimating $T_\gamma(F_Z)$ from the observed data $Y_n$. We do this by applying the optimal threshold functional $T_{p/n}(\cdot)$ on a judiciously transformed version of $F_{Y_n}$, the empirical singular value distribution of $Y_n$. The continuity of the functional with respect to the CDF and the shape parameter then implies that the resulting quantity is a

Figure 3: Several empirical noise singular value distributions that come from the model in Section 3.2. Left to right: covariance eigenvalue distribution: (i) $dF_S = \delta_1$ (giving a Marcenko-Pastur bulk); (ii) An equal mix of two atoms, $dF_S = \frac{1}{2}\delta_1 + \frac{1}{2}\delta_{10}$; (iii) $F_S$ uniform on [1,10]. Top: shape $\gamma = 1$; bottom: $\gamma = 0.5$. Each plot is the histogram of singular values from a single random $n \times p$ matrix, with $p = 1000$ and $n = p/\gamma$.

As a final remark, we mention that when the covariance matrix $S_n$ is invertible and known (or can be consistently estimated with respect to operator norm), estimating $X_n$ using the leading singular vectors of $Y_n$ is sub-optimal. Instead, it is better to first “whiten” the noise, that is, compute $Y_n^\omega = Y_n S_n^{-1/2} = X_n S_n^{-1/2} + W_n$. Letting $u_{i,n}^\omega$ and $v_{i,n}^\omega$ be respectively the left and right singular vectors of $Y_n$, we “re-color” the right singular vectors, $v_{i,n}^\omega = S_n^{1/2} v_{i,n}^\omega / \|v_{i,n}^\omega\|$. Under a uniform prior on the signal singular vectors, as we assume in this paper, and when $W_n$ is i.i.d Gaussian, the correlations between the signal singular vectors and empirical singular vectors can be shown to be stronger in the whiten-then-recolor scheme:

$$\lim_{n \to \infty} \langle a_{i,n}, u_{i,n}^\omega \rangle \langle b_{i,n}, v_{i,n}^\omega \rangle \geq \lim_{n \to \infty} \langle a_{i,n}, u_{i,n} \rangle \langle b_{i,n}, v_{i,n} \rangle.$$  

For details see [Leeb and Romanov, 2018, Hong et al., 2018].

4 Results

Outline. We start by developing a theory for optimal hard thresholding, under the assumption that the noise singular value distribution $F_Z$ is known. We show that there is an asymptotically uniquely admissible hard threshold $T_\gamma(F_Z)$, which is given as a certain functional $T_\gamma$ of the asymptotic aspect ratio $\gamma$ and the limiting noise CDF $F_Z$. Relying on the fact that SE$_n$[$x|\theta$] can only take a finite number of values as $\theta$ varies, we show that thresholding at $T_\gamma(F_Z)$ has rather strong optimality properties: it in fact attains oracle loss, at finite $n$, with probability increasing to 1 as $n \to \infty$. We then move on to the practical setting of interest, in which $F_Z$ is unknown. We propose a method for consistently estimating $T_\gamma(F_Z)$ from the observed data $Y_n$. We do this by applying the optimal threshold functional $T_{p/n}(\cdot)$ on a judiciously transformed version of $F_{Y_n}$, the empirical singular value distribution of $Y_n$. The continuity of the functional with respect to the CDF and the shape parameter then implies that the resulting quantity is a
consistent estimator for \( T_\gamma(F_Z) \); the optimality properties of the adaptive algorithm then follow from the previously developed theory. Unless otherwise stated, we always operate under assumptions (1)-(6) of Section 3.

### 4.1 A theory for optimal singular value thresholding

Consider the function \( \theta \mapsto ASE[x|\theta] \) defined for \( \theta > 0 \) by

\[
ASE[x|\theta] = \sum_{i=1}^{r} R(x_i|\theta), \quad \text{where} \quad R(x_i|\theta) = I_{y_i,\infty \leq \theta} \cdot R_0(x_i) + I_{y_i,\infty > \theta} \cdot R_1(x_i),
\]

and

\[
R_0(x) = x^2, \quad R_1(x) = x^2 + y(x)^2 - 2x y(x) c(x),
\]

and recall that \( y_i,\infty = z_+ (\equiv Z_+(F_Z)) \) when \( x_i \leq x_+ (= \lambda'_+ (F_Z, \gamma)) \) and \( y_i,\infty = y(x_i) \) when \( x > x_+ \). Define also

\[
ASE^*[x] = \sum_{i=1}^{r} R^*(x_i), \quad \text{where} \quad R^*(x_i) = \begin{cases} R_0(x_i) & \text{when } x_i < x_+, \\ \min \{ R_0(x_i), R_1(x_i) \} & \text{when } x_i \geq x_+. \end{cases}
\]

Clearly, \( R^*(x) \leq R(x|\theta) \) for any \( x \) and \( \theta \), which means \( ASE^*[x] \leq ASE[x|\theta] \).

It is easy to verify that for almost every \( \theta > Z_+(F_Z) \), the loss of thresholding at the fixed point \( \theta \) converges: \( \lim_{n \to \infty} SE_n[x|\theta] = ASE[x|\theta] \) almost surely; see Lemma 7 for a precise statement.

We start by finding the threshold that attains minimum asymptotic loss.

**Definition 1 (Optimal threshold functional).** For a compactly supported CDF \( H \) and \( \gamma \in (0,1] \), let

\[
\Psi_\gamma(y; H) = y \cdot \frac{D'_\gamma(y; H)}{D_\gamma(y; H)} = y \cdot \left( \frac{\phi'(y; H)}{\phi(y; H)} + \frac{\Phi'(y; H)}{\Phi(y; H)} \right);
\]

this is well-defined for \( y > Z_+(H) \). Define the functional of \( H \)

\[
T_\gamma(H) = \inf \{ y : y > Z_+(H) \text{ and } \Psi_\gamma(y; H) \geq -4 \}.
\]

we call this the **optimal threshold functional**.

**Lemma 1.** The following holds:

1. For any \( H \) and \( \gamma \), \( y \mapsto \Psi_\gamma(y; H) \) is negative and increasing, with \( \Psi_\gamma(\infty) = -2 \).
2. Assume that \( H \) is compactly supported and satisfies \( \lim_{y \to Z_+(H)} \int (y-z)^{-2} dH(z) = \infty \) (note that, by assumption, \( H = F_Z \) satisfies this). Then \( T_\gamma(H) \) is the unique number \( > Z_+(H) \) satisfying \( \Psi_\gamma(T_\gamma(H); H) = -4 \).
3. Thresholding at \( \theta^* = T_\gamma(F_Z) \) universally minimizes the asymptotic loss:

\[
ASE[x|\theta^*] = \min_{\theta} ASE[x|\theta] = ASE^*[x].
\]

Moreover, \( \theta^* \) is the unique threshold for which the above holds **universally**, for all signals \( x \).

**Lemma 1** is proved in Section 6.1.

Note that \( \theta \mapsto ASE[x|\theta] \) is piecewise constant, with jumps at \( y_1,\infty, \ldots, y_r,\infty \). This means that its minimum is actually attained on an **interval**.
Definition 2 (The asymptotic optimal interval). Let
\[
\Theta(x) = \max \{ y_{i,\infty} : y_{i,\infty} < T_\gamma(F_Z) \}, \quad \overline{\Theta}(x) = \min \{ y_{i,\infty} : y_{i,\infty} > T_\gamma(F_Z) \}. \tag{26}
\]
Note that since \( T_\gamma(F_Z) > z_+ = Z_+(F_Z, \gamma) \) and \( y_{r+1,\infty} = z_+ \), we always have, by definition, \( \Theta(x) \geq z_+ \). Moreover, if \( y_{1,\infty} \leq T_\gamma(F_Z) \) then we define \( \overline{\Theta}(x) = \infty \).

Lemma 2. 1. Throughout the interval \( \theta \in (\Theta(x), \overline{\Theta}(x)) \), \( \text{ASE}[x|\theta] \) is constant. Moreover, it attains its minimum there; if \( \theta_0 \in (\Theta(x), \overline{\Theta}(x)) \), then
\[
\text{ASE}[x|\theta_0] = \min_{\theta \geq 0} \text{ASE}[x|\theta] = \text{ASE}^*[x].
\]
2. Any \( \theta_1 > Z_+(F_Z) \) outside \( (\Theta(x), \overline{\Theta}(x)) \) has
\[
\text{ASE}[x|\theta_1] > \text{ASE}^*[x].
\]
3. Unique asymptotic admissibility: \( T_\gamma(F_Z) \) is in the interior of the asymptotic optimal interval. In fact, it is the only threshold which has optimal asymptotic loss simultaneously for all signals \( x \):
\[
\bigcap_{x \text{ signal}} (\Theta(x), \overline{\Theta}(x)) = \{ T_\gamma(F_Z) \}.
\]

Lemma 2 is proved in Section 6.1.

It is clear at this point that thresholding at any point in the interior of the asymptotic optimal interval achieves the best asymptotic loss, among all other fixed hard thresholds. Our main result states that, remarkably, one cannot come up with a consistently better thresholding strategy, even if given access to the true unknown signal \( X_n \):

Theorem 1. 1. Almost surely,
\[
\lim_{n \to \infty} \text{SE}^*_n[x] = \text{ASE}^*[x].
\]
2. Let \( \theta \in (\Theta(x), \overline{\Theta}(x)) \) be in the interior of the asymptotic optimal interval, and \( \theta_n \) be any sequence of thresholds (possibly depending on \( Y_n \)) such that \( \theta_n \overset{a.s.}{\to} \theta \). Then
\[
\text{SE}_n[x|\theta_n] \overset{a.s.}{\to} \text{ASE}^*[x].
\]

Our next result states that thresholding inside the asymptotic optimal interval in fact achieves oracle risk with high probability, for finite \( n \):

Theorem 2. Suppose that \( T_\gamma(F_Z) \notin \{ y_{1,\infty}, \ldots, y_{r,\infty} \} \). Then:
1. Let \( \theta_0 \in (\Theta(x), \overline{\Theta}(x)) \) and \( \theta_n \) be a sequence with \( \theta_n \overset{a.s.}{\to} \theta_0 \). Then
\[
\mathbb{P} \{ \exists N \text{ s.t. } \forall n \geq N : \text{SE}_n[x|\theta_n] = \text{SE}^*_n[x] \} = 1.
\]
2. Let \( \theta_1 \notin (\Theta(x), \overline{\Theta}(x)) \) and \( \theta_n \overset{a.s.}{\to} \theta_1 \). There exists \( \delta > 0, \delta = \delta(x; F_Z, \gamma) \) such that
\[
\mathbb{P} \{ \exists N \text{ s.t. } \forall n \geq N : \text{SE}_n[x|\theta_n] > \text{SE}^*_n[x] + \delta \} = 1.
\]

Theorems 1 and 2 are proved in Section 6.2.

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14If \( y_{i,\infty} = T_\gamma(F_Z) \) for some \( i \), thresholding either slightly above or below \( y_{i,\infty} \) (but still inside the asymptotic optimal interval) will achieve the same (optimal) asymptotic risk. However, we cannot deduce that for finite \( n \), one option is consistently better than the other.
4.2 The ScreeNOT algorithm

In practice, the noise distribution $F_Z$ is generally unknown to the statistician. Theorems 1 and 2, along with the unique admissibility property of Lemma 2, tell us that our goal should be to estimate the optimal threshold $T_{\gamma}(F_Z)$.

We start by showing that the functional $(\gamma, H) \mapsto T_{\gamma}(H)$ is continuous with respect to weak convergence of CDFs, with the additional requirement that the edge of the support converges as well:

**Lemma 3** (Continuity of the optimal threshold functional). Suppose that $H$ is compactly supported and satisfies the condition $\lim_{y \to Z_+(H)} \int (y-z)^{-2}dH(z) = \infty$. Let $H_n$ be a sequence of CDFs such that

1. $H_n$ converges weakly to $H$, denoted $H_n \xrightarrow{d} H$.
2. $Z_+(H_n) \to Z_+(H)$.

Then $T_{p/n}(H_n) \to T_{\gamma}(H)$.

Lemma 3 is proved in Section 6.3.

Recall that the empirical singular value distribution of the noise matrix, $F_{Z_n}$, converges, by assumption, weakly almost surely to $F_Z$, with $Z_+(F_{Z_n}) \xrightarrow{a.s.} Z_+(F_Z)$. The matrix noise $Z_n$, and consequently $F_{Z_n}$, is of course unknown to the statistician. However, since $Y_n$ is a rank-$r$ additive perturbation of $Z_n$, the interlacing inequalities for singular values imply for example the convergence of CDF’s in Kolmogorov-Smirnov distance $\|F_{Y_n} - F_{Z_n}\|_{KS} \to 0$ (by the same arguments used in Lemma 4 below) and hence also in weak convergence. The obstacle preventing the would-be use of $T_{p/n}(F_{Y_n})$ to estimate $T_{\gamma}(F_Z)$ lies with the fact that $T$ is not continuous in Kolmogorov-Smirnov metric convergence or other topologies involving CDF convergence such as weak convergence. More concretely, $T_{p/n}(F_{Y_n})$ can be very different than $T_{\gamma}(F_Z)$ because the top masspoints of $F_{Y_n}$ don’t converge to the bulk edge $F_Z$. Indeed, recall that $Z_+(F_{Y_n}) = y_{1,n} \xrightarrow{a.s.} y_{1,\infty}$, which is $> Z_+(F_Z)$ when $x_i > X_+$.

To get a reasonable simulacrum of $F_{Z_n}$ built from knowledge only of $F_{Y_n}$, we perform “surgery” on $F_{Y_n}$ “amputating” the top $k$ masspoints and fitting a “prosthesis” to replace them. Post-surgery, we get an estimate for the unknown empirical noise CDF $F_{Z_n}$.

As indicated in Section 2 above, the user of our proposed procedure supplies an upper bound (which can be potentially very loose) $k \geq r$ on the rank of the unknown low-rank matrix.

We could, in principle, propose any one of the following “pseudo-noise” CDFs, derived from $F_{Y_n}$:

- **Transport to zero**: We construct a CDF $F_{n,k}^0$, obtained by removing the $k$ largest singular values of $Y_n$, and adding $k$ additional zeros. That is,

$$F_{n,k}^0(y) = \frac{1}{p} \sum_{i=k+1}^{p} 1_{\{y_{i,n} \leq y\}} + \frac{k}{p} 1_{\{y \geq 0\}}.
$$

- **“Winsorization” (clipping)**: As in the previous construction, we remove the leading $k$ singular values. Instead of adding $k$ zeros, we add $k$ copies of $y_{k+1,n}$. Equivalently, we

\[Of course, this does not prevent convergence of ECDFs. Recall that $F_{Y_n} \xrightarrow{d} F_Z$ means that for bounded and continuous functions $f$, $\int f(z)dF_{Y_n}(z) \to \int f(z)dF_Z(z).$
Lemma 4. Suppose that \(k \geq r\) and \(k \geq k_n\) satisfies \(k_n \geq r\) and \(k_n/p \to 0\) (in particular, \(k\) can be any constant \(\geq r\)). Then for any choice \(* \in \{0, w, i\}\):

1. Almost surely, \(F_{n,k}^* \xrightarrow{d} F_Z\).
2. \(Z_+(F_{n,k}^*) \xrightarrow{d.s.} Z_+(F_Z)\).
3. We have the following bound on the Kolmogorov-Smirnov distance between \(F_{n,k}^*\) and \(F_{Z_n}^\ast\):

\[
\|F_{n,k}^* - F_Z\|_{KS} = \sup_z |F_{n,k}^*(z) - F_{Z_n}(z)| \leq \frac{k}{p}.
\]
Lemma 4 is proved in Section 6.3.

The following theorem states the optimality properties of the proposed ScreeNOT algorithm. It is an immediate corollary of Theorems 1, 2 and Lemma 4:

**Theorem 3.** Suppose that \( k = k_n \) satisfies \( k_n \geq r \) and \( k_n / p \to 0 \). For any \( \ast \in \{0, w, i\} \), \( \theta_n = T_{p/n}(F^*_{n,k}) \) satisfies:

1. \( \theta_n \xrightarrow{a.s.} T_\gamma(F_Z) \).
2. \( \text{SE}_n[x|\theta_n] \xrightarrow{a.s.} \text{ASE}^*[x] \).
3. Assume that \( T_\gamma(F_Z) \notin \{y_{1,\infty}, \ldots, y_{r,\infty}\} \). Then
   \[ \mathbb{P} \left\{ \exists N \text{ s.t. } \forall n \geq N : \text{SE}_n[x|\theta_n] = \text{SE}^*_n[x] \right\} = 1. \]

Regarding the assumption in item 3 above, we note the following.

**Lemma 5.** The condition \( T_\gamma(F_Z) \notin \{y_{1,\infty}, \ldots, y_{r,\infty}\} \) is **generic**, i.e. in the space of possible singular value \( r \)-vectors \( x \) this condition holds on an open dense set.

Fix the noise bulk \( F_Z \); then \( \theta^* = T_\gamma(F_Z) \) is a constant not varying as the underlying signal \( x \) changes. Moreover, it always strictly exceeds the bulk edge \( Z_+(F_Z) \). So \( x^* = \gamma^{-1}(\theta^*;F_Z,\gamma) \) is a uniquely defined constant which exceeds \( \mathcal{X}_+(F_Z,\gamma) \). The set of vectors \( x \) with all entries distinct from \( x^* \) is open and dense.

### 4.3 Stability of ScreeNOT

A natural question is how fast \( T_{p/n}(F^*_{n,k}) \) converges to the limit \( T_\gamma(F_Z) \). We show that in the case of noise matrices with correlated columns, the noise model described in Section 3.2, the typical deviations are of order \( O(k/p) \).

We start with a “quantitative” version of Lemma 3:

**Lemma 6.** Adopt the setting of Lemma 3. Set
\[
\Delta_{1,n} = |\varphi'(T_\gamma(H);H) - \varphi(T_\gamma(H);H_n)|, \quad \Delta_{2,n} = |\varphi'(T_\gamma(H);H) - \varphi'(T_\gamma(H);H_n)|,
\]
where \( \varphi \) and \( \varphi' \) are given in Eqs (13) and (14). Then
\[
|T_\gamma(H) - T_{p/n}(H_n)| = \mathcal{O} \left( \Delta_{1,n} + \Delta_{2,n} + |\frac{p}{n} - \gamma| \right).
\]

Lemma 6, along with the Kolmogorov-Smirnov distance bound from Lemma 4 and the tightness result for linear spectral statistics from [Bai and Silverstein, 2004] (see Section 3.2), gives the following:

**Proposition 1.** Suppose that \( (Z_n) \) is a sequence of noise matrices with correlated columns, as described in Section 3.2; and let \( F_3 \) denote the LECDF of eigenvalues of the cross-column covariances \( S_n \). Assume, in addition, that \( T_\gamma(F_Z) > \bar{\gamma}^{1/2} = (1 + \sqrt{\gamma}) \cdot \sqrt{\lambda_+(F_3)} \).\(^\text{16}\) Suppose that \( k \geq r \) with \( k/p \to 0 \). Then for any \( \ast \in \{0, w, i\} \),
\[
|T_\gamma(F_Z) - T_{p/n}(F^*_{n,k})| = \mathcal{O}_p \left( \frac{k + 1}{p} \right).
\]

Lemma 6 and Proposition 1 are proved in Section 6.3.

\(^{16}\)This additional assumption is used due to a technical requirement in the results of [Bai and Silverstein, 2004]. We suspect that it can be removed.


5 Numerical experiments

Appendix C contains comprehensive experiments conducted on a large variety of noise distributions. For space considerations we include here results for the white noise (Marcenko-Pastur) case with $\gamma = 0.5$. Simulation results and code reproducing all figures here and in Appendix C is permanently available at [Donoho et al., 2020]. See Appendix C for full details on each experiment reported here.

Figure 4: The functions $R_0(x)$ and $R_1(x)$ from Lemma 8. Observe that $x^* = \mathcal{Y}^{-1}(T_\gamma(F_Z))$ is their unique crossing point $x > \mathcal{X}_+$. Here, $\gamma = 0.5$, $p = 500$ and $n = p/\gamma$.

Figure 5: A single problem instance, corresponding to the rank $r = 5$ signal $x = (0.5, 1.0, 1.3, 2.5, 5.2)$. Shown are the functions $SE|x|t|$ and $ASE|x|t|$ on top of each other. Here $\gamma = 0.5$, $p = 500$ and $n = p/\gamma$. We indicate the locations of $Z_+$, $T_\gamma(F_Z)$ and the estimates $T_{p/n}(F_{n,k}^\star)$ for $\star \in \{0, w, i\}$, with $k = 4r = 20$. 

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Figure 6: For various choices of \( p \), and \( T = 50 \) denoising experiments, shown are the fraction of experiments where each threshold \( \in \{ T_\gamma(F_Z), T_{p/n}(F_{n,k}^0), T_{p/n}(F_{n,k}^w), T_{p/n}(F_{n,k}^i) \} \) attains oracle loss. Here, \( x = (0.5, 1.0, 1.3, 2.5, 5.2) \) so that \( r = 5 \) and \( k = 4r = 20 \).

Figure 7: Oracle loss \( \text{SE}^*_n[x] \) compared with \( \text{SE}_n[x|\hat{\theta}] \) for the choices \( \hat{t} \in \{ T_\gamma(F_Z), T_{p/n}(F_{n,k}^0), T_{p/n}(F_{n,k}^w), T_{p/n}(F_{n,k}^i) \} \), for a single spike. We let the spike intensity \( x \) vary and plot \( \text{SE}_n[x|\hat{t}]/\text{SE}^*_n[x] \) for each choice of estimator. The ratios shown are averages across \( T = 20 \) experiments.
Figure 8: Rate of convergence of $T_{p/n}(F_{\gamma,n}^{*})$ towards $T_{\gamma}(F_{Z})$. Here, $r = 10$ with $x = (1, \ldots, 10)$, set $k = 20$. Shown is the relative absolute error $\left| T_{p/n}(F_{\gamma,n}^{*}) - T_{\gamma}(F_{Z}) \right| / T_{\gamma}(F_{Z})$ as $p$ varies and $n = p/\gamma$. A logarithmic scale is used to observe the polynomial rate of decay in $p$. All points are generated by averaging the error of $T = 50$ experiments.

6 Proofs

6.1 The asymptotic loss at a fixed threshold

Throughout this section, $F_{Z}$ and $\gamma$ will be held fixed, and we will leave them implicit where possible, so as to make the notation less cumbersome. In particular, we set $z_{+} = Z_{+}(F_{Z})$, $x_{+} = X_{+}(F_{Z}, \gamma)$ throughout and we suppress mention of $F_{Z}$ and $\gamma$ in entities like $C$, $Y$, $D$.

We start by investigating $\lim_{n \to \infty} \text{SE}_{n}[x|\theta]$ for fixed $\theta$. Note that when $\theta < z_{+}$, it is clear that $\lim_{n \to \infty} \text{SE}_{n}[x|\theta] = \infty$; the reason being that, for small enough $\epsilon > 0$, with probability 1, $(1 - F_{Z}(t + \epsilon)) \cdot n = \Omega(n)$ empirical singular values $y_{i,n}$ pass the threshold $t$, so that $\text{rank}(\tilde{X}_{t}(Y_{n}))$ increases indefinitely (this argument will be made more precise later).

The following is an easy calculation:

**Lemma 7.** For any $\theta > z_{+}$, almost surely:

1. $\liminf_{n \to \infty} \text{SE}_{n}[x|\theta] \geq \text{ASE}^{*}[x]$.

2. If, in addition, $\theta \notin \{y_{1,\infty}, \ldots, y_{r,\infty}\}$, then $\lim_{n \to \infty} \text{SE}_{n}[x|\theta] = \text{ASE}[x|\theta]$.

The quantities $\text{ASE}[x|\theta]$ and $\text{ASE}^{*}[x]$ appear in Eqs. (21) and (23) respectively.

**Proof.** Since $y > z_{+}$ and $y_{r+1,\infty} \xrightarrow{a.s.} z_{+}$, we see that with probability 1, for large enough $n$,
The lemma follows by recalling that $y_{i,n} \xrightarrow{a.s.} y_{i,\infty}$ for all $i = 1, \ldots, r$, where $y_{i,\infty} = \mathcal{Y}(x_i)$ if $x_i > x_+$ and $y_{i,\infty} = z_+ < \theta$ whenever $x_i \leq x_+$, and that

$$\langle a_{i,n}, u_{i,n} \rangle \langle b_{i,n}, v_{i,n} \rangle \rightarrow \begin{cases} C(x_i) & \text{when } i = j \text{ and } x_i > x_+, \\ 0 & \text{otherwise} \end{cases}$$

and also the fact that $\mathbb{I}_{\{y_{i,n} > \theta\}} \xrightarrow{a.s.} \mathbb{I}_{\{y_{i,\infty} > \theta\}}$ whenever $\theta \neq y_{i,\infty}$. \hfill \Box

Our goal for the moment is to characterize the minimum of $\text{ASE}[x|\theta]$ with respect to thresholds $\theta$ strictly above the noise bulk edge, $\theta > z_+$. This will give us the optimal fixed threshold, in the sense of minimal asymptotic loss (though, at this point, we cannot exclude the possibility that thresholding precisely at $\theta = z_+$ might achieve better asymptotic risk).

Recall, by Eqs. (21) and (23), that the asymptotic loss decouples across the signal spikes as

$$\text{ASE}[x|\theta] = \sum_{i=1}^r R(x_i|\theta), \quad \text{ASE}^*[x] = \sum_{i=1}^r R^*(x_i),$$

where $R(x|\theta) = R^*(x) = x^2$ when $x \leq X_+$, and for $x > X_+$,

$$R(x|\theta) = \mathbb{I}_{\{\mathcal{Y}(x) \leq \theta\}} \cdot R_0(x) + \mathbb{I}_{\{\mathcal{Y}(x) > \theta\}} \cdot R_1(x), \quad R^*(x) = \min(R_0(x), R_1(x)), $$

with

$$R_0(x) = x^2, \quad R_1(x) = x^2 + \mathcal{Y}(x)^2 - 2x\mathcal{Y}(x)C(x).$$

If we were able to find $\theta > z_+$ such that $R(x|\theta) = R^*(x)$ for all $x > x_+$, then, clearly, it achieves minimal asymptotic loss. To do that, it is convenient to introduce a re-parameterization $y = \mathcal{Y}(x)$, where recall that $\mathcal{Y}(\cdot)$ is an increasing bijection, mapping $(x_+, \infty)$ to $(z_+, \infty)$. Using Eqs. (18) and (19), assuming $x > x_+$, we get

$$x^2 = (D(y))^{-1}, \quad C(x) = -2 \frac{(D(y))^{3/2}}{D'(y)},$$

so that

$$R_1(x) - R_0(x) = y^2 - 2xyC(x) = y^2 + 4y \cdot \frac{D(y)}{D'(y)} = y^2 \left(1 + \frac{4}{\Psi_\gamma(y)}\right),$$

where

$$\Psi_\gamma(y) = y \cdot \frac{D'(y)}{D(y)}$$

is as defined in Eq. (24). Since $\Psi_\gamma(\cdot)$ is negative ($D$ is positive and decreasing), we conclude that

$$R^*(x) = \mathbb{I}_{\{\Psi_\gamma(y) \leq -4\}} \cdot R_0(x) + \mathbb{I}_{\{\Psi_\gamma(y) > -4\}} \cdot R_1(x). \quad (27)$$

The next lemma establishes some essential properties of $\Psi_\gamma(y)$:
Lemma 8. Let $H$ be a compactly supported CDF, with $Z_+(H) > 0$. Let $\gamma \in (0, 1]$, and let $\Psi_\gamma(y; H)$ be defined as in Eq. (24). Then

1. The function $y \mapsto \Psi_\gamma(y; H)$ is strictly increasing on $y \in (Z_+(H), \infty)$, with $\lim_{y \to \infty} \Psi_\gamma(y; H) = -2$.

2. Assume that
   $$\lim_{y \to Z_+(F_Z)} (y - z)^{-2}dH(z) = \infty.$$  
   (This is Assumption 6 for $H = F_Z$). Then $\lim_{y \to Z_+(F_Z)} \Psi_\gamma(y; H) = -\infty$, and there is a unique point $y^* \in (Z_+(F_Z), \infty)$ such that $\Psi_\gamma(y^*; H) = -4$.

The proof of Lemma 8 is deferred to the Appendix, Section A.

Figure 9: A numerical illustration of Lemma 8 and its consequences. Assuming a rank-1 signal $X = x \cdot a_{1,n}b_{1,n}^T$, set $R_0(x) = \|X\|_F^2 = x^2$ and $R_1(x) = \lim_{n \to \infty} \|X - y_{1,n}a_{1,n}b_{1,n}^T\|_F^2$. The point $x^* = \mathcal{Y}^{-1}(T_\gamma(F_Z))$ is the unique crossing point $R_0(x^*) = R_1(x^*)$. When $x < x^*$, the principal components of $Y$ are “too noisy”, so that estimating $\hat{X} = 0$ gives better squared error; when $x > x^*$, the situation reverses. At each plot, $R_0(x)$ and $R_1(x)$ are plotted as $x$ varies, for finite $n$, fixed signal components $a_{1,n}b_{1,n}^T$ and a single instance of $Z_n$. The dashed vertical line is an estimate of $x^*$, obtained by applying the functional $T_{p/n}(\cdot)$ on $F_{Z_n}$, as well as computing the inverse map $\mathcal{Y}^{-1}(T_{p/n}(F_{Z_n}))$ numerically from $F_{Z_n}$. In all cases, $p = 500$ and $n = p/\gamma$. From left to right, top to bottom: (i) Marcenko-Pastur law with shape $\gamma = 1$; (ii) Noise matrix with correlated columns, with $F_S = \frac{1}{2}\delta_1 + \frac{1}{2}\delta_{10}$ and $\gamma = 0.5$; (iii) Likewise, with $F_S = \text{Unif}[1, 10]$; (iv) $F_Z = \delta_1$ and $\gamma = 1$ (specifically, $Z_n = I$).
Proof of Lemma 1. The lemma follows as a straightforward corollary of Lemma 8. Lemma 8 implies that there is a unique number $T_\gamma(F_Z) > Z_+(F_Z)$ such that $\Psi_\gamma(T_\gamma(F_Z);F_Z) = -4$. Since $y \mapsto \Psi_\gamma(y;F_Z)$ is increasing, plugging into Eq. (27),

$$R^*(x) = R(x|T_\gamma(F_Z)) = \mathbf{1}_{\{y \leq T_\gamma(F_Z)\}} \cdot R_0(x) + \mathbf{1}_{\{y > T_\gamma(F_Z)\}} \cdot R_1(x),$$  

(28)

where $x > X_+$ and $y = \mathcal{Y}(x)$. We conclude that $\text{ASE}^*_\mathbb{E}[x] = \text{ASE}[x|T_\gamma(F_Z)]$. This is the minimum of $\text{ASE}[x|\theta]$ over all $\theta > 0$ since, clearly, $\text{ASE}[x|\theta] \geq \text{ASE}^*_\mathbb{E}[x]$ by definition. Moreover, for any $\theta \neq T_\gamma(F_Z)$, we can find some $y > Z_+(F_Z)$ such that either $\theta < y < T_\gamma(F_Z)$ or $T_\gamma(F_Z) < y < \theta$. Taking $x = \mathcal{Y}^{-1}(x)$, we find that $R(x|\theta) > R(x|T_\gamma(F_Z)) = R^*(x)$, since there is a unique crossing point $x > X_+$ with $R_0(x) = R_1(x)$ (this is because $y \mapsto \Psi_\gamma(y;F_Z)$ is strictly increasing). Thus, we can construct a signal $x$ for which $\text{ASE}[x|\theta] > \text{ASE}^*_\mathbb{E}[x]$; we conclude that $T_\gamma(F_Z)$ is the unique threshold which minimizes $\text{ASE}[x|\theta]$ universally for all $x$.

Proof of Lemma 2. Part (1) of the Lemma follows from Lemma 1, along with the observation that if $\mathcal{Y}(x) = T_\gamma(F_Z)$, then $R_0(x) = R_1(x) = R^*(x)$; this means that regardless of whether we threshold slightly above or below $\mathcal{Y}(x)$, we get the same asymptotic loss. Part (2) follows by the same argument as in the proof of Lemma 3, in the paragraph above. Finally, part (3) follows right from the definition of $\Theta(x)$ and $\Theta(x)$.

6.2 Achieving oracle loss

We move on to study the oracle loss $\text{SE}^*_\mathbb{E}[x]$. This random variable depends on both $X_n$ and the noise $Z_n$.

Denote

$$\hat{X}_{[k]} = \sum_{i=1}^{k} y_{n,i} u_{i,n} v_{i,n}^T, \quad k = 0, \ldots, p.$$  

(29)

That is, $\hat{X}_{[k]}$ is obtained from $Y$ by keeping only the top $k = 0, \ldots, p$ singular values (equivalently, hard thresholding at $t = y_{k+1,n}$). Any hard thresholding estimator $\hat{X}_\theta$ obviously corresponds to some $\hat{X}_{[k]}$, specifically, $y_{k,n} > \theta \geq y_{k+1,n}$ (for notational consistency, set $y_{0,n} = \infty$). Thus,

$$\text{SE}^*_\mathbb{E}[x] = \min_{0 \leq k \leq p} \|X - \hat{X}_{[k]}\|^2_F.$$  

We first show that keeping too many singular values is consistently sub-optimal:

Lemma 9. Set $M = r + 1 + \left\lceil \frac{\text{ASE}^*_\mathbb{E}[x]}{\varepsilon_y} \right\rceil$. Then

$$\mathbb{P} \left\{ \exists N \text{ s.t. } \forall n \geq N : \text{SE}^*_\mathbb{E}[x] < \min_{k \geq M} \|X - \hat{X}_{[k]}\|^2_F \right\} = 1.$$  

Proof. Recall that for any matrix $A \in \mathbb{R}^{n \times p}$ with SVD $A = \sum_{i=1}^{p} \sigma_i u_i v_i^T$, its best rank-$r$ approximation with respect to Frobenius norm is obtained by taking its $r$ leading principal components. Since $X$ has rank $r$, for any $k \geq M$,

$$\|X - \hat{X}_{[k]}\|^2_F \geq \min_{\text{rank}(B) = r} \|B - \hat{X}_{[k]}\|^2_F = \sum_{i=r+1}^{k} y_{i,n}^2 \geq \sum_{i=r+1}^{M} y_{i,n}^2.$$  

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Recall that any fixed \( i \geq r + 1 \) satisfies \( y_{i,n} \xrightarrow{a.s.} y_{i,\infty} = z_+ \). Since \( M \) is constant, and satisfies \( M > r + \text{ASE}^*|x|/z_+ \), we obtain that

\[
\sum_{i=r+1}^{\infty} y_{i,n}^2 \xrightarrow{a.s.} (M - r)z_+ > \text{ASE}^*|x|.
\]

Since \( \text{SE}_n^*|x| \leq \text{SE}_n|x|T_\gamma(F_Z) \xrightarrow{a.s.} \text{ASE}^*|x| \), we conclude that almost surely, for all large enough \( n, \text{SE}_n^*|x| < \min_{n \geq M} \|X - \hat{X}_{[k]}\|_{F}^2 \).

\( \square \)

Lemma 9 tells us that to study the oracle loss \( \text{SE}_n^*|x| \) as \( n \to \infty \), we only need, essentially, to study the risk of a bounded number of estimators; specifically, \( X_{[k]} \) for \( 0 \leq k < M \). In order to obtain formulas for \( \lim_{n \to \infty} \|X_n - \hat{X}_{[k]}\|_{F}^2 \), we need to compute the limiting correlations between the underlying signal dyads, \( a_{i,n}, b_{i,n}, \ldots, a_{r,n}, b_{r,n} \) and the corresponding empirical dyads \( u_{i,n}v_{i,n}^\top \), for all \( 1 \leq i < M \). For empirical spikes up to \( i = r \), these limiting correlations are computed in [Benaych-Georges and Nadakuditi, 2012a] (recall Eq. (12)).

The next result shows that, as one would expect, the \( j \)-th singular vectors of \( Y \), for any bounded \( j \geq r + 1 \), are asymptotically uncorrelated with the signal singular vectors:

**Proposition 2.** For any \( 1 \leq i \leq r \) and fixed \( j \neq i \) (not necessarily \( j \leq r \)), one has

\[
\langle a_{i,n,j}, b_{i,n,j} \rangle \rightarrow 0.
\]

We provide a proof of Proposition 2, assuming that \( r = 1 \). This restriction is due to our proof technique, and numerical results indicate that this results holds generally in the multi-spiked case. The proof is technical, and provided in Section B.

The following Lemma is an immediate corollary of Proposition 2:

**Lemma 10.** For any \( k \geq r \),

\[
\|X - \hat{X}_{[k]}\|_{F}^2 \xrightarrow{a.s.} \sum_{i=1}^{r} \left[ x_i^2 + y_{i,\infty}^2 - 2x_i \cdot y_{i,\infty} \cdot C(x_i) \right] + (k - r)z_+,
\]

where, by way of notation, we use \( C(x_i) = 0 \) for \( x_i \leq x_+ \). In particular,

\[
\mathbb{P}\left\{ \exists N \text{ s.t. } \forall n \geq N : \text{SE}_n^*|x| < \min_{k \geq r + 1} \|X - \hat{X}_{[k]}\|_{F}^2 \right\} = 1.
\]

**Proof.** The calculation is straightforward, as in the proof of Lemma 7. For the last part, simply recall that

\[
\text{SE}_n|x|T_\gamma(F_Z) \xrightarrow{a.s.} \text{ASE}^*|x| \leq \sum_{i=1}^{r} \left[ x_i^2 + y_{i,\infty}^2 - 2x_i \cdot y_{i,\infty} \cdot C(x_i) \right] .
\]

\( \square \)

We are ready to prove Theorems 1 and 2.
Proof of Theorem 1. By Lemmas 9 and 10, almost surely, there exists $N$ such that $\forall n \geq N$,

$$SE_n^*[x] = \min_{0 \leq k \leq r} \|X - \hat{X}_k\|_F^2.$$

Part (1) then follows from the observation that $\min_{0 \leq k \leq r} \|X - \hat{X}_k\|_F^2 \overset{a.s.}{\rightarrow} \text{ASE}^*[x]$, as can be deduced from the calculations of Section 6.1. We now prove (2). Let’s assume, for ease of notation, that $T_\gamma(F_Z) \notin \{y_1, \ldots, y_{r, \infty}\}$. In that case, the asymptotic optimal interval is just the interval between some two consecutive spikes, say,

$$\Omega(x) = y_{k^* + 1, \infty}, \quad \overline{\Omega}(x) = y_{k^*, \infty},$$

with the notation $y_{0, \infty} = \infty$. With probability one, for large enough $n$, $X_{\hat{\theta}_n} = \hat{X}_{[k^*]}$. Now, recall that $\|X_n - \hat{X}_{[k^*]}\|_F^2 \overset{a.s.}{\rightarrow} \text{ASE}^*[x]$.

Proof of Theorem 2. Let $k^*$ be as in the proof of Theorem 1. We know, from Lemmas 9, 10 and the definition of the asymptotic optimal interval, that $\|X - \hat{X}_{[k^*]}\|_F^2 \overset{a.s.}{\rightarrow} \text{ASE}^*[x]$ and that almost surely, $\liminf_{n \to \infty} \min_{k \neq k^*} \|X - \hat{X}_k\|_F^2 > \text{ASE}^*[x]$ (here we assume that there is no $y_{i, \infty}$ that equals $T_\gamma(F_Z)$). Thus,

$$\mathbb{P}\left\{ \exists N \text{ s.t. } \forall n \geq N : SE_n^*[x] = \|X - \hat{X}_{[k^*]}\|_F^2 < \min_{k \neq k^*} \|X - \hat{X}_k\|_F^2 \right\} = 1.$$

The proof follows by noting that: (i) If $\theta \in (\Omega(x), \overline{\Omega}(x))$, then with probability 1, for all large enough $n$, $X_{\hat{\theta}_n} = \hat{X}_{[k^*]}$; (ii) If $\theta \notin (\Omega(x), \overline{\Omega}(x))$ then with probability 1, for large enough $n$, $X_{\hat{\theta}_n} = \hat{X}_{[k^*]}$.

6.3 Estimating $T_\gamma(F_Z)$

Proof of Lemma 3. Let $\epsilon > 0$ be small. By assumption, $T_\gamma(H) > Z_+(H)$, and it is the unique number satisfying $\Psi_\gamma(T_\gamma(H); H) = -4$. Let $y_1 = T_\gamma(H) - \epsilon/2$, $y_2 = T_\gamma(H) + \epsilon/2$, where $\epsilon$ was chosen small enough so that $Z_+(H) < y_1 < y_2$. Note that $\Psi_\gamma(y_1; H) < -4 < \Psi_\gamma(y_2; H)$.

Since $H_n \overset{d}{\rightarrow} H$ (and $|p/n - \gamma| \leq 1/n \to 0$) we find that for all large enough $n$, $\Psi_{p/n}(y_1; H_n) < -4 < \Psi_{p/n}(y_2; H_n)$. Since also $Z_+(H_n) \overset{d}{\rightarrow} Z_+(H) < y_1$, we deduce that for large enough $n$, $y_1 < T_{p/n} H_n < y_2$, that is, $|T_{p/n} H_n - T_\gamma(H)| < \epsilon$.

Proof of Lemma 4. Part (1) will follow from (3), since convergence in KS distance implies weak convergence, and $F_{Z_n} \overset{d}{\rightarrow} F_Z$ almost surely. For part (3), denote by $z_{i,n}$, $i = 1, \ldots, p$, the singular values of $Z_n$. By Weyl’s interlacing inequality, since $Y_n = X_n + Z_n$ and rank($X$) = $r \leq k$,

$$z_{i,n} \leq y_{i,n} \leq z_{i-k,n}, \text{ for } i = k + 1, \ldots, p.$$

Fix some $y$, and let $j$ be the smallest index $j \geq k + 1$ such that $y_{j,n} \leq y$ (set $j = 0$ if no such index exists). The interlacing inequality states that $z_{j,n} \leq y$ as well. If $j = k + 1$, then at worst the interval contains all of $z_{k,n}, \ldots, z_{1,n}$ and none of the additional “pseudo-singular values” we have introduced. Hence, in that case, $|F_{Z_n}(y) - F_{n,k}^*| \leq k/p$. Now, suppose that $j > k + 1$. Since $y_{j+1,n} > y$, the interlacing inequality gives $z_{j+1-k,n} \geq y_{j+1,n} > y$, hence in addition to $z_{p,n}, \ldots, z_{j,n}$, the interval $(-\infty, y]$ contains at most $k$ additional singular values of $Z_n$, specifically $z_{j+1,n}, \ldots, z_{j-k,n}$. In the worst case, we have added no “pseudo-singular values” with $\leq y$, hence again $|F_{Z_n}(y) - F_{n,k}^*| \leq k/p$. Lastly, to prove (2), note that for any
\( \epsilon > 0, F_Z(Z_+(F_Z) - \epsilon) < 1 \), which means that almost surely, for large enough \( n \) there are \( \Omega(n) \) singular values of \( Z_n \) bigger than \( Z_+(F_Z) - \epsilon \). By interlacing, for any \( m_n = o(n) \) with \( m_n < r, y_{m,n} \geq z_{m,n}, \) and \( z_{m,n} \) must eventually be among those singular values bigger than \( Z_+(F_Z) - \epsilon \). But this is true for any \( \epsilon > 0 \), meaning that \( y_{m,n} \overset{a.s.}{\rightarrow} Z_+(F_Z) \) whenever \( r < m_n = o(n) \).

**Proof of Lemma 6.** Fix any \( a \) satisfying \( Z_+(H) < a < T_\gamma(H) \). Observe that one can find a neighborhood \( \mathcal{N} \) of \( T_\gamma(H) \) and \( c_1, c_2 > 0 \) such that \( c_2 < \Psi_\gamma'(y; G) < c_1 \) for any distribution \( G \) supported on \([0, a]\) and \( \gamma' \) (to see this, simply follow calculations in the proof of Lemma 8). Thus, since \( T_{p/n}(H_n) \rightarrow T_\gamma(H) \), for all large enough \( n \),

\[
c_2(T_{p/n}(H_n) - T_\gamma(H)) < \Psi_{p/n}(T_{p/n}(H_n); H_n) - \Psi_{p/n}(T_\gamma(H); H_n) \leq c_1(T_{p/n}(H_n) - T_\gamma(H)).
\]

Using \( \Psi_{T_\gamma(H); H} = \Psi_{p/n}(T_{p/n}(H_n); H_n) = -4 \), and the fact that \( \Psi \) is increasing, we conclude that

\[
|T_{p/n}(H_n) - T_\gamma(H)| \leq \max(1/c_1, 1/c_2) \cdot |\Psi_{p/n}(T_{p/n}(H_n); H_n) - \Psi_{p/n}(T_\gamma(H); H_n)|
\]

\[
= \max(1/c_1, 1/c_2) \cdot \left| \Psi_{T_\gamma(H); H} - \Psi_{p/n}(T_{p/n}(H_n); H_n) \right|.
\]

The right-hand-side is now \( O(\Delta_{1,n} + \Delta_{2,n} + |p/n - \gamma|) \).

**Proof of Proposition 1.** By Lemma 6, we need to show that

\[
|\varphi(T_\gamma(F_Z); F_Z) - \varphi(T_\gamma(F_Z); F^*_n)|, \ |\varphi'(T_\gamma(F_Z); F_Z) - \varphi'(T_\gamma(F_Z); F^*_n)| = O(\Psi(k/p))
\]

(by definition, \( |\gamma_n - \gamma| \leq 1/n \)). Write

\[
\varphi(T_\gamma(F_Z); F_Z) - \varphi(T_\gamma(F_Z); F^*_n) = \left[ \varphi(T_\gamma(F_Z); F_Z) - \varphi(T_\gamma(F_Z); F_n) \right]
+ \left[ \varphi(T_\gamma(F_Z); F_n) - \varphi(T_\gamma(F_Z); F^*_n) \right],
\]

we bound each bracket separately (the argument when \( \varphi \) is replaced by \( \varphi' \) is the same). The expression \( \varphi(T_\gamma(F_Z); F_Z) = \int T_\gamma(F_Z) \varphi\left( \frac{t}{T_\gamma(F_Z)} \right) dF_Z(z) \) is a linear spectral statistic, and satisfies the requirement of [Bai and Silverstein, 2004], by assumption - see Section 3.2. Hence,

\[
|\varphi(T_\gamma(F_Z); F_Z) - \varphi(T_\gamma(F_Z); F_n)| = O(1/p).
\]

For the second term, recall that if \( F_1 \) and \( F_2 \) are CDFs supported on the interval \( I \) and \( g : I \rightarrow \mathbb{R} \) is bounded and continuously differentiable, then

\[
\left| \int g(t)(dF_1(t) - dF_2(t)) \right| \leq \left( \|g\|_{L^\infty(I)} + \|g'\|_{L^1(I)} \right) \cdot \|F_1 - F_2\|_{KS}.
\]

Since both \( Z_+(F_n), Z_+(F^*_n) \overset{a.s.}{\rightarrow} Z_+(F_Z) \), by Lemma 4, almost surely for large enough \( n \),

\[
|\varphi(T_\gamma(F_Z); F_n) - \varphi(T_\gamma(F_Z); F^*_n)| = O(k/p).
\]

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References


A Proof of Lemma 8

Define the probability distribution $d\tilde{H} = \gamma dH + (1 - \gamma)\delta_0$, so that, by definition, $\bar{\phi}_\gamma(y; H) = \Phi(y; \tilde{H})$. Since

$$\Psi(y; H) = y \cdot \frac{D'(y; H)}{D(y; H)} = y \cdot \left( \frac{\phi'(y; H)}{\Phi(y; H)} + \frac{\phi'(y; H)}{\phi(y; H)} \right),$$

to show that $\Psi$ is increasing, it suffices to show that $y \mapsto y \cdot \frac{\phi'(y; H)}{\phi(y; H)}$ is increasing for any CDF $H$ and $y > Z_+(H)$.

Introduce a change of variables $w = \log(y)$ and set $\psi(w) = \phi(e^w; H)$. We have

$$y \cdot \frac{\phi'(y; H)}{\phi(y; H)} = y \cdot \frac{d}{dy} \left( \log \phi(y; H) \right) = y \cdot \frac{d}{dw} \left( \log \phi(e^w; H) \right) \cdot \frac{dw}{dy} = \frac{d}{dw} \left( \log \psi(w) \right).$$

Since $w$ is strictly increasing in $y$, it remains to show that $w \mapsto \left( \log \psi(w) \right)'$ is increasing, equivalently, that $w \mapsto \psi(w)$ is log-convex. Write

$$\psi(w) = \int \psi_z(w) dH(z), \quad \text{where} \quad \psi_z(w) = \frac{e^w}{e^{2w} - z^2}.$$

Since a convex combination of log-convex functions is log-convex, it suffices to verify that each $\psi_z(w)$ is log-convex, whenever $y^2 = e^{2w} > z^2$. A straightforward calculation gives:

$$(\log \psi_z(w))' = 1 - \frac{2e^{2w}}{e^{2w} - z^2} = -\frac{z^2 + e^{2w}}{e^{2w} - z^2} = -1 - \frac{2z^2}{e^{2w} - z^2},$$

which is negative and clearly increasing in $w$. Thus, $\psi_z(w)$ is log-convex, and so we conclude that $y \mapsto D(y; H)$ is strictly increasing. For the limit as $y \to \infty$, write

$$\phi(y; H) = \int \frac{y}{y^2 - z^2} dH(z) = \frac{1}{y} + o \left( \frac{1}{y^2} \right), \quad \phi(y; H) = -\int \frac{y^2 + z^2}{(y^2 - z^2)^2} dH(z) = -\frac{1}{y^2} + o \left( \frac{1}{y^3} \right),$$

as $y \to \infty$. Thus, $\Psi(\gamma(y; H)) = -2 + o(1)$ as $y \to \infty$.

For part (2), observe that the additional assumption on $H$ implies that $\frac{\phi'(y; H)}{\phi(y; H)} \to -\infty$ as $y \to Z_+(H)$ from the right, hence $\Psi(y) \to -\infty$. Now, since $\Psi(y)$ is continuous on $y \in (Z_+(H), \infty)$, it must attain $\Psi(y^*) = -4$ for some $y^*$. This $y^*$ must be unique since, as we have proved in (1), $\Psi(y; H)$ is strictly increasing.

B Proof of Proposition 2

We provide a proof assuming $r = 1$ (in fact the case $j \leq r$ already follows from the result of [Benaych-Georges and Nadakuditi, 2012b]).

The argument below relies on ideas from [Nadler, 2008].

When $r = 1$, the measurement matrix $Y_n$ has the form $Y_n = x_1 a_{1,n} b_{1,n}^\top + Z_n$. Of course, the eigenvectors of $Y_n^\top Y_n$ are exactly the right singular vectors of $Y_n$, namely, $\mathbf{v}_{1,n}, \ldots, \mathbf{v}_{p,n}$. Let $P_n = I - b_{1,n} b_{1,n}^\top$ be the projection onto the orthogonal complement of $b_{1,n}$, and let $\mathbf{q}_{2,n}, \ldots, \mathbf{q}_{p,n}$ be an eigenbasis of $P_n Y_n Y_n^\top P_n$, corresponding to its restriction onto range($P_n$) = $\{b_{1,n}\}$ in $\mathbb{R}^p$. Of course, the ordered tuple $B = (b_{1,n}, \mathbf{q}_{2,n}, \ldots, \mathbf{q}_{p,n})$ constitutes an orthonormal basis of $\mathbb{R}^p$. 33
We now write the matrix $Y_n^\top Y_n$ in terms of the basis $\mathcal{B}$ (that is, we conjugate it by the appropriate orthogonal change-of-basis matrix). The resulting matrix has the form

$$M = \begin{bmatrix} a_n & w \top \\ w & D \end{bmatrix},$$

where

- $a_n = b_{1,n}^\top Y_n^\top Y_n b_{1,n}$.
- $w \in \mathbb{R}^{p-1}$ is given by

$$w \top = \begin{bmatrix} b_{1,n}^\top Y_n^\top Y_n q_{2,n}, \ldots, b_{1,n}^\top Y_n^\top Y_n q_{p,n} \end{bmatrix}.$$  

Note that, using $b_{1,n} \perp q_{i,n}$, we can write, for $i = 2, \ldots, p$,

$$w_{i,n} = b_{1,n}^\top Y_n^\top Y_n q_{i,n} = \left(x_1a_{1,n} + b_{1,n}^\top Z_n^\top \right) Z_n q_{i,n} = x_1 a_{1,n} q_{i,n} + b_{1,n}^\top Z_n^\top Z_n q_{i,n},$$

where $w = (w_2, \ldots, w_{n,n})$.

- $D$ is a diagonal matrix, $D = \text{diag}(\mu_{2,n}, \ldots, \mu_{p,n})$ where $\mu_{i,n}$ is the eigenvalue of $P_n Y_n^\top Y_n P_n = P_n Z_n^\top Z_n P_n$ corresponding to the eigenvector $q_{i,n}$.

The matrix $M$ is a so-called arrowhead matrix. Recall that, by definition, its eigenvalues are $y_{1,n}^2, \ldots, y_{p,n}^2$; the corresponding eigenvectors are known to have the form

$$p_{j,n} \propto \left(1, \frac{w_{2,n}}{y_{2,n} - \mu_{2,n}}, \ldots, \frac{w_{n,n}}{y_{n,n} - \mu_{n,n}} \right), \quad j = 1, \ldots, p.$$  

Of course, recall that $p_{j,n}$ is simply $v_{j,n}$ written in the basis $\mathcal{B}$. Now, the first entry of $p_{j,n}$ is (up to the ambiguous sign) the inner product $\langle b_{1,n}, v_{j,n} \rangle$, since $b_{1,n}$ is represented by $e_1$ in the basis $\mathcal{B}$. Thus,

$$|\langle b_{1,n}, v_{j,n} \rangle| = \left(1 + \sum_{i=2}^n \frac{w_{i,n}^2}{(y_{i,n}^2 - \mu_{i,n})^2} \right)^{-1/2}.$$  

We claim that for any fixed $j \geq 2$,

$$\sum_{i=2}^n \frac{w_{i,n}^2}{(y_{i,n}^2 - \mu_{i,n})^2} \xrightarrow{a.s.} \infty,$$

from which the claimed result follows. Recall that, by assumption, $a_{1,n}$ is uniform on the unit sphere $S^{n-1}$. Introduce a Gaussian random vector, $g \sim \mathcal{N}(0, I)$, independent of $Z_n$ and $b_{1,n}$, such that $a_{1,n} = g / \|g\|$. Note that the basis $q_{2,n}, \ldots, q_{n,n}$ can be chosen such that $b_{1,n}^\top Z_n^\top Z_n q_{i,n} \geq 0$ for all $2 \leq i \leq n$; indeed assume that this is the case. Setting $\eta_i = (\mu_{i,n})^{-1/2}Z_n q_{i,n}$, the random variables $\eta_2, \ldots, \eta_p$ are standard Gaussians, independent of $Z_n$ and $b_{1,n}$, and independent of one another, as

$$\text{Cov}(\eta_i, \eta_k) = (\mu_{i,n}\mu_{k,n})^{-1/2} q_{i,n}^\top Z_n^\top Z_n q_{k,n} = 1_{\{i=k\}},$$

and this is true because the vectors $q_{i,n}$ are eigenvectors of $P_n Y_n^\top Y_n P_n = P_n Z_n^\top Z_n P_n$, with eigenvalues $\mu_{i,n}$. Clearly,

$$w_{i,n}^2 = \left(x_1a_{1,n} q_{i,n} + b_{1,n}^\top Z_n^\top Z_n q_{i,n} \right)^2 \geq \frac{x_1 \sqrt{\mu_{i,n}}}{\|g\|} \eta_i + b_{1,n}^\top Z_n^\top Z_n q_{i,n} \right)^2 \geq \frac{x_1^2 \mu_{i,n}}{\|g\|^2} \eta_i^2 1_{\{\eta_i \geq 0\}}.$$  

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We have conducted experiments using the following noise distributions.

To conclude the proof, recall that the quantity on the right tends to \( \infty \). Fixing any \( \varepsilon > 0 \), we know that with probability 1, for large enough \( n \), \( y_{j,n}^2 \leq (Z_+ + \varepsilon)^2 \), since \( y_{j,n} \stackrel{d}{\rightarrow} y_{j,\infty} = Z_+ + \varepsilon \) (and \( j > r = 1 \)). Since \( \mu_{2,n} \stackrel{a.s.}{\rightarrow} Z_+ + \varepsilon \), we deduce that with probability 1, for large enough \( n \),

\[
\sum_{i=2}^{n} \frac{w_{2,n}^2}{\left( y_{j,n}^2 - \mu_{i,n} \right)^2} \geq \sum_{i=2}^{n} \frac{w_{2,n}^2}{\left( (Z_+ + \varepsilon)^2 - \mu_{i,n} \right)^2} \geq \frac{x_1^2}{\|g\|^2} \sum_{i=2}^{n} \frac{\eta_i^2 1_{\{\eta_i \geq 0\}} \cdot \mu_{i,n}}{(Z_+ + \varepsilon)^2 - \mu_{i,n}} .
\]

Since \( \mathbb{E}[\eta_i^2 1_{\{\eta_i \geq 0\}}] = 1/2 \), and \( \|g\|^2/n \stackrel{a.s.}{\rightarrow} 1 \), appealing to the strong law of large numbers,

\[
\frac{x_1^2}{\|g\|^2} \sum_{i=2}^{n} \frac{\eta_i^2 1_{\{\eta_i \geq 0\}} \cdot \mu_{i,n}}{(Z_+ + \varepsilon)^2 - \mu_{i,n}} \stackrel{a.s.}{\rightarrow} \frac{1}{2} x_1^2 \int \frac{t^2}{(Z_+ + \varepsilon)^2 - t^2} \, dF_Z(t).
\]

Thus, almost surely, for any \( \varepsilon > 0 \)

\[
\liminf_{n \to \infty} \left\{ \sum_{i=2}^{n} \frac{w_{2,n}^2}{\left( y_{j,n}^2 - \mu_{i,n} \right)^2} \right\} \geq \frac{1}{2} x_1^2 \int \frac{t^2}{(Z_+ + \varepsilon)^2 - t^2} \, dF_Z(t) .
\]

To conclude the proof, recall that the quantity on the right tends to \( \infty \) as \( \varepsilon \to 0 \).

## C Additional numerical experiments

In this section we provide extensive numerical experiments validating different aspects of our results under various noise distributions.

### C.1 Noise distributions

We have conducted experiments using the following noise distributions:

- **Marcenko-Pastur**: the matrix \( Z \) is an i.i.d Gaussian matrix, so that \( F_Z \) is a Marcenko-Pastur with shape parameter \( \gamma \).

- **Chi10**: A noise matrix with correlated columns, such that \( W \) is i.i.d Gaussian and \( F_S \) is the law of a \( \chi^2 \)-squared random variable with 10 degrees of freedoms, normalized to have variance 1: \( T = \frac{1}{m} \sum_{i=1}^{10} g_i \) where \( g_1, \ldots, g_{10} \sim \mathcal{N}(0,1) \).

- **Mix2**: A noise matrix with correlated columns, such that \( W \) is i.i.d Gaussian, and \( F_S \) is an equal mixture of two atoms: \( dF_S = \frac{1}{2} \delta_1 + \frac{1}{2} \delta_{10} \).

- **Unif[1,10]**: A noise matrix with correlated columns, such that \( W \) is i.i.d Gaussian, and \( F_S \) is the uniform distribution on \([1,10]\).
• **Fisher3n**: $Z$ has the form $Z = W_1 S_2^{-1/2}$ where $W_1 \in \mathbb{R}^{n \times p}$ is i.i.d Gaussian $\mathcal{N}(0, 1/n)$, and $S_2 = W_2^2 W_2$ where $W_2 \in \mathbb{R}^{3p \times p}$ is an i.i.d Gaussian matrix with entries $\mathcal{N}(0, 1/(3n))$. Matrices of this form have been studied in the literature under the name F-matrices (also F-ratios, Fisher matrices). Their limiting singular value distribution is given by Wachter’s law [Wachter et al., 1980], see also [Yin et al., 1983, Silverstein, 1985, Bai and Silverstein, 2010].

• **PaddedIdentity**: All the singular values of $Z$ are 1, that is, $dF_Z = \delta_1$. Specifically, $Z$ is the matrix $Z = [I_{p \times p}, 0_{p \times (n-p)}]$ T, that is, a $p$-by-$p$ identity matrix, padded by zeros.

In the table below, one can find some useful quantities corresponding to the distributions above (with select choices of $\gamma$): the bulk edge $Z_+(F_Z)$, the location of the BBP PT $\mathcal{X}_+$, optimal threshold $T_\gamma(F_Z)$ and $x^* = \mathcal{Y}^{-1}(T_\gamma(F_Z))$. All these quantities are estimated by sampling a large noise matrix $Z$ (specifically, we take $p = 3000$ and $n = p/\gamma$) and estimating all the necessary functionals by their plugin estimates, putting $F_Z$ in place of $F_Z$, and rounding all numbers to 2 digits after the decimal point. Estimating $\mathcal{X}_+$ in this manner is especially problematic, since for any counting measure $H$, in our case $H = F_{Z_\gamma}$, $\mathcal{X}_+(H) = \lim_{y \rightarrow Z_+(H)} (D_{p/n}(y; H))^{-1/2} = 0$, since $D(\cdot; H)$ has 1/2 singularity near $Z_+(H)$. For our purposes, we use the heuristic $\mathcal{X}_+ \approx (D_{p/n}(Z_+(F_{Z_\gamma}) + 0.01; F_{Z_\gamma}))^{-1/2}$, which may be somewhat off from the true PT location. In the case of PaddedIdentity, it is obvious that $\mathcal{X}_+ = 0$, and this is what we give below.

<table>
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<tr>
<th>Distribution:</th>
<th>$\gamma$</th>
<th>$Z_+(F_Z)$</th>
<th>$\mathcal{X}_+(F_Z)$</th>
<th>$T_\gamma(F_Z)$</th>
<th>$\mathcal{Y}^{-1}(T_\gamma(F_Z))$</th>
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<td>Marcenko-Pastur</td>
<td>0.5</td>
<td>1.7</td>
<td>0.91</td>
<td>1.98</td>
<td>1.48</td>
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<td></td>
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<td>2.0</td>
<td>1.07</td>
<td>2.31</td>
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<td>1.59</td>
<td>2.17</td>
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</tr>
<tr>
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<td>1.89</td>
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<td>Fisher3n</td>
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<td>2.57</td>
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<td>1.0</td>
<td>0.0</td>
<td>1.73</td>
<td>1.15</td>
</tr>
</tbody>
</table>

C.2 Description of experiments

For each noise distribution we conduct the following experiments:

• **Hist**: We give a histogram singular values of a large noise matrix, in the case where the description of $F_Z$ is not trivial. We do this to get a some sense for how the noise bulk looks like. Specifically, the noise matrix we sample has dimensions $p = 3000$ and $n = p/\gamma$.

• **R0-vs-R1**: We compare the functions $R_0(x)$ and $R_1(x)$ from Lemma 8, and demonstrate that $x^* = \mathcal{Y}^{-1}(T_\gamma(F_Z))$ is their unique crossing point $x > \mathcal{X}_+$; this is done in the following way: we consider a rank 1 signal $X = x a b^T$ and $Y = X + Z$, where the signal directions $a, b$ and noise matrix $Z$ are sampled once, and we let the intensity $x$ vary. The dimensions used are $p = 500$ and $n = p/\gamma$. We plot the quantities $R_0(x) = \|X\|_F^2 = x^2$ (the error of the estimator $\hat{X} = 0$) and $R_1(x) = \|X - y_1 u v^T\|_F^2$, the error obtained by for

\footnote{For instance, when the noise is Marcenko-Pastur, exact expressions are available, see e.g [Gavish and Donoho, 2014], and $\mathcal{X}_+ = \gamma^{1/4}$. This is quite off from the expression in the table!}
estimating $X$ using the principal component of $Y$. The theory states that $\widehat{R}_1(x)$ converges to converges to $R_1(x)$, and we also plot this, as well as show that $x^*$ is the unique intersection point of $R_0(x)$ and $R_1(x)$. Thresholding at the intersection of $R_1(x)$ and $R_0(x)$ is optimal (for this problem instance), and we see that indeed this intersection point is quite close to $x^*$.

- **SE-vs-ASE**: Our theory states that as $n, p$ grow, the random function $\theta \mapsto SE_n|x[θ]$ tends to the deterministic function $θ \mapsto ASE|x[θ]$, when $θ > Z_+(F_2)$. We illustrate this phenomenon. We consider a single problem instance, corresponding to the rank $r = 5$ signal $x = (0.5, 1.0, 1.3, 2.5, 5.2)$, and plot the function $SE_n|x[θ]$ and $ASE|x[θ]$ on top of each other (we plot $SE_n|x[θ]$ for very few thresholds $θ ≤ y_{r+1,n}$; as the rank of $X_i$ grows, the MSE blows up quickly). We use dimensions $p = 500$ and $n = p / γ$. We indicate the locations of $z_+, T_γ(F_2)$ and the estimates $T_{p/n}(F^*_{n,k})$ for $* ∈ \{0, w, i\}$, where we use $k = 4r = 20$. We see that for a “typical” problem instance, $ASE|x[θ]$ is indeed a good proxy for $SE_n|x[θ]$.

- **Oracle Attainment**: We test Theorems 2 and 3, whereby the probability that thresholding at $T_{p/n}(F^*_{n,k})$ attains oracle loss with probability tending to 1 as $n, p → ∞$. For various choices of $p$, we run $T = 50$ denoising experiments, and report the fraction of experiments where each threshold $θ ∈ \{T_γ(F_2), T_{p/n}(F^*_0_{n,k}), T_{p/n}(F^w_{n,k}), T_{p/n}(F^i_{n,k})\}$ attains oracle loss ($T_γ(F_2)$ is computed as described in experiment R0-vs-R1). In all experiments, we use the signal $x = (0.5, 1.0, 1.3, 2.5, 5.2)$ which has rank $r = 5$ (the same signal as in experiment SE-vs-ASE), and the upper bound $k = 4r = 20$. Note that we have chosen the spikes $x_i$ to be all far from $x^* = Y^{-1}(T_γ(F_2))$, in accordance with the condition in Theorem 2.

- **Regret**: We compare the oracle loss $SE_n|x$ with $SE_n|x[θ]$ for the choices

$$\hat{θ} ∈ \{T_γ(F_2), T_{p/n}(F^0_{n,k}), T_{p/n}(F^w_{n,k}), T_{p/n}(F^i_{n,k})\},$$

in the single-spiked setup, as described in experiment R0-vs-R1 above. We let the spike intensity $x$ vary and plot $SE_n|x[θ]/SE_n|x|$ for each choice of estimator. We expect the choice of estimator to especially matter when $x$ is close to $x^* = Y^{-1}(T_γ(F_2))$ (indicated in the plots by a dashed vertical line), and this can indeed be seen in the plots. The ratios we report are averages across $T = 20$ experiments.

- **Convergence Rate**: We study the rate of convergence of $T_{p/n}(F^*_{n,k})$ towards $T_γ(F_2)$. To that end, we consider a rank $r = 10$ signal $x = (1, \ldots, 10)$, set $k = 20$ and plots the relative absolute error $|T_{p/n}(F^*_{n,k}) - T_γ(F_2)|/T_γ(F_2)$ as $p$ varies and $n = p / γ$. We plot the error in a logarithmic scale, to get a sense of its polynomial rate of decay in $p$. Note that by Proposition 1, we expect the slope in most cases to be, roughly, $≤ 1$. We find that almost always, $T_{p/n}(F^w_{n,k})$ (imputation) approximates $T_γ(F_2)$ much better than $T_{p/n}(F^e_{n,k})$ (winsorization) or $T_{p/n}(F^0_{n,k})$ (transport to zero). All points on the plots are generated by averaging the error of $T = 50$ experiments.
C.3 Distribution: Marcenko-Pastur, $\gamma = 1.0$

Figure 10: Experiment: Hist

Figure 11: Experiment: R0-vs-R1
Figure 12: Experiment: SE-vs-ASE

Figure 13: Experiment: OracleAttainment
Noise = Marcenko-Pastur, $\gamma = 1.0$

Figure 14: Experiment: Regret

Noise = Marcenko-Pastur, $\gamma = 1.0$

Figure 15: Experiment: Convergence Rate
C.4 Distribution: Chi10, $\gamma = 0.5$

Figure 16: Experiment: Hist

Figure 17: Experiment: R0-vs-R1
Figure 18: Experiment: **SE-vs-ASE**

Figure 19: Experiment: **OracleAttainment**
Figure 20: Experiment: Regret

Figure 21: Experiment: ConvergenceRate
C.5 Distribution: Chi10, $\gamma = 1.0$

Figure 22: Experiment: Hist

Figure 23: Experiment: R0-vs-R1
Noise = Chi10, \( \gamma = 1.0 \)

Figure 24: Experiment: **SE-vs-ASE**

Noise = Chi10, \( \gamma = 1.0 \)

Figure 25: Experiment: **OracleAttainment**
Figure 26: Experiment: Regret

Figure 27: Experiment: Convergence Rate
C.6  Distribution: Fisher3n, $\gamma = 0.5$

![Distribution: Fisher3n, $\gamma = 0.5$](image)

Figure 28: Experiment: Hist

![Figure 29: Experiment: R0-vs-R1](image)

Figure 29: Experiment: R0-vs-R1
Figure 30: Experiment: SE-vs-ASE

Figure 31: Experiment: OracleAttainment
Noise = Fisher3n, $\gamma = 0.5$

Figure 32: Experiment: Regret

Figure 33: Experiment: ConvergenceRate
C.7 Distribution: Fisher3n, $\gamma = 1.0$

Figure 34: Experiment: Hist

Figure 35: Experiment: R0-vs-R1
Figure 36: Experiment: **SE-vs-ASE**

Figure 37: Experiment: **OracleAttainment**
Figure 38: Experiment: Regret

Figure 39: Experiment: ConvergenceRate
C.8 Distribution: Mix2, $\gamma = 0.5$

Figure 40: Experiment: Hist

Figure 41: Experiment: R0-vs-R1
Noise = Mix2, $\gamma = 0.5$

Figure 42: Experiment: **SE-vs-ASE**

Figure 43: Experiment: **OracleAttainment**
Noise = Mix2, $\gamma = 0.5$

Figure 44: Experiment: Regret

Figure 45: Experiment: ConvergenceRate
C.9 Distribution: Mix2, $\gamma = 1.0$

![Histogram](image1.png)

Figure 46: Experiment: Hist

![Line graph](image2.png)

Figure 47: Experiment: R0-vs-R1
Figure 48: Experiment: **SE-vs-ASE**

Figure 49: Experiment: **OracleAttainment**
Noise = Mix2, $\gamma = 1.0$

![Graph showing Regret](image)

Figure 50: Experiment: **Regret**

Noise = Mix2, $\gamma = 1.0$

![Graph showing Convergence Rate](image)

Figure 51: Experiment: **Convergence Rate**
C.10 Distribution: Unif[1,10], $\gamma = 0.5$

Figure 52: Experiment: Hist

Figure 53: Experiment: R0-vs-R1
Figure 54: Experiment: **SE-vs-ASE**

Figure 55: Experiment: **OracleAttainment**
Noise = Unif[1,10], $\gamma = 0.5$

Figure 56: Experiment: Regret

Figure 57: Experiment: ConvergenceRate
C.11 Distribution: Unif[1,10], $\gamma = 1.0$

![Histogram](image1)

**Figure 58: Experiment: Hist**

![Graph](image2)

**Figure 59: Experiment: R0-vs-R1**
Figure 60: Experiment: **SE-vs-ASE**

Figure 61: Experiment: **OracleAttainment**
Figure 62: Experiment: Regret

Figure 63: Experiment: Convergence Rate
C.12 Distribution: PaddedIdentity, $\gamma = 0.5$

Figure 64: Experiment: Hist

Figure 65: Experiment: R0-vs-R1
Noise = PaddedIdentity, $\gamma = 0.5$

Figure 66: Experiment: **SE-vs-ASE**

Figure 67: Experiment: **OracleAttainment**
Figure 68: Experiment: **Regret**

Figure 69: Experiment: **ConvergenceRate**
C.13 Distribution: PaddedIdentity, $\gamma = 1.0$

Figure 70: Experiment: Hist

Figure 71: Experiment: R0-vs-R1
Noise = PaddedIdentity, $\gamma = 1.0$

Figure 72: Experiment: SE-vs-ASE

Noise = PaddedIdentity, $\gamma = 1.0$

Figure 73: Experiment: OracleAttainment
Noise = PaddedIdentity, $\gamma = 1.0$

Figure 74: Experiment: **Regret**

Figure 75: Experiment: **ConvergenceRate**