Selecting the number of components in PCA via random signflips

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Abstract

Principal component analysis (PCA) is a foundational tool in modern data analysis, and a crucial step in PCA is selecting the number of components to keep. However, classical selection methods (e.g., scree plots, parallel analysis, etc.) lack statistical guarantees in the increasingly common setting of large-dimensional data with heterogeneous noise, i.e., where each entry may have a different noise variance. Moreover, it turns out that these methods, which are highly effective for homogeneous noise, can fail dramatically for data with heterogeneous noise. This paper proposes a new method called signflip parallel analysis (FlipPA) for the setting of approximately symmetric noise: it compares the data singular values to those of “empirical null” matrices generated by flipping the sign of each entry randomly with probability one-half. We develop a rigorous theory for FlipPA, showing that it has nonasymptotic type I error control and that it consistently selects the correct rank for signals rising above the noise floor in the large-dimensional limit (even when the noise is heterogeneous). We also rigorously explain why classical permutation-based parallel analysis degrades under heterogeneous noise. Finally, we illustrate that FlipPA compares favorably to state-of-the art methods via numerical simulations and an illustration on data coming from astronomy.

Keywords: rank estimation, parallel analysis, large-dimensional data, heterogeneous noise, entrywise heteroscedasticity.

1 Introduction

Discovering latent low-dimensional structure in large and noisy datasets is one of the central challenges faced in modern data analysis. Indeed, examples arise across virtually all of science and engineering, and unsupervised dimensionality reduction is a standard element of statistical analysis. In particular, Factor Analysis (FA) and Principal Component Analysis (PCA) remain incredibly popular and successful techniques. They continue to be integral parts of myriad data analysis pipelines, being performed routinely in thousands of studies every year. Applications abound in psychology and education (Horn, 1965; Tran and Formann, 2009), public health (Patil et al., 2010), management and marketing (Stewart, 1981), economics and finance (Bai and Ng, 2002; Ahn and Horenstein, 2013), genomics (Lin et al., 2016; Yano et al., 2019), environmental sensing (Subbarao et al., 1996), and manufacturing (Apley and Shi, 2001), to name just a few. See, e.g., Anderson (2003); Jolliffe (2002); Yao et al. (2015), for further references.

Given measurements of \( p \) features (covariates) over a set of \( n \) observations (datapoints), FA and PCA identify components driving variation in the data. However, these components do not all capture meaningful variation, i.e., signal; many capture variation simply due to noise. Hence, an important question is: how many components capture signals rising above the noise? Informally stated, we have data that consists of a low-rank signal \( S \) plus noise \( N: X = S + N \in \mathbb{R}^{n \times p}, \) \( k := \text{rank} S \ll n. \) The problem is to estimate the

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rank \( k \) given only \( X \). This paper tackles this problem in the increasingly common setting where the noise can be heterogeneous. As we will show below, methods that do not appropriately account for heterogeneity can dramatically degrade, and theory developed for homogeneous cases does not directly apply.

1.1 Related work

Estimating the rank is well known to significantly impact downstream data analyses, with the standard textbook Brown (2014) calling it “the most crucial decision” in exploratory FA. Choosing too few factors deprives downstream steps of potentially crucial information, while choosing too many passes on unnecessary noise. Moreover, data in many important applications have weak “emergent” factors that are nontrivial to identify, making this a challenging problem. Such settings are common, e.g., in behavioral and biological sciences. As a result, a tremendous amount of work has gone into the development of effective methods for this problem; we give a brief overview of some related literature here.

Classical and standard methods include Cattell’s scree plot (Cattell, 1966; Cattell and Vogelmann, 1977), sphericity tests based on likelihood ratios (Bartlett, 1954; Lawley, 1956), the Kaiser-Guttman criterion for correlation matrices (Guttman, 1954; Kaiser, 1960), the minimum average partial test (Velicer, 1976), and approaches based on minimum description length (Wax and Kailath, 1985; Fishler et al., 2002). A popular choice is parallel analysis (Horn, 1965; Buja and Eyuboglu, 1992), which computes a parallel set of singular values (typically by computing singular values after applying random permutations to each column of the data matrix), and selects all the components whose singular values rise above some quantile of their parallel counterparts. Owen and Wang (2016) note that “there is a large amount of evidence that PA is one of the most accurate […] classical methods for determining the number of factors”. Indeed many works find parallel analysis (PA) to be highly effective; see, e.g., Dobriban (2020, Section 1.2) and references therein.

More recently, tremendous progress has been made in developing and analyzing methods for large-dimensional data by using modern insights from high-dimensional probability and random matrix theory. For example, several works have developed methods based on the asymptotic behavior of the eigenvalues of sample covariance matrices (including the behavior of the differences or the ratios of consecutive eigenvalues) under various assumptions (Kapetanios, 2004, 2010; Kritchman and Nadler, 2009; Onatski, 2010; Lam and Yao, 2012; Ahn and Horenstein, 2013; Passemier and Yao, 2014; Li et al., 2017). Others works have studied methods based on various information criterion (Bai and Ng, 2002; Nadakuditi and Edelman, 2008; Alessi et al., 2010), including very recent work by Bai et al. (2018) and Hu et al. (2020). Other recently proposed approaches include bi-cross-validation (Owen and Wang, 2016), double cross validation (Zeng et al., 2019), and a random matrix theoretic thresholding of eigenvalues from the sample correlation matrix (Fan et al., 2020). A few works focus specifically on rank estimation for heterogeneous noise (Ke et al., 2021; Landa et al., 2022), which we will discuss in greater detail below. Related to parallel analysis, Dobriban (2020) analyzed permutation-based parallel analysis for large-dimensional data, and Dobriban and Owen (2019) proposed a derandomized variant. Finally, we note that rank estimation for large-dimensional data under various assumptions remains an incredibly active research field; see, e.g., Cai et al. (2020); Xu et al. (2023) for some recent works that study other settings (e.g., diverging spikes, correlated data, etc.).

1.2 Heterogeneous noise and the need for new methods

In modern applications, data are now commonly not only large-dimensional but also heterogeneous. Heterogeneous noise in particular occurs often in modern settings, whether due to heteroscedasticity in the features or due to heterogeneous quality among the observations. For example, the noise level in medical imaging varies both within images and from image to image. Likewise, atmospheric corruptions in astronomical image data vary both from night to night and from pixel to pixel, and the quality of environmental sensors can vary from location to location. These types of effects all contribute to noise heterogeneity.

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1A key point is that weak signal components can get buried in the noise, and as a result the corresponding principal components of \( X \) completely fail to capture the signal (see, e.g., Baik et al., 2005; Johnstone and Paul, 2018). In this case, the goal is to estimate only the number of components that actually capture the signal and not the noise, i.e., the number of signal components rising above the noise.

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Figure 1: Illustrative example of permutation-based parallel analysis (PermPA) for a simple rank-one signal in homogeneous and heterogeneous noise. PermPA is incredibly effective for homogeneous noise, but can substantially over-estimate when the noise is heterogeneous.

However, much of the existing work to date has been for data with homogeneous noise, and methods made for homogeneous noise can dramatically degrade when the noise is heterogeneous. For example, as mentioned above, permutation-based parallel analysis (which we will refer to as “PermPA”) (Buja and Eyuboglu, 1992) is highly effective for homogeneous noise and even remains effective when the data is large-dimensional (Dobriban, 2020). It turns out, however, that PermPA can substantially over-estimate the rank when the noise is heterogeneous, as shown in the example of Fig. 1. The entries of the noise in Fig. 1b have heterogeneous variances: the data matrix is moderately noisy on the right side, least noisy in the upper left, and most noisy in the lower left. PermPA correctly selects one component in the homogeneous setting of Fig. 1a, but incorrectly selects eleven components in the heterogeneous setting of Fig. 1b. Similarly, we will show in experiments that other highly effective methods for homogeneous noise can substantially degrade for heterogeneous noise.

Consequently, recent works have begun to study how to properly account for noise heterogeneity when carrying out PCA for large data. Great progress has been made on improving the quality of the estimated components (see, e.g., Zhang et al., 2022; Leeb and Romanov, 2021; Leeb, 2021; Hong et al., 2016, 2018, 2023), but relatively fewer works have addressed how to estimate the number of components in these heterogeneous settings. For heterogeneity across features, Leeb and Romanov (2021) consider selecting the singular values rising above the asymptotic operator norm of the noise matrix, which can be predicted when the noise is whitened or when the noise variances are well-estimated. Ke et al. (2021) consider noise variances drawn from a Gamma distribution, and propose setting a threshold based on fitting the associated Marčenko-Pastur distribution to the bulk singular values. Landa et al. (2022) propose rescaling the rows and columns of the data matrix to biwhiten the data, then selecting the singular values rising above the same cut-off as applies for large-dimensional homogeneous noise. They show that the biwhitening procedure makes the formerly heterogeneous noise behave like homogeneous noise, making this a good choice of cut-off.

Overall, the analysis of large-dimensional data with heterogeneous noise is an actively developing area. In this paper, we develop an elegant and flexible method in the style of parallel analysis that is not only effective for homogeneous noise but also remains effective for heterogeneous noise. The method is intuitive and simple to implement, and we provide theoretical guarantees (including not only asymptotic consistency, but also nonasymptotic type I error control in selecting incorrect components) leveraging modern insights.

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2 The over-estimation in Fig. 1b is not unique to this particular example and is a general result (which we rigorously characterize in Section 3.2) that occurs when the noise is heterogeneous.
Algorithm 1: Signflip parallel analysis (FlipPA)

**Input**: Data $X \in \mathbb{R}^{n \times p}$, quantile $q \in [0, 1]$, number of trials $T$, threshold $\tau \geq 0$.

**Output**: Selected number of factors $\hat{k}$.

1. **for** $t = 1$ **to** $T$ **do**
2. Randomly signflip the entries of $X$:
   $$X_{i,j}^{(t)} \overset{\text{ind}}{\sim} \begin{cases} +X_{i,j}, & \text{with probability 1/2,} \\ -X_{i,j}, & \text{with probability 1/2,} \end{cases}$$
   i.e., $X^{(t)} \leftarrow R^{(t)} \circ X$ where $R^{(t)} \in \{-1, 1\}^{n \times p}$ has i.i.d. Rademacher entries;
3. $\tilde{\sigma}^{(t)} \leftarrow$ singular values of $X^{(t)}$;
4. **end**
5. $\sigma \leftarrow$ singular values of $X$;
6. $\hat{k} \leftarrow$ first $k$ for which
   $$\begin{align*}
   &\sigma_{k+1} \leq q\text{-quantile of } \left(\tilde{\sigma}_{k+1}^{(1)}, \ldots, \tilde{\sigma}_{k+1}^{(T)}\right) + \tau, &\text{if using pairwise comparison,} \\
   &\sigma_{k+1} \leq q\text{-quantile of } \left(\tilde{\sigma}_{1}^{(1)}, \ldots, \tilde{\sigma}_{1}^{(T)}\right) + \tau, &\text{if using upper-edge comparison.}
   \end{align*}$$

from random matrix theory and randomization-based testing. In contrast to other approaches, the proposed signflip parallel analysis (FlipPA) method allows for entry-wise noise heterogeneity, does not need exact or distributional knowledge of the variances, does not modify the data, and provides nonasymptotic type I error control. We show in a broad range of experiments that our method compares favorably to prior approaches (Buja and Eyuboglu, 1992; Bai et al., 2018; Hu et al., 2020; Fan et al., 2020; Ke et al., 2021; Landa et al., 2022).

1.3 Organization

The remainder of the paper is organized as follows. Section 2 describes the proposed signflip parallel analysis (FlipPA) method. Section 3 rigorously analyzes FlipPA, discussing nonasymptotic type I error control and establishing asymptotic consistency (Section 3.1); Section 3.2 rigorously explains why PermPA degrades under heterogeneous noise. Section 4 demonstrates the performance of FlipPA through numerical simulations and compares with several state-of-the-art methods. Section 5 demonstrates FlipPA on an empirical dataset coming from astronomy. Finally, Section 6 concludes with a discussion of future directions.

2 Proposed method: Signflip parallel analysis (FlipPA)

We propose a new method for rank estimation called signflip parallel analysis (FlipPA). FlipPA is a method in the style of parallel analysis (Horn, 1965; Buja and Eyuboglu, 1992) that largely retains the excellent battle-tested performance of parallel analysis under homogeneous noise, while expanding these benefits to data with heterogeneous noise. The idea is to generate parallel matrices that look like pure noise, then select the components whose singular values rise above data-driven cut-offs determined by their parallel counterparts. FlipPA generates parallel matrices from the data matrix by randomly flipping the signs of its entries, i.e., each entry is signflipped independently with probability 1/2. Each parallel matrix is formed using a new independent set of random signflips. A feature of this approach is that it provides non-asymptotic type I error control at a user-specified level (see Section 3).
Algorithm 1 provides a detailed description of FlipPA, and Fig. 2 illustrates the process using the heterogeneous data from Fig. 1b. The first step (Lines 1 to 4) is to compute $T \geq 1$ sets of parallel singular values $	ilde{\sigma}(1), \ldots, \tilde{\sigma}(T)$ from the signflipped data matrices $\tilde{X}(1), \ldots, \tilde{X}(T)$ in (1).\(^3\) Fig. 2 illustrates the signflipped data matrix from one of the trials. The next and final step (Lines 5 and 6) is to compute the singular values of the data $X$ and compare them against a chosen quantile $q$ (e.g., 50%, 95%, or 99%) computed with their parallel counterparts. There are two choices for the comparison method:\(^4\)

- pairwise comparison (2a) selects all the leading components for which the data singular value $\sigma_k$ rises $\tau$-above the $q$-quantile of its parallel counterparts $\tilde{\sigma}_k^{(1)}, \ldots, \tilde{\sigma}_k^{(T)}$.
- upper-edge comparison (2b) selects all the leading components for which the data singular value $\sigma_k$ rises $\tau$-above the $q$-quantile of the parallel upper-edges $\tilde{\sigma}_1^{(1)}, \ldots, \tilde{\sigma}_1^{(T)}$.

The scatter plot in Fig. 2 shows the singular values $\sigma_k$ of the original data $X$, overlaid with each empirical distribution for the parallel singular values $\tilde{\sigma}_k^{(1)}, \ldots, \tilde{\sigma}_k^{(T)}$ and the resulting $q$-quantiles. Both comparison methods correctly select one component with $\tau = 0$ here.

While pairwise comparison is the classical selection method (Horn, 1965; Buja and Eyuboglu, 1992), upper-edge comparison can have some benefits. For example, upper-edge comparison never selects more factors than pairwise comparison, making it more conservative and less likely to over-estimate the rank. Moreover, upper-edge comparison can be computationally cheaper, since it only requires computing and storing the first singular value $\tilde{\sigma}_1^{(t)}$ of the signflipped data (i.e., the operator norm $\|\tilde{X}^{(t)}\|$) in each trial. At the same time, upper-edge comparison is also more likely to under-estimate the rank, which can be an issue if strong signals are shadowing weak signals in the data. The two comparison methods also agree in many cases, especially when the data dimensions are large. When they disagree, which comparison method to choose will depend on the application and the salient priorities. We suggest using upper-edge comparison as a default if over-selection of the number of components or a large computational cost are important issues.

As a parallel analysis method, FlipPA has the same structure as the permutation-based parallel analysis (PermPA) of Buja and Eyuboglu (1992). The crucial difference is that PermPA creates parallel matrices by randomly permuting the entries of each column of the data matrix while FlipPA uses random entrywise signflips. Thus, FlipPA immediately shares many of the practical benefits of PermPA, being intuitive and

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\(^3\)Note that only the singular values $\tilde{\sigma}(1), \ldots, \tilde{\sigma}(T)$ need to be saved; the memory for storing $\tilde{X}(t)$ can be reused across trials.

\(^4\)Note that both comparison methods are sequential: the selection ends once a data singular value $\sigma_k$ falls below its appropriate parallel cut-off, even if singular values later on rise above again.
simple to implement. Moreover, it is a flexible method. As we will demonstrate in Section 4.3, it can be straightforwardly modified, e.g., to handle noise whose entries have blockwise dependence.

The remaining sections investigate the performance of FlipPA theoretically (Section 3), via simulations (Section 4), and via an illustration on data from astronomy (Section 5).

3 Theoretical Properties

This section studies the theoretical properties of the proposed FlipPA method. Throughout this section, we consider data of the following signal-plus-noise form:

\[ X = \sum_{i=1}^{k} \theta_i u_i z_i^\top + N \in \mathbb{R}^{n \times p}. \]  

(3)

The signal \( S \) is of rank at most \( k \), and \( \theta_i \geq 0, u_i \in \mathbb{R}^n, \) and \( z_i \in \mathbb{R}^p, \) for \( i \in \{1, \ldots, k\} \) may be deterministic or random and are not necessarily orthogonal, as discussed below. Furthermore, the signal component coefficients \( \theta_i \) and the number of terms \( k \) may both change with \( n \) and \( p \). The noise matrix \( N \) has independent entries with symmetric distributions, i.e., \( N_{ij} = -N_{ij} \) for all \( i, j \). A slightly subtle point is that the precise output of FlipPA can depend on how one computes sample quantiles; all the results in this section hold for sample quantiles computed using any of the nine commonly used definitions enumerated in Hyndman and Fan (1996).

Consider first the nonasymptotic type I error rate of FlipPA under the null hypothesis of \( H_0 : k = 0 \). There is no signal here, and the type I error rate of FlipPA is \( \Pr_{H_0} [\hat{k} > 0] \), where \( \hat{k} \) is the output of FlipPA. Combining some general arguments for randomization tests (Hemerik and Goeman, 2017) with some careful but straightforward additional analysis (to connect sample quantiles to order statistics) yields the following fact:

**Type I error control:** The type I error rate of FlipPA, for both upper-edge and pairwise comparison methods, is bounded above as \( \Pr_{H_0} [\hat{k} > 0] \leq 1 - \frac{qT}{T+1} \).

For completeness, we provide a proof in Appendix A. Note that the type I error bound holds for any chosen threshold \( \tau \geq 0 \) and takes values in increments of \( 1/(T+1) \), starting at \( 1/(T+1) \) and going up. These bounds provide a simple way to control the type I error of FlipPA. Namely, to obtain a type I error rate below level \( \alpha \), simply choose the number of trials \( T \) and the quantile \( q \) so that \( 1 - \frac{|qT|}{T+1} \leq \alpha \), e.g., one can choose \( q = 1 \) and \( T = \lceil 1/\alpha \rceil - 1 \), yielding a type I error rate bounded as \( \Pr_{H_0} [\hat{k} > 0] \leq 1/\lceil 1/\alpha \rceil \leq \alpha \). One may choose a larger \( T \) to reduce the variability in FlipPA due to the random signflips, and a correspondingly smaller \( q \) to control type I error at level \( \alpha \).

The following subsections present our main theoretical results. Section 3.1 considers the alternative hypothesis (i.e., nonzero components) and proves asymptotic consistency under suitable conditions. Section 3.2 provides a rigorous explanation of why permutation-based parallel analysis degrades under heterogeneous noise.

3.1 Consistency of FlipPA

Here, we consider the asymptotic consistency of FlipPA in the large-dimensional limit where \( n, p \to \infty \) with \( p/n \to \gamma > 0 \). This asymptotic regime captures many modern datasets, for which the number of features is comparable to the number of observations. For practical purposes, this asymptotic consistency means that FlipPA provides accurate rank estimates with high probability when there are sufficiently many features and many observations.

The key insight is the observation that the signflipping operation in FlipPA scrambles the signal in the data while preserving heterogeneous noise, producing matrices that look like the noise, as illustrated in

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5 A Julia package implementing the method is available at: https://github.com/dahong67/FlipPA.jl
Figure 3: Example illustrating how FlipPA scrambles the signal while preserving heterogeneous noise, resulting in singular values similar to those of the noise.

Fig. 3. Specifically, the signflipped signal has a much reduced operator norm, while the signflipped noise is similar to the original noise. As a result, the singular values of the signflipped data are very similar to those of the original noise (which we do not observe directly) and hence lead to a good choice for cut-off in estimating the rank.⁶ The remainder of this section develops this intuition into a rigorous theory. To simplify the presentation, here we will focus on FlipPA with the upper-edge comparison method. Similar statements can be shown for the pairwise comparison method under similar conditions.

To carry out the rigorous analysis, we consider the following two conditions.

**Condition 3.1** (Well-defined asymptotic noise upper-edge). The noise has a well-defined asymptotic upper-edge \( \bar{\sigma} \), i.e., \( \| N \|_{\text{i.p.}} \to \bar{\sigma} \).

This first condition simply ensures a well-defined asymptotic noise limit. Essentially it means that the variability of the noise operator norm is small relative to its value, since one can always re-scale the data by the order of the noise operator norm without loss of generality. This condition is satisfied in many natural models studied in random matrix theory (see, e.g., Benaych-Georges and Nadakuditi, 2012), including ones with heterogeneous noise (see, e.g., Husson (2022); Ajanki et al. (2016, 2019)).

**Condition 3.2** (Asymptotically perceptible signal). The signal is asymptotically perceptible, i.e., there exists some \( \varepsilon > 0 \) such that \( \Pr[\sigma_k(X) > \| N \| + \varepsilon] \to 1 \).

This second condition ensures that the signal rises above the noise and is perceptible as a result. As is well known (see, e.g., Baik et al., 2005; Johnstone and Paul, 2018), signals that are too weak can get buried in the noise for large-dimensional data, and the corresponding components can consequently completely fail to recover them. Our goal is to identify only the components above the noise level.

⁶Similar observations were also used to derive properties of PermPA in Dobriban (2020) and to derive general properties of randomization-based tests in Dobriban (2022). However, the results from those works cannot be used to derive the results presented here.


We are now ready to state the main consistency results; see Appendix B for their proofs.

**Theorem 3.3** (Asymptotic consistency of FlipPA). Suppose the signal-plus-noise model (3) satisfies Conditions 3.1 and 3.2. Then FlipPA using the upper-edge comparison method with threshold \( \tau \in (0, \varepsilon) \) is consistent, i.e., \( \Pr[\hat{k} = k] \to 1 \), as long as the signal components are delocalized as follows:

\[
E \left\{ \sum_{i=1}^{k} \theta_i \| u_i \|_2 z_i \cdot \left( \frac{\| u_i \|_\infty / \| u_i \|_2 + \| z_i \|_\infty / \| z_i \|_2}{2} \right) \right\} \to 0. \tag{4}
\]

Theorem 3.3 follows from the more general Theorem 3.5 below, and its proof is provided in Appendix B.2. We are now ready to state the main consistency results; see Appendix B for their proofs.

**Corollary 3.4** (Asymptotic consistency of FlipPA in terms of growth rates). Suppose the signal-plus-noise model (3) satisfies Conditions 3.1 and 3.2, where

1. the signal rank \( k \) and component coefficients \( \theta_1, \ldots, \theta_k \) are deterministic and grow at the following rates:
   \[ k = O(p^{\alpha_1} \log^{\alpha_2} p) \quad \text{and} \quad \max_{i=1, \ldots, k} \theta_i = O(p^{\beta_1} \log^{\beta_2} p) \]
   for some \( \nu_1, \nu_2, \beta_1, \beta_2 \geq 0 \),

2. the component vectors \( u_1, \ldots, u_k \) and \( z_1, \ldots, z_k \) are all jointly independent, are normalized such that
   \[ E \| u_i \|_2 = E \| z_i \|_2 = 1 \]
   for \( i \in \{1, \ldots, k\} \), and delocalize at the following rates:
   \[ \max_{i=1, \ldots, k} E \| u_i \|_\infty = O(p^{-\alpha_1} \log^{-\alpha_2} p) \]
   and
   \[ \max_{i=1, \ldots, k} E \| z_i \|_\infty = O(p^{-\alpha_1} \log^{-\alpha_2} p) \]
   for some \( \alpha_1, \alpha_2 \in \mathbb{R} \).

Then FlipPA using the upper-edge comparison method with threshold \( \tau \in (0, \varepsilon) \) is consistent, i.e., \( \Pr[\hat{k} = k] \to 1 \), as long as: a) \( \alpha_1 > \nu_1 + \beta_1 \), or b) \( \alpha_1 = \nu_1 + \beta_1 \) and \( \alpha_2 > \nu_2 + \beta_2 \).

Corollary 3.4 covers many important settings. For example, in the commonly studied settings where the component vectors \( u_i \) and \( z_i \) either: a) have i.i.d. sub-Gaussian entries, or b) are uniformly distributed on the unit spheres in \( \mathbb{R}^n \) and \( \mathbb{R}^p \), respectively, it follows that \( \max_{i=1, \ldots, k} E \| u_i \|_\infty = O(p^{-1/2} \log^{1/2} p) \) and

\[ \max_{i=1, \ldots, k} E \| z_i \|_\infty = O(p^{-1/2} \log^{1/2} p). \]

Hence, in these settings, \( \alpha_1 = 1/2 \) and \( \alpha_2 = -1/2 \), and FlipPA remains consistent even if the signal rank and component coefficients both grow, as long as their combined rate is small enough, i.e., \( k \cdot \max_{i=1, \ldots, k} \theta_i = O(p^{\delta_1} \log^{\delta_2} p) \) with \( \zeta_1 < 1/2 \) or \( \zeta_1 = 1/2 \) with \( \zeta_2 < -1/2 \). For instance, this allows \( k = p^{1/4} \) and \( \max_{i=1, \ldots, k} \theta_i = p^{1/4-\delta} \) for any fixed \( \delta > 0 \). Moreover, it is common in many applications for the rank to be fixed or bounded, i.e., \( \nu_1 = \nu_2 = 0 \), in which case the condition simply reduces to \( \max_{i=1, \ldots, k} \theta_i = O(p^{\beta_1} \log^{\beta_2} p) \) with \( \beta_1 < 1/2 \) or \( \beta_1 = 1/2 \) with \( \beta_2 < -1/2 \). Overall, FlipPA remains consistent even if the signal rank and component coefficients grow, as long as the component vectors delocalize sufficiently quickly to compensate.

We conclude this section with a discussion of the more general sufficient conditions for FlipPA consistency, of which Theorem 3.3 (and consequently Corollary 3.4) are actually special cases. The following theorem shows that FlipPA remains consistent under an even weaker form of signal delocalization than that of (4).

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7 To simplify the presentation, here we suppose the rank \( k \) and the signal component coefficients \( \theta_1, \ldots, \theta_k \) are deterministic, and that the component vectors \( u_1, \ldots, u_k \) and \( z_1, \ldots, z_k \) are all jointly independent.

8 This can be verified using, e.g., Vershynin (2018, Exercise 2.5.10 and Theorem 3.4.6).
This weaker form of delocalization is stated in terms of properties of the signal matrix $S$ directly, rather than the component coefficients $\theta_i$ and vectors $u_i$ and $z_i$. In particular, we define the delocalization coefficients

$$\rho_2(S) := \| S^\top S \|_{2,\infty} \quad \sqrt{\log(n + p)},$$

$$\rho_\infty(S) := \max_{i = 1, \ldots, n + p} \| S^\top S \|_{\infty,(i)} \quad \sqrt{\log t},$$

(5)

where $\| \cdot \|_{2,\infty}$ denotes the maximum row $\ell_2$ norm, and $\| \cdot \|_{\infty,(i)}$ denotes the $i$-th largest row $\ell_\infty$ norm, i.e., for any matrix $A \in \mathbb{R}^{m \times t}$, $\| A \|_{\infty,(1)} \geq \cdots \geq \| A \|_{\infty,(m)}$ sorts the row $\ell_\infty$ norms $\| A_1 : \|, \ldots, \| A_m : \|$ in descending order. We are now ready to state the theorem.

**Theorem 3.5** (Asymptotic consistency of FlipPA: general condition). Suppose the signal-plus-noise model (3) satisfies Conditions 3.1 and 3.2. Then FlipPA using the upper-edge comparison method with threshold $\tau \in (0, \varepsilon)$ is consistent, i.e., $\Pr[\hat{k} = k] \to 1$, as long as $\mathbb{E}\|S\|_{2,\infty} \to 0$, $\mathbb{E}\|S^\top\|_{2,\infty} \to 0$, and $\min\{\mathbb{E}\rho_2(S), \mathbb{E}\rho_\infty(S)\} \to 0$.

The proof involves showing that the noise is preserved (so that the signflipped noise looks like the true noise), while the signal is destroyed by signflipping (so that the signflipped data looks like the signflipped noise). See Appendix B.4. We leverage recent advances in a line of work in random matrix theory on nonhomogeneous random matrices (Segnier, 2000; Latala, 2005; Schuett and Riemer, 2013; Bandeira and Van Handel, 2016; Van Handel, 2017; Latala et al., 2018). The delocalization conditions $\mathbb{E}\|S\|_{2,\infty} \to 0$ and $\mathbb{E}\|S^\top\|_{2,\infty} \to 0$ ensure that the signal is not localized on any particular row or column. The condition $\min\{\mathbb{E}\rho_2(S), \mathbb{E}\rho_\infty(S)\} \to 0$ ensures that the decay of row and column norms is sufficiently fast with respect to either of the delocalization coefficients $\rho_2$ or $\rho_\infty$ in (5). The coefficient $\rho_2$ captures a dimension-dependent form of decay: $\mathbb{E}\rho_2(S) \to 0$ is equivalent to saying that both $\mathbb{E}\|S\|_{2,\infty}$ and $\mathbb{E}\|S^\top\|_{2,\infty}$ decay at a rate of $o(\log^{-1/4}(n + p))$. The coefficient $\rho_\infty$ captures a dimension-free form of decay, and is satisfied in many natural circumstances, as described by the following theorem (see Appendix B.5 for its proof).

**Theorem 3.6** (Sufficient conditions for $\rho_\infty$ decay). We have $\mathbb{E}\rho_\infty(S) \to 0$, under either of the following conditions: (1) there is $t \geq 2$ such that $\mathbb{E}\|S\|_{t,t} \to 0$; (2) the rank grows slowly enough that $\mathbb{E}\left\{\text{rank}^{1/2}(S) \sqrt{\|S\|_{2,\infty} \cdot \|S^\top\|_{2,\infty}}\right\} \to 0$.

The mixed norm $\| \cdot \|_{t,t}$ denotes the $\ell_t$ norm of the vector made of the row $\ell_t$ norms, i.e., $\|S\|_{t,t} = \|\|S_1\|_{1}, \ldots, \|S_n\|_{1}\|_{t}$, which is equivalent to the $\ell_1$ norm of the vectorized matrix. The row-wise and column-wise delocalization conditions $\mathbb{E}\|S\|_{2,\infty} \to 0$ and $\mathbb{E}\|S^\top\|_{2,\infty} \to 0$ imply the second sufficient condition in Theorem 3.6 when the rank of $S$ is bounded, and hence are already sufficient in that case. Overall, Theorems 3.5 and 3.6 show that FlipPA is consistent as long as the signal is sufficiently delocalized in an even weaker sense than in Theorem 3.3 and Corollary 3.4.

### 3.2 Degradation of PermPA under heterogeneous noise

This section gives a rigorous explanation of why PermPA degrades under heterogeneous noise. The key insight is that randomly permuting the entries of each column, as is done by PermPA, has the effect of homogenizing the noise variance in each column. More precisely, let $\pi_1, \ldots, \pi_p \in \{0, 1\}^{n \times n}$ be the $p$ PermPA permutation matrices (drawn i.i.d. uniformly at random) for a single trial, and let $N_{\pi} := [\pi_1 N_1; \cdots; \pi_p N_p] \in \mathbb{R}^{n \times p}$ be the resulting parallel noise matrix generated by PermPA. Then it immediately follows that for all $i, j$,

$$\mathbb{E}\{(N_{\pi})_{ij}\}^2 = \mathbb{E}\{(\pi_j N_j)_{ij}\}^2 = \mathbb{E}\{(\pi_j)_{ij} N_j\}^2 = \mathbb{E}\left[N_j^\top (\pi_j)_{ij}^\top (\pi_j)_{ij} N_j\right]$$

$$= \mathbb{E}\left[N_j^\top (\pi_j)_{ij}^\top (\pi_j)_{ij} N_j\right] = \mathbb{E}\left[N_j^\top \left(\frac{1}{n} I_n\right) N_j\right] = \frac{1}{n} \sum_{m=1}^{n} \mathbb{E}|N_{mj}|^2.$$

Namely, the variances of all entries within a given column of $N_{\pi}$ equal the average of the variances in that column of $N$. PermPA homogenizes the noise variances, and hence one might expect the parallel singular
values to look more like those of a noise matrix with the homogenized variances (6) rather than those of the actual noise $N$.

Indeed, this distortion of the noise singular values is exactly what can happen, as shown in Fig. 4. The empirical singular value distribution of the permuted noise is very different from that of the original noise and instead closely matches that of a noise matrix with independent Gaussian entries generated using the homogenized variance profile (6). The consequence of such a distortion is that PermPA incorrectly estimates the noise floor, which can then lead to incorrect rank estimates. For example, in Fig. 4, running PermPA directly on the original noise (which has zero signal components) would incorrectly select many components since the permuted noise has substantially smaller leading singular values than the original noise.

The following theorem makes this intuition rigorous; see Appendix C for the proof.

**Theorem 3.7** (PermPA homogenizes heterogeneous noise). Let $N \in \mathbb{R}^{n \times p}$ have independent entries with zero mean and uniformly bounded fourth moments, let $N_\pi$ be the corresponding permuted noise, and let $\bar{N}$ be the homogenized noise matrix defined as $\bar{N}_{ij} \overset{\text{iid}}{\sim} N(0, v_j)$, where $v_j := (1/n) \sum_{m=1}^n E|N_{mj}|^2$. Then as $n, p \to \infty$ with $p/n \to \gamma > 0$, the empirical singular value distribution of $N_\pi / \sqrt{n}$ converges to the same almost sure weak limit as $\bar{N} / \sqrt{n}$, as long as the empirical distribution of the column-wise variances $v_1, \ldots, v_p$ converges to some deterministic distribution $H$. In particular, their empirical singular value distributions both converge to the generalized Marchenko-Pastur distribution defined by $H$.

Note that proving Theorem 3.7 is more nontrivial than may initially appear. Even though $N_\pi$ has the same variance profile as $\bar{N}$, the entries of $N_\pi$ are *not independent*; one must show that the dependence induced by the permutations has no impact in the limit. This requires showing a generalized Marchenko-Pastur law under relaxed independence conditions, related to, but different from those of Hui and Pan (2010); Wei et al. (2016); Bryson et al. (2021), and then showing that the permuted matrix satisfies these conditions by controlling the variance of certain quadratic forms.

### 4 Simulation Studies

This section demonstrates the empirical performance of FlipPA through numerical simulations. We compare with the following state-of-the-art methods for high-dimensional data:

- **PermPA** (Buja and Eyuboglu, 1992): traditional permutation-based parallel analysis, which is highly effective for homoscedastic noise but not for heteroscedastic noise. We use $T = 100$ trials, a quantile of

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9Codes for reproducing the figures in this section are available online at: [https://gitlab.com/dahong/rank-selection-via-random-signflips](https://gitlab.com/dahong/rank-selection-via-random-signflips)
\( q = 1.0, \) and a threshold of \( \tau = 0 \) with the upper-edge comparison; this choice of comparison and quantile discourages overestimation.

- **BCF and GIC (Bai et al., 2018; Hu et al., 2020):** the Bai-Choi-Fujikoshi (BCF) method studied in Bai et al. (2018) and the generalized information criterion (GIC) proposed by Hu et al. (2020) are penalization-based model selection approaches; they each select the rank that minimizes an associated selection criterion. For BCF, we use the presentation from Equations (4.5)–(4.6) of Hu et al. (2020). For GIC, we use Equation (4.9) of Hu et al. (2020) with \( \gamma \) chosen as suggested in Remark 6 of Hu et al. (2020).

- **ACT (Fan et al., 2020):** the adjusted correlation thresholding (ACT) method uses the eigenvalues of the correlation matrix instead of the covariance matrix to address observed variables with heterogeneous scales. The method has a maximum rank parameter, which we set to 100. We use the implementation provided online in their supplementary materials: https://www.tandfonline.com/doi/suppl/10.1080/01621459.2020.1825448.

- **BEMA0 and BEMA (Ke et al., 2021):** two methods based on bulk eigenvalue matching analysis (BEMA). BEMA0 is designed for homoscedastic noise; it estimates the noise variance by fitting the sample covariance matrix eigenvalues to a standard scaled Marcenko-Pastur distribution, then uses the estimated noise variance to determine an appropriate cut-off from the Tracy-Widom distribution. BEMA is a generalization designed to allow for heteroscedasticity in the noise across features; instead of estimating a single noise variance for the data, it assumes that the feature-wise noise variances are drawn from a Gamma distribution and estimates the parameters of this Gamma distribution from the data to determine an appropriate cut-off. We use the R implementations (with the default values) provided online by the authors: https://github.com/ZhengTracyKe/BEMA.

- **Biwhitening (Landa et al., 2022, Section 4):** a method that addresses heteroscedasticity by rescaling the rows and columns of the data matrix to whiten the data along both axes; the necessary rescaling is determined via the Sinkhorn-Knopp algorithm. The rank is estimated by counting how many singular values the biwhitened matrix has that exceed the homoscedastic cut-off of \( \sqrt{n} + \sqrt{p} \). For Sinkhorn-Knopp, which is an iterative algorithm, we used 1000 iterations.

For FlipPA, we use the same parameters as PermPA, i.e., we use \( T = 100 \) trials, a quantile of \( q = 1.0 \), and a threshold of \( \tau = 0 \). For simplicity, we focus on the upper-edge comparison method; the results for the pairwise comparison method are similar. Overall, we find that FlipPA compares favorably to the existing methods.

### 4.1 Homogeneous noise variances

This section considers an \( n \times p \) data matrix \( X \) with a rank-1 signal generated as \( X = \theta uz^\top + N \), where \( N_{ij} \overset{iid}{\sim} N(0, v/n) \), \( u \in \mathbb{R}^n \) and \( z \in \mathbb{R}^p \) are drawn uniformly from the respective unit spheres, \( \theta \) is swept from zero to two, and we take \( v = 1 \) without loss of generality. As \( \theta \) increases, the signal transitions from being buried in the noise to rising above it. The noise is homogeneous, so we expect the existing methods to also work well.

Fig. 5 shows the resulting performance of each method across 100 runs, where \( n = 500 \) and \( p = 300 \). The left plot shows the average selected rank \( \mathbb{E}[\hat{k}] \) across the runs; the second column of plots shows the proportion \( \Pr[\hat{k} > 1] \) of runs resulting in over-estimation, correct estimation (i.e., \( \Pr[\hat{k} = 1] \)), and under-estimation (i.e., \( \Pr[\hat{k} < 1] \)).

As expected, all the methods were highly effective once \( \theta \) was large enough, i.e., once the signal rose above the noise, and they estimated the rank correctly in most of the runs. Interestingly, ACT also correctly estimated a rank of one for small \( \theta \); using the eigenvalues of the correlation matrix may have helped here. However, ACT also incorrectly estimated a rank of one for \( \theta = 0 \), where the data is pure noise and the correct rank is zero.
The behavior at $\theta = 0$ illustrates the type I error properties of the methods since the data is pure noise in that case. PermPA rejected the pure noise null hypothesis in 2 of the 100 trials (achieving an empirical type I error rate of 2%); BEMA0 and Biwhitening rejected the null in 8 of the 100 trials (achieving empirical type I error rates of 8%); and ACT rejected the null in all of the 100 trials (achieving an empirical type I error rate of 100%). The other methods (BCF, GIC, BEMA, and FlipPA) never rejected the null, but FlipPA seemed to have the most power among them; for $\theta > 0$, FlipPA correctly rejected the null (and selected one component) more often than BCF, GIC, and BEMA.

We also considered a higher dimensional setting ($n = 60, p = 5000$) in Appendix D; Fig. 11 provides the analogue to Fig. 5. With the exceptions of BCF, GIC, and ACT (all of which dramatically over-estimated the rank), the remaining methods performed similarly: PermPA, BEMA0, Biwhitening, and FlipPA were all highly effective once $\theta$ was large enough. The empirical type I error rates (seen at $\theta = 0$) for this setting were better for BEMA0 (4%) and Biwhitening (3%), and were fairly similar for PermPA (1%) and FlipPA (1%). They were dramatically worse for BCF (100%) and GIC (100%), matching ACT (100%) here. Only PermPA and FlipPA seem to have controlled the type I error for both data sizes here, highlighting the rigorously guaranteed nonasymptotic type I error control of these randomization-based methods. This benefit makes them especially appealing in practice.

4.2 Block-structured noise variance profiles

To study how the various methods perform for heterogeneous noise, this section considers the same experiment as Section 4.1, but now the noise matrix is generated with a block-structured noise variance profile as follows:

$$N_{ij} \sim \mathcal{N}(0, V_{ij}/n) \quad \text{where} \quad V = \begin{pmatrix} (1 - \Delta) \cdot 1_{n_1 \times p_1} & 1 \cdot 1_{n_1 \times p_2} \\ (1 + \Delta) \cdot 1_{n_2 \times p_1} & 1 \cdot 1_{n_2 \times p_2} \end{pmatrix},$$

and $\Delta$ is swept from zero to one. As $\Delta$ increases from zero to one, the noise transitions from being homoscedastic (when $\Delta = 0$) to being increasingly heteroscedastic (as $\Delta$ grows).

Fig. 6 shows the resulting performance of each method across 100 runs, where $\theta = 1.5$, $n = 500$, $p = 300$, $n_1 = n_2 = 250$, $p_1 = 240$, and $p_2 = 60$. As before, the left plot shows the average selected rank $E[\hat{k}]$ across the runs; the second column of plots shows the proportion $\Pr[\hat{k} > 1]$ of runs resulting in over-estimation, correct estimation (i.e., $\Pr[\hat{k} = 1]$), and under-estimation (i.e., $\Pr[\hat{k} < 1]$).

All methods were highly effective for small $\Delta$: they all properly accounted for the high-dimensionality of the data in this homoscedastic regime. However, only FlipPA and Biwhitening correctly estimated the rank across the entire sweep, with only a few runs where they either over-estimated or under-estimated. BEMA correctly estimated the rank until $\Delta \approx 0.5$; for $\Delta > 0.5$ it began to under-estimate the rank. The block-structured variance profile is outside of the assumptions under which BEMA was designed, since the
noise variances are not uniform across the observations. The remaining methods significantly over-estimated the rank as \( \Delta \) grew, because they do not properly account for the heteroscedasticity.

We also considered a higher dimensional setting \((n = 60, p = 5000)\) in Appendix D; Fig. 12 provides the analogue to Fig. 6. With the exceptions of BCF, GIC, and ACT (all of which dramatically over-estimated the rank), the remaining methods again performed similarly: PermPA, BEMA0, Biwhitening, and FlipPA were all effective when \( \Delta \) was small, but only FlipPA and Biwhitening remained effective in the heteroscedastic case of larger \( \Delta \).

### 4.3 Noise with dependent entries

To illustrate the flexibility of FlipPA, here we consider the experiment from Section 4.2 but add blockwise dependence among the noise entries. Namely, suppose the data matrix \( X \) has a rank-one signal as in Section 4.1 but now the noise matrix \( N \) is generated with blockwise dependence on top of the block-structured noise variance profile of (7). Specifically, \( N = \Sigma_1^{1/2} \tilde{N} \Sigma_2^{1/2} \), where \( \tilde{N} \) has a block-structured variance profile similar to (7):

\[
\tilde{N}_{ij} \overset{iid}{\sim} N(0, V_{ij} / n) \quad \text{with} \quad V = \begin{bmatrix} 0.25 \cdot 1_{n_1 \times p_1} & 1 \cdot 1_{n_1 \times p_2} \\ 1.75 \cdot 1_{n_2 \times p_1} & 1 \cdot 1_{n_2 \times p_2} \end{bmatrix}.
\]

Further, \( \Sigma_1 \) and \( \Sigma_2 \) induce blockwise dependence across both observations and features as

\[
\Sigma_1 = I_{n/b_1} \otimes (\gamma \cdot 1_{b_1 \times b_1} + (1 - \gamma) \cdot 1_{b_1}), \quad \Sigma_2 = I_{p/b_2} \otimes (\gamma \cdot 1_{b_2 \times b_2} + (1 - \gamma) \cdot 1_{b_2}),
\]

and \( \gamma \) is swept from zero to 1/2. As \( \gamma \) increases from zero to 1/2, the noise transitions from entrywise independence (when \( \gamma = 0 \)) to increasing blockwise dependence (as \( \gamma \) grows), i.e., consecutive block of \( b_1 \times b_2 \) entries are no longer independent. Blockwise dependence can arise in settings where observations and features may form groups, e.g., blockwise dependence across both features and observations can arise in genomics data from a combination of linkage disequilibrium and kinship among subjects (see, e.g., Conomos et al., 2016).

In addition to the methods in the previous comparisons, we add a straightforward variant of FlipPA called BlockFlipPA that flips the sign of all entries in a block together, i.e., the signflip matrix \( R = \tilde{R} \otimes 1_{b_1 \times b_2} \), where \( \tilde{R}_{ij} \overset{iid}{\sim} \pm 1 \), with probability 1/2. This method is simply FlipPA applied at the block level\(^{10}\) so it preserves the distribution of the noise \( N \) and is a valid group-invariance based method, just like FlipPA is for noise with independent entries.

\(^{10}\)Note that the blocks of entries need not be regular and consecutive as in this case.
Figure 7: Performance across 100 runs of each method for a rank-one signal in noise having a block-structured noise variance profile with blockwise dependence, where the amount of dependence increases as $\gamma$ increases from zero (independent entries) to $1/2$ (increasing blockwise dependence).

Figure 8: Performance for the same setting as Fig. 7 across 100 runs of each method with prewhitening using $\Sigma_1$, $\Sigma_2$.

Fig. 7 shows the resulting performance of each method across 100 runs, where $\theta = 6$, $n = 500$, $p = 300$, $n_1 = n_2 = 250$, $p_1 = 240$, $p_2 = 60$, $b_1 = 25$, $b_2 = 15$. As before, the left plot shows the average selected rank $E[\hat{k}]$ across the runs; the second column of plots shows the proportion $Pr[\hat{k} > 1]$ of runs resulting in over-estimation, correct estimation (i.e., $Pr[\hat{k} = 1]$), and under-estimation (i.e., $Pr[\hat{k} < 1]$). When $\gamma$ is small, several methods are fairly effective. However, only BlockFlipPA correctly estimates the rank across the entire sweep; the rest overestimate it. Notably, this straightforward modification of FlipPA allows it to remain effective even in the presence of significant dependence, highlighting the flexibility of the approach.

It is perhaps less obvious how one would modify the other methods to account for the dependence. A common approach might be to instead prewhiten the data, then apply one of the other methods, in hopes that the prewhitening will sufficiently remove the dependence. For example, one might form the estimates $\Sigma_1 = (I_{n_1/b_1} \otimes 1_{b_1 \times b_1}) \circ (X X^\top)$, $\Sigma_2 = (I_{p_2/b_2} \otimes 1_{b_2 \times b_2}) \circ (X^\top X)$, then apply the methods to the prewhitened data $\tilde{X} = \Sigma_1^{-1/2} X \Sigma_2^{-1/2}$. Doing so improved their performance at small to moderate $\gamma$, as shown in Fig. 8, but only to a point. BlockFlipPA was again the only method that correctly estimated the rank across the entire sweep. For $\gamma > 0.3$, BEMA with prewhitening under-estimated the rank and the other methods with prewhitening over-estimated the rank.

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11Note that the estimates $\Sigma_1$, $\Sigma_2$ use the same knowledge of the blockwise dependence structure as BlockFlipPA; they do so by zeroing out all entries except those corresponding to within-block dependence. We also considered forming the estimates $\Sigma_1$ and $\Sigma_2$ without zeroing out these entries; this form of prewhitening did not generally perform better.
We also considered a higher dimensional setting \((n = 60, p = 5000)\) in Appendix D; Figs. 13 and 14 provide the analogues to Figs. 7 and 8. Similar to the lower dimensional setting here, only BlockFlipPA was effective across the entire sweep. Moreover, prewhitening did not significantly improve the methods, perhaps due to poor estimates of the prewhitening operators in the higher dimensional setting. To summarize, this experiment demonstrates the ease of adapting FlipPA to allow for dependence among the entries and highlights the flexibility of the approach.

5 Empirical Data Illustration from Astronomy

This section illustrates the behavior of FlipPA on an empirical dataset coming from astronomy.\(^{12}\) We consider quasar spectra obtained from the 16th data release of the Sloan Digital Sky Surveys (SDSS) (Ahumada et al., 2020) using the associated DR16Q quasar catalog (Lyke et al., 2020). The spectra are each composed of flux measurements at various wavelengths, and each spectrum comes with associated variance estimates for the flux measurements. To illustrate FlipPA and the methods considered in Section 4, we selected and preprocessed (i.e., interpolated, centered, and normalized) a subset of the data in a manner similar to Section 8 of Hong et al. (2023); see Appendix E for details.

Fig. 9a shows the resulting data matrix \(Y \in \mathbb{R}^{5000 \times 1081}\) of 5000 spectra across 1081 wavelengths, as well as the corresponding variance profiles \(V \in \mathbb{R}^{5000 \times 1081}\). As can be seen from the variance profile, the data is heteroscedastic along both observations (here, spectra) and features (here, wavelengths). Fig. 9b shows the associated scree plot, i.e., a scatter plot of the singular values of \(Y\).

Table 1: Rank selections for the quasar spectroscopy data

| Method                  | Rank | Algorithm |
|-------------------------|------|-----------|
| PermPA (pairwise)      | 133  | BEMA0     | 168 |
| PermPA (upper-edge)    | 1    | BEMA      | 4   |
| BCF                     | 1080 | Biwhitening| 7   |
| GIC                     | 1080 | FlipPA (pairwise) | 4 |
| ACT (max rank = 1000)  | 107  | FlipPA (upper-edge) | 2 |

Table 1 shows the ranks selected by FlipPA and the methods considered in Section 4. For PermPA and FlipPA, we include both the pairwise comparison and upper-edge comparison options. For ACT, we set the max rank parameter here to be 1000 because it selected up to the max rank when we set it to 100.

\(^{12}\)Codes for reproducing the figures in this section are available online at: https://gitlab.com/dahong/rank-selecction-via-random-signflips
We observe that PermPA with pairwise comparisons, BCF, GIC, ACT, and BEMA0 all selected over 100 components for this dataset. Comparing with the scree plot in Fig. 9b, such large selections seem unlikely to be correct. Notably, BCF and GIC selected all the components. In stark contrast to PermPA with pairwise comparisons, PermPA with upper-edge comparisons selected only one component for this dataset. The reason is likely that permutations were not able to sufficiently suppress the largest singular value, leading to shadowing of smaller components in this case.

The remaining methods are roughly similar, and seem fairly reasonable when compared with the scree plot in Fig. 9b. The selection of 2 components by FlipPA with upper-edge comparisons corresponds to selecting the two strong components that are substantially above the rest, while the selection of 4 components by BEMA and FlipPA with pairwise comparisons corresponds to including the next two weaker components that nonetheless appear to rise slightly above the rest. Biwhitening selects several more components, which is likely because the biwhitening operation changes the data singular values and can cause components that were previously “buried” in the noise to rise above it.

Fig. 10 shows eigenspectra computed by taking the leading right singular vectors of the data matrix $Y$. The rank selections by FlipPA, BEMA, and Biwhitening seem to correspond to relatively “clean” eigenspectra, providing some further evidence that they are selecting meaningful signal components rather than components buried in the noise. Overall, this example illustrates the potential benefits of FlipPA for rank selection in practice.

6 Discussion

This paper proposed a new method (FlipPA) for tackling the problem of rank estimation from data with heterogeneous noise. In future work, there are opportunities to sharpen the theoretical analysis of FlipPA; for example, we suspect that the delocalization conditions in Section 3.1 can likely be weakened. Another unexplored aspect is the interplay of the matrix size and the number of trials to run. When the matrix is large, it can be computationally expensive to carry out many trials, but the singular values also tend to be less variable, so FlipPA may not require many trials. Finally, a major challenge for parallel analysis methods like FlipPA remains overcoming the shadowing of weak signals by strong signals.

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A Proof of Type I error control

We use the same overall approach as the proof of (Hemerik and Goeman, 2017, Theorem 2). Note first that for both pairwise and upper-edge comparison methods
\[
\ell > 0 \iff \sigma_1 > q\text{-quantile of } \left(\hat{\sigma}_1^{(1)}, \ldots, \hat{\sigma}_1^{(T)}\right) + \tau
\]
\[
\iff \sigma_1 > q\text{-quantile of } \left(\tilde{\sigma}_1^{(1)}, \ldots, \tilde{\sigma}_1^{(T)}\right).
\]

Now, whenever \(\sigma_1 > q\text{-quantile of } \left(\tilde{\sigma}_1^{(1)}, \ldots, \tilde{\sigma}_1^{(T)}\right)\) then it must also be the case that
\[
\#\left\{ t \in \{1, \ldots, T\} : \tilde{\sigma}_1^{(t)} < \sigma_1 \right\}
\]
\[
\geq \#\left\{ t \in \{1, \ldots, T\} : \hat{\sigma}_1^{(t)} \leq q\text{-quantile of } \left(\hat{\sigma}_1^{(1)}, \ldots, \hat{\sigma}_1^{(T)}\right) \right\} \geq \lfloor qT \rfloor,
\]
where the second inequality holds for sample quantiles computed using any of the nine commonly used definitions enumerated in Hyndman and Fan (1996).\(^{13}\) Moreover, note that
\[
\left\{ t \in \{1, \ldots, T\} : \tilde{\sigma}_1^{(t)} < \sigma_1 \right\} = \left\{ t \in \{0, \ldots, T\} : \sigma_1(R^{(t)} \circ X) < \sigma_1(X) \right\}
\]
where \(R^{(0)} = 1_{n \times p}\) and \(R^{(1)}, \ldots, R^{(T)} \text{iid } \text{Unif}(\{-1, 1\}^{n \times p})\) are the \(T\) signflip matrices in FlipPA, since \(\sigma_1 = \sigma_1(X)\) and \(\tilde{\sigma}_1^{(t)} = \sigma_1(R^{(t)} \circ X)\) for \(t = 1, \ldots, T\). Combining (8) to (10) yields
\[
\Pr[\hat{\ell} > 0] = \Pr \left[ \sigma_1 > q\text{-quantile of } \left(\tilde{\sigma}_1^{(1)}, \ldots, \tilde{\sigma}_1^{(T)}\right) \right]
\]
\[
\leq \Pr \left[ \sigma_1 > q\text{-quantile of } \left(\hat{\sigma}_1^{(1)}, \ldots, \hat{\sigma}_1^{(T)}\right) \right]
\]
\[
\leq \Pr \left[ \#\left\{ t \in \{1, \ldots, T\} : \hat{\sigma}_1^{(t)} < \sigma_1 \right\} \geq \lfloor qT \rfloor \right]
\]
\[
= \Pr \left[ \#\left\{ t \in \{0, \ldots, T\} : \sigma_1(R^{(t)} \circ X) < \sigma_1(X) \right\} \geq \lfloor qT \rfloor \right],
\]
where these probabilities are with respect to the randomness in \(X\) and \(R^{(1)}, \ldots, R^{(T)}\), all under the null hypothesis \(H_0\) of no signal.

So, it remains to bound the final probability in (11), for which we will exploit the invariance properties of the signflips. Namely, note that for any \(j \in \{0, \ldots, T\}\),
\[
\left\{ \{R^{(0)}, \ldots, R^{(T)}\} \right\} = \left\{ \{R^{(0)} \circ R^{(j)}, \ldots, R^{(T)} \circ R^{(j)}\} \right\},
\]
where the double braces here denote a multiset, i.e., a set with multiplicities for its elements. Additionally, under \(H_0\), for any \(j \in \{0, \ldots, T\}\),
\[
X = \text{d} R^{(j)} \circ X.
\]
Thus, for any \(j \in \{0, \ldots, T\}\),
\[
\Pr \left[ \#\left\{ t \in \{0, \ldots, T\} : \sigma_1(R^{(t)} \circ X) < \sigma_1(X) \right\} \geq \lfloor qT \rfloor \right]
\]
\[
= \Pr \left[ \#\left\{ t \in \{0, \ldots, T\} : \sigma_1(R^{(t)} \circ R^{(j)} \circ X) < \sigma_1(X) \right\} \geq \lfloor qT \rfloor \right]
\]
\[
= \Pr \left[ \#\left\{ t \in \{0, \ldots, T\} : \sigma_1(R^{(t)} \circ R^{(j)} \circ R^{(j)} \circ X) < \sigma_1(R^{(j)} \circ X) \right\} \geq \lfloor qT \rfloor \right]
\]
\[
= \Pr \left[ \#\left\{ t \in \{0, \ldots, T\} : \sigma_1(R^{(t)} \circ X) < \sigma_1(R^{(j)} \circ X) \right\} \geq \lfloor qT \rfloor \right],
\]
\(^{13}\)Specifically, the second inequality corresponds to Property P2 in Hyndman and Fan (1996), with the correction posted online by the authors (Hyndman, 2024).
where the first equality uses (12), the second equality uses (13), and the final equality follows by simplifying. Thus, averaging (14) across \( j \in \{0, \ldots, T\} \) yields

\[
\Pr \left[ \# \left\{ t \in \{0, \ldots, T\} : \sigma_1(R^{(i)} \circ X) < \sigma_1(X) \right\} \geq \lfloor qT \rfloor \right] = \frac{1}{T+1} \sum_{j=0}^T \Pr \left[ \# \left\{ t \in \{0, \ldots, T\} : \sigma_1(R^{(i)} \circ X) < \sigma_1(R^{(j)} \circ X) \right\} \geq \lfloor qT \rfloor \right]
\]

\[
= \frac{1}{T+1} \sum_{j=0}^T \mathbb{E} \left[ 1 \left( \# \left\{ t \in \{0, \ldots, T\} : \sigma_1(R^{(i)} \circ X) < \sigma_1(R^{(j)} \circ X) \right\} \geq \lfloor qT \rfloor \right) \right]
\]

\[
= \frac{1}{T+1} \mathbb{E} \left[ \sum_{j=0}^T 1 \left( \# \left\{ t \in \{0, \ldots, T\} : \sigma_1(R^{(i)} \circ X) < \sigma_1(R^{(j)} \circ X) \right\} \geq \lfloor qT \rfloor \right) \right]
\]

\[
\leq \frac{1}{T+1} \mathbb{E}[T+1] - \lfloor qT \rfloor = 1 - \frac{\lfloor qT \rfloor}{T+1},
\]

where \( 1(\cdot) \) denotes the indicator function, which equals one when the argument is true and zero otherwise. Combining (11) and (15) concludes the proof. \( \square \)

## B Proofs for Section 3.1

This appendix provides proofs for the consistency guarantees in Section 3.1.

### B.1 Useful lemmas

This section states some lemmas that will be useful for proving the results from Section 3.1. The first provides a simple expression for the \( \| \cdot \|_{2,\infty} \) norm of a rank-one matrix.

**Lemma B.1** (\( \| \cdot \|_{2,\infty} \) norm of a rank-one matrix). Let \( u \in \mathbb{R}^n \) and \( z \in \mathbb{R}^p \) be arbitrary. Then \( \| uz^\top \|_{2,\infty} = \| u \|_\infty \| z \|_2 \).

The proof of Lemma B.1 is straightforward; we provide it here for the reader’s convenience.

**Proof of Lemma B.1.** Since the \( i \)-th row of \( uz^\top \) is \( (uz^\top)_i = u_i \cdot z \), we immediately have

\[
\| uz^\top \|_{2,\infty} = \max_{i=1,\ldots,n} \| (uz^\top)_i \|_2 = \max_{i=1,\ldots,n} \| u_i \cdot z \|_2 = \max_{i=1,\ldots,n} \| u_i \|_\infty \| z \|_2 = \| u \|_\infty \| z \|_2,
\]

which completes the proof. \( \square \)

The next lemma provides an elegant relationship between the entrywise matrix norm \( \| \cdot \|_{t,t} \) and a corresponding maximum row norm \( \| \cdot \|_{t/2,\infty} \).

**Lemma B.2** (Bound for \( \| \cdot \|_{t,t} \) norm in terms of \( \| \cdot \|_{t/2,\infty} \)). Let \( A \in \mathbb{R}^{n \times p} \) and \( t \geq 2 \) be an arbitrary even number. Then \( \| A \|_{t,t} \leq \text{rank}^{1/2}(A) \sqrt{\| A \|_{t/2,\infty} \cdot \| A^\top \|_{t/2,\infty}}. \)

**Proof of Lemma B.2.** Note first that

\[
\| A \|_{t,t} = \sum_{i=1}^n \sum_{j=1}^p |A_{i,j}|^t = \sum_{i=1}^n \sum_{j=1}^p |A_{i,j}|^{t/2} \cdot |A_{i,j}|^{t/2} = \| B \|_F^2,
\]

where

\[
B_{i,j} = |A_{i,j}|^{t/2}.
\]
where \( \| \cdot \|_F \) denotes the Frobenius norm and \( B \in \mathbb{R}^{n \times p} \) has entries \( B_{i,j} := A_{i,j}^{t/2} \), i.e.,

\[
B := A \odot \cdots \odot A,
\]

where \( \odot \) denotes the Hadamard product. Now, recall that for any matrix \( B \),

\[
\| B \|_F^2 \leq \operatorname{rank}(B) \| B \|_2^2,
\]

\[
\| B \|_2 \leq \sqrt{\| B \|_1 \| B \|_\infty},
\]

where \( \| \cdot \|_2 \), \( \| \cdot \|_1 \), and \( \| \cdot \|_\infty \) denote the \( \ell_2 \), \( \ell_1 \), and \( \ell_\infty \) operator norms, respectively. Thus, we have

\[
\| A \|_{t,1} = \| B \|_F^2 \leq \operatorname{rank}(B) \| B \|_1 \| B \|_\infty.
\]

Next, note that

\[
\| B \|_1 = \max_{j=1,\ldots,p} \sum_{i=1}^n |B_{ij}| = \max_{j=1,\ldots,p} \sum_{i=1}^n |A_{ij}^{t/2}| = \max_{j=1,\ldots,p} \sum_{i=1}^n |A_{ij}|^{t/2} = \| A^T \|_{t/2,\infty}^{t/2},
\]

\[
\| B \|_\infty = \max_{i=1,\ldots,n} \sum_{j=1}^p |B_{ij}| = \max_{i=1,\ldots,n} \sum_{j=1}^p |A_{ij}^{t/2}| = \max_{i=1,\ldots,n} \sum_{j=1}^p |A_{ij}|^{t/2} = \| A \|_{t/2,\infty}^{t/2},
\]

and

\[
\operatorname{rank}(B) = \operatorname{rank}(A \odot \cdots \odot A) \leq \left[ \operatorname{rank}(A) \right]^{t/2}.
\]

Substituting (17) to (19) into (16) and taking the \( t \)-th root completes the proof.

The final lemma collects and combines some recent results on the operator norms of nonhomogeneous random matrices (Segner, 2000; Latala, 2005; Schnett and Riemer, 2013; Bandeira and Van Handel, 2016; Van Handel, 2017; Latala et al., 2018) and writes the result in our notation.

**Lemma B.3** (Operator norms of signflipped matrices). Let \( A \in \mathbb{R}^{n \times p} \) be arbitrary and let \( R \sim \operatorname{Unif}\{-1,1\}^{n \times p} \) be a Rademacher random matrix. Then \( \mathbb{E} \| A \odot R \| \lesssim \| A \|_{2,\infty} + \| A^T \|_{2,\infty} + \min \left[ \rho_2(A), \rho_\infty(A) \right] \).

**Proof of Lemma B.3.** Consider the two symmetric \((n+p) \times (n+p)\) matrices

\[
\bar{A} := \begin{bmatrix} A & A^T \end{bmatrix},
\]

\[
\bar{R} := \begin{bmatrix} R & R^T \end{bmatrix}.
\]

Several existing results provide dimension-dependent bounds for this case, e.g., writing (Bandeira and Van Handel, 2016, Corollary 4.7) in our notation and simplifying yields

\[
\mathbb{E} \| \bar{A} \odot \bar{R} \| \lesssim \| \bar{A} \|_{2,\infty} \sqrt{\log(n+p)} = \left\| A \right\|_{2,\infty} \sqrt{\log(n+p)} = \rho_2(A).
\]

Next, we develop a bound using the dimension-free bounds of Latala et al. (2018), which apply to nonhomogeneous Gaussian matrices. For this, let \( \bar{G} \) be a symmetric \((n+p) \times (n+p)\) Gaussian random matrix, i.e., \( G_{ij} \sim \mathcal{N}(0,1) \) for \( i \geq j \). Then writing (Latala et al., 2018, Theorem 1.1) in our notation and simplifying yields the following bound for \( \bar{A} \odot \bar{G} \):

\[
\mathbb{E} \| \bar{A} \odot \bar{G} \| \lesssim \| \bar{A} \|_{2,\infty} + \max_{i=1,\ldots,n+p} \| \bar{A} \|_{\infty,(i)} \sqrt{\log i}
\]

\[
= \left\| A \right\|_{2,\infty} + \max_{i=1,\ldots,n+p} \left\| A \right\|_{\infty,(i)} ^{\sqrt{\log i}}
\]

\[
= \max \left( \| A \|_{2,\infty}, \| A^T \|_{2,\infty} \right) + \rho_\infty(A).
\]
We next use the following relationship between $\tilde{A} \circ \tilde{G}$ and $\tilde{A} \circ \tilde{R}$ (also used in Latala (2005)):

$$E\|\tilde{A} \circ \tilde{G}\| = E\|\tilde{A} \circ \tilde{R} \circ |\tilde{G}|\| = E_{\tilde{R}} \left[E_{\tilde{G}}\|\tilde{A} \circ \tilde{R} \circ |\tilde{G}|\|\right] \geq E_{\tilde{R}} \left[E_{\tilde{G}}\|\tilde{A} \circ \tilde{R} \circ |\tilde{G}|\|\right] = E_{\tilde{R}} \left[E_{\tilde{G}}\|\tilde{A} \circ \tilde{R} \circ |\tilde{G}|\|\right] = \sqrt{\frac{2}{\pi}} E\|\tilde{A} \circ \tilde{R}\|,$$

(22)

where $|\tilde{G}| \in \mathbb{R}^{(n+p) \times (n+p)}$ is the elementwise absolute value of $\tilde{G}$, i.e., $|\tilde{G}_{ij}| = |\tilde{G}_{ij}|$. The first equality holds because $\tilde{A} \circ \tilde{G} = d \circ \tilde{A} \circ \tilde{R} \circ |\tilde{G}|$, the second equality is the law of total expectation, the inequality follows by applying Jensen’s inequality to the operator norm $\| \cdot \|$, and the final two equalities hold by linearity of the expectation and the fact that $E|\tilde{G}_{ij}| = \sqrt{2/\pi}$.

Combining (21) and (22) yields the following dimension-free bound for $\tilde{A} \circ \tilde{R}$:

$$E\|\tilde{A} \circ \tilde{R}\| \lesssim E\|\tilde{A} \circ \tilde{G}\| \lesssim \max (\|A\|_{2,\infty}, \|A^\top\|_{2,\infty}) + \rho_\infty (A),$$

(23)

and finally combining (20) and (23) and simplifying yields

$$E\|\tilde{A} \circ \tilde{R}\| \lesssim \min \left[\rho_2 (A), \max (\|A\|_{2,\infty}, \|A^\top\|_{2,\infty}) + \rho_\infty (A)\right] \leq \|A\|_{2,\infty} + \|A^\top\|_{2,\infty} + \min \left[\rho_2 (A), \rho_\infty (A)\right].$$

Since the nonzero eigenvalues of $\tilde{A} \circ \tilde{R}$ consist of positive and negative copies of the singular values of $A \circ R$ (see, e.g., Stewart and Sun, 1990, Theorem 4.2), it follows that $E\|A \circ R\| = E\|\tilde{A} \circ \tilde{R}\|$, which concludes the proof.

### B.2 Proof of Theorem 3.3

Theorem 3.3 can be proved using similar techniques as in the proof of Theorem 3.5, but doing so can make it less obvious that Theorem 3.3 is actually a special case of Theorem 3.5. So, here we will prove Theorem 3.3 by showing that it follows from Theorem 3.5. Namely, we show that the signal matrix $S = \sum_{i=1}^k \theta_i u_i z_i^\top$ satisfies the conditions of Theorem 3.5, i.e.,

$$E\|S\|_{2,\infty} \rightarrow 0, \quad E\|S^\top\|_{2,\infty} \rightarrow 0, \quad \text{and} \quad \min \left[\mathbb{E}\rho_2 (S), \mathbb{E}\rho_\infty (S)\right] \rightarrow 0.$$

We begin with the first two conditions. Note that

$$E\|S\|_{2,\infty} = E \left[\sum_{i=1}^k \theta_i u_i z_i^\top\right]_{\|\cdot\|_{2,\infty}} \leq E \left[\sum_{i=1}^k \theta_i \|u_i\|_\infty \|z_i\|_2\right] = E \left[\sum_{i=1}^k \theta_i \|u_i\|_\infty \|z_i\|_2\right],$$

(24)

$$E\|S^\top\|_{2,\infty} = E \left[\sum_{i=1}^k \theta_i z_i u_i^\top\right]_{\|\cdot\|_{2,\infty}} \leq E \left[\sum_{i=1}^k \theta_i \|z_i\|_\infty \|u_i\|_2\right] = E \left[\sum_{i=1}^k \theta_i \|z_i\|_\infty \|u_i\|_2\right].$$

(25)

where the inequality in each line follows from the triangle inequality and the final equality in each line follows from Lemma B.1. Thus, we have

$$\max (E\|S\|_{2,\infty}, E\|S^\top\|_{2,\infty}) \leq E\|S\|_{2,\infty} + E\|S^\top\|_{2,\infty} \leq E \left[\sum_{i=1}^k \theta_i \|u_i\|_\infty \|z_i\|_2\right] + E \left[\sum_{i=1}^k \theta_i \|u_i\|_2 \|z_i\|_\infty\right] = 2 \cdot E \left[\sum_{i=1}^k \theta_i \|u_i\|_2 \|z_i\|_2 \cdot \frac{\|u_i\|_\infty / \|u_i\|_2 + \|z_i\|_\infty / \|z_i\|_2}{2}\right] \rightarrow 0.$$
where the first inequality holds because $\mathbb{E}\|S\|_{2,\infty}$ and $\mathbb{E}\|S^T\|_{2,\infty}$ are nonnegative, the second inequality follows from (24) and (25), and the final limit follows from the delocalization condition (4) in the theorem. So, we are done with the first two conditions of Theorem 3.5.

To show that the final condition of Theorem 3.5 is satisfied, we will show that $\mathbb{E}\|S\|_{4,4} \rightarrow 0$ then apply Theorem 3.6. Note first that

$$\mathbb{E}\|S\|_{4,4} = \mathbb{E} \left\{ \sum_{i=1}^{k} \theta_i \|u_i\|_2 \|z_i\|_2 \right\} \leq \mathbb{E} \left\{ \sum_{i=1}^{k} \|\theta_i u_i z_i^T\|_{4,4} \right\}$$

$$\leq \mathbb{E} \left\{ \sum_{i=1}^{k} \text{rank}^{1/2}(\theta_i u_i z_i^T) \sqrt{\|\theta_i u_i z_i^T\|_{2,\infty} \cdot \|\theta_i z_i u_i^T\|_{2,\infty}} \right\},$$

where the first inequality follows from the triangle inequality, and the second inequality follows from Lemma B.2. Noting that $\text{rank}(\theta_i u_i z_i^T) = 1$, applying Lemma B.1, and simplifying then yields

$$\mathbb{E}\|S\|_{4,4} = \mathbb{E} \left\{ \sum_{i=1}^{k} \theta_i \|u_i\|_2 \|z_i\|_2 \cdot \frac{\|u_i\|_\infty / \|u_i\|_2 + \|z_i\|_\infty / \|z_i\|_2}{2} \right\} \rightarrow 0,$$

where the inequality follows from the AM-GM inequality, and the limit follows from the delocalization condition (4) in the theorem. Finally, applying Theorem 3.6 yields

$$\min \left[ \mathbb{E}\rho_2(S), \mathbb{E}\rho_\infty(S) \right] \leq \mathbb{E}\rho_\infty(S) \rightarrow 0,$$

so we are done with the final condition of Theorem 3.5.

The proof concludes by combining Theorem 3.5 with (26) and (27).

\[\square\]

### B.3 Proof of Corollary 3.4

We prove Corollary 3.4 by showing that the signal matrix $S = \sum_{i=1}^{k} \theta_i u_i z_i^T$ satisfies the delocalization condition (4) from Theorem 3.3. Note first that

$$\mathbb{E} \left\{ \sum_{i=1}^{k} \theta_i \|u_i\|_2 \|z_i\|_2 \cdot \frac{\|u_i\|_\infty / \|u_i\|_2 + \|z_i\|_\infty / \|z_i\|_2}{2} \right\}$$

$$= \mathbb{E} \left\{ \sum_{i=1}^{k} \theta_i \left[ \frac{\|u_i\|_\infty \|z_i\|_2 + \|u_i\|_2 \|z_i\|_\infty}{2} \right] \right\} = \sum_{i=1}^{k} \theta_i \left[ \mathbb{E}\|u_i\|_\infty \mathbb{E}\|z_i\|_2 + \mathbb{E}\|u_i\|_2 \mathbb{E}\|z_i\|_\infty \right],$$

because the signal rank and component coefficients are deterministic and the component vectors are jointly independent. Substituting the rates yields

$$\sum_{i=1}^{k} \theta_i \left[ \mathbb{E}\|u_i\|_\infty \mathbb{E}\|z_i\|_2 + \mathbb{E}\|u_i\|_2 \mathbb{E}\|z_i\|_\infty \right] \leq \sum_{i=1}^{k} p^{\beta_1} \log^{\beta_2} p \left[ p^{-\alpha_1} \log^{-\alpha_2} p + p^{-\alpha_1} \log^{-\alpha_2} p \right]$$

$$= k \cdot p^{\beta_1 - \alpha_1} \log^{\beta_2 - \alpha_2} p \leq (p^{\nu_1} \log^{\nu_2} p) \cdot (p^{\beta_1 - \alpha_1} \log^{\beta_2 - \alpha_2} p) = p^{\nu_1 + \beta_1 - \alpha_1} \log^{\nu_2 + \beta_2 - \alpha_2} p.$$

Thus we have

$$\mathbb{E} \left\{ \sum_{i=1}^{k} \theta_i \|u_i\|_2 \|z_i\|_2 \cdot \frac{\|u_i\|_\infty / \|u_i\|_2 + \|z_i\|_\infty / \|z_i\|_2}{2} \right\} \leq p^{\nu_1 + \beta_1 - \alpha_1} \log^{\nu_2 + \beta_2 - \alpha_2} p,$$

which converges to zero if either $\alpha_1 > \nu_1 + \beta_1$, or $\alpha_1 = \nu_1 + \beta_1$ and $\alpha_2 > \nu_2 + \beta_2$. \[\square\]
B.4 Proof of Theorem 3.5

By Condition 3.2, there exists $\varepsilon > 0$ for which $\Pr[\sigma_k > \|N\| + \varepsilon] \to 1$. Now note that for the upper-edge comparison method

$$ \hat{k} = k \quad \iff \quad \sigma_{k+1} \leq q\text{-quantile of } \left( \tilde{\sigma}_1^{(1)}, \ldots, \tilde{\sigma}_1^{(T)} \right) + \tau < \sigma_k, $$

which occurs for $\tau \in (0, \varepsilon)$ whenever the following conditions are simultaneously met:

$$ \sigma_k > \|N\| + \varepsilon \quad \text{and} \quad \sigma_{k+1} \leq \|N\| $$

and $\|N\| - \tau \leq \tilde{\sigma}_1^{(t)} \leq \|N\| + (\varepsilon - \tau)$ for $t = 1, \ldots, T$,

since in that case we have

$$ \sigma_{k+1} \leq \|N\| \leq \min \left( \tilde{\sigma}_1^{(1)}, \ldots, \tilde{\sigma}_1^{(T)} \right) + \tau \leq q\text{-quantile of } \left( \tilde{\sigma}_1^{(1)}, \ldots, \tilde{\sigma}_1^{(T)} \right) + \tau, $$

$$ \sigma_k > \|N\| + \varepsilon \geq \max \left( \tilde{\sigma}_1^{(1)}, \ldots, \tilde{\sigma}_1^{(T)} \right) + \tau > q\text{-quantile of } \left( \tilde{\sigma}_1^{(1)}, \ldots, \tilde{\sigma}_1^{(T)} \right) + \tau. $$

As a result, we have the simple bound

$$ \Pr[\hat{k} = k] \geq \Pr \left[ \begin{array}{c} \sigma_k > \|N\| + \varepsilon \text{ and } \sigma_{k+1} \leq \|N\| \\ \text{and } \|N\| - \tau \leq \tilde{\sigma}_1^{(t)} \leq \|N\| + (\varepsilon - \tau) \text{ for } t = 1, \ldots, T \end{array} \right] \geq 1 + (\Pr[\sigma_k > \|N\| + \varepsilon] - 1) + (\Pr[\sigma_{k+1} \leq \|N\|] - 1) $$

$$ + \sum_{t=1}^{T} \left( \Pr[\|N\| - \tau \leq \tilde{\sigma}_1^{(t)} \leq \|N\| + (\varepsilon - \tau)] - 1 \right), $$

where the second inequality comes from applying a union bound to the complement of the event. Now, by Condition 3.2, we already have

$$ \Pr[\sigma_k > \|N\| + \varepsilon] \to 1. \quad (29) $$

Moreover, it follows from Weyl's inequality (see, e.g., Stewart and Sun, 1990, Corollary 4.10) that $\sigma_{k+1} = \sigma_{k+1}(S + N) \leq \sigma_{k+1}(S) + \|N\| = \|N\|$ since rank$(S) \leq k$, so

$$ \Pr[\sigma_{k+1} \leq \|N\|] = 1. \quad (30) $$

Hence, it remains to show that $\Pr[\|N\| - \tau \leq \tilde{\sigma}_1^{(t)} \leq \|N\| + (\varepsilon - \tau)] \to 1$ for $t = 1, \ldots, T$. Namely, we need to show that the signflipped data singular value $\tilde{\sigma}_1^{(t)}$ is close to the noise operator norm $\|N\|$. To do so, we first decompose the difference of the two using triangle inequality:

$$ |\tilde{\sigma}_1^{(t)} - \|N\|| = |\sigma_1(R^{(t)} \circ X) - \sigma_1(N)| $$

$$ \leq \underbrace{|\sigma_1(R^{(t)} \circ X) - \sigma_1(R^{(t)} \circ N)|}_{\text{signal destruction}} + \underbrace{|\sigma_1(R^{(t)} \circ N) - \sigma_1(N)|}_{\text{noise preservation}}, $$

where $R^{(t)} \sim \text{Unif} \{-1,1\}^{n \times p}$ is the signflip matrix for trial $t$. The first term captures destruction of the signal by signflipping (so that the signflipped data looks like the signflipped noise) and the second term captures preservation of the noise (so that the signflipped noise looks like the true noise). We now analyze each term separately, starting with the noise preservation:

1. noise preservation $|\sigma_1(R^{(t)} \circ N) - \sigma_1(N)|$: For this term, note that

$$ |\sigma_1(R^{(t)} \circ N) - \sigma_1(N)| \leq |\sigma_1(R^{(t)} \circ N) - \tilde{\sigma}| + |\tilde{\sigma} - \sigma_1(N)| \xrightarrow{i.p.} 0, \quad (32) $$

because $\sigma_1(N) = \|N\| \xrightarrow{i.p.} \tilde{\sigma}$ by Condition 3.1 and $R^{(t)} \circ N = d N$ since $N_{ij} = d - N_{ij}$. 

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2. **signal destruction** \(|\sigma_1(\mathbf{R}^{(t)} \circ \mathbf{X}) - \sigma_1(\mathbf{R}^{(t)} \circ \mathbf{N})|\): For this term, note that Weyl's inequality (see, e.g., Stewart and Sun, 1990, Corollary 4.10) yields
\[
|\sigma_1(\mathbf{R}^{(t)} \circ \mathbf{X}) - \sigma_1(\mathbf{R}^{(t)} \circ \mathbf{N})| \leq \|\mathbf{R}^{(t)} \circ \mathbf{S}\|,
\]
since \(\mathbf{R}^{(t)} \circ \mathbf{X} = \mathbf{R}^{(t)} \circ (\mathbf{S} + \mathbf{N}) = \mathbf{R}^{(t)} \circ \mathbf{S} + \mathbf{R}^{(t)} \circ \mathbf{N}\). Now, using Lemma B.3 we have
\[
E|\sigma_1(\mathbf{R}^{(t)} \circ \mathbf{X}) - \sigma_1(\mathbf{R}^{(t)} \circ \mathbf{N})| \leq E\|\mathbf{R}^{(t)} \circ \mathbf{S}\| \\
\lesssim E\|\mathbf{S}\|_{2,\infty} + E\|\mathbf{S}^\top\|_{2,\infty} + \min \left[ E\rho_2(\mathbf{S}), E\rho_\infty(\mathbf{S}) \right] \to 0,
\]
since each of these terms go to zero by assumption; note that the expectations in the final line are only with respect to \(\mathbf{S}\). So, we have shown that \(|\sigma_1(\mathbf{R}^{(t)} \circ \mathbf{X}) - \sigma_1(\mathbf{R}^{(t)} \circ \mathbf{N})|\) converges to zero in \(L^1\), and thus we have
\[
|\sigma_1(\mathbf{R}^{(t)} \circ \mathbf{X}) - \sigma_1(\mathbf{R}^{(t)} \circ \mathbf{N})| \overset{L^1}{\to} 0. \tag{33}
\]
Combining (31) to (33) yields
\[
|\tilde{\sigma}_1^{(t)} - \|\mathbf{N}\| | \leq |\sigma_1(\mathbf{R}^{(t)} \circ \mathbf{X}) - \sigma_1(\mathbf{R}^{(t)} \circ \mathbf{N})| + |\sigma_1(\mathbf{R}^{(t)} \circ \mathbf{N}) - \sigma_1(\mathbf{N})| \overset{L^1}{\to} 0,
\]
i.e., \(\tilde{\sigma}_1^{(t)} \overset{L^1}{\to} \|\mathbf{N}\|\), and so for all \(t = 1, \ldots, T\)
\[
Pr[|\|\mathbf{N}\| - \tau \leq \tilde{\sigma}_1^{(t)} \leq \|\mathbf{N}\| + (\varepsilon - \tau)] \to 1. \tag{34}
\]
The proof concludes by combining (28) to (30) and (34).

### B.5 Proof of Theorem 3.6

Borrowing an argument from Latala et al. (2018), note that for any matrix \(\mathbf{A} \in \mathbb{R}^{m \times t}\), \(t \geq 2\), and \(i \in \{1, \ldots, m\}\), we have
\[
i \cdot \|\mathbf{A}\|_{\infty, (i)}^t \leq \sum_{j=1}^{i} \|\mathbf{A}\|_{\infty, (j)}^t \leq \sum_{j=1}^{m} \|\mathbf{A}\|_{\infty, (j)}^t = \sum_{j=1}^{m} \|\mathbf{A}_j\|_{\infty}^t \leq \sum_{j=1}^{m} \sum_{s=1}^{t} |A_{js}|^t = \|\mathbf{A}\|_{t, t},
\]
so \(\|\mathbf{A}\|_{\infty, (i)} \leq i^{-1/t} \|\mathbf{A}\|_{t, t}\). Thus, for any \(t \geq 2\)
\[
\rho_\infty(\mathbf{S}) = \max_{i=1, \ldots, n+p} \|S^\top\|_{\infty, (i)}^t \leq \max_{i=1, \ldots, n+p} i^{-1/t} \|S^\top\|_{t, t} \leq \max_{i=1, \ldots, n+p} \sqrt{\log i} \|S^\top\|_{t, t} \leq \sqrt{\log i} \|S^\top\|_{t, t}
\]
and so \(E\rho_\infty(\mathbf{S}) \to 0\) if \(E\|S\|_{t, t} \to 0\), which establishes the first condition of Theorem 3.6. Setting \(t = 4\) and applying Lemma B.2 yields
\[
\rho_\infty(\mathbf{S}) \lesssim \|\mathbf{S}\|_{4,4} \leq \text{rank}^{1/2}(\mathbf{S}) \sqrt{\|\mathbf{S}\|_{2, \infty} \cdot \|\mathbf{S}^\top\|_{2, \infty}},
\]
so \(E\rho_\infty(\mathbf{S}) \to 0\) if \(E \left\{ \text{rank}^{1/2}(\mathbf{S}) \sqrt{\|\mathbf{S}\|_{2, \infty} \cdot \|\mathbf{S}^\top\|_{2, \infty}} \right\} \to 0\), which establishes the second condition of Theorem 3.6 and completes the proof. \(\square\)
C Proof of Theorem 3.7

Note first that the homogenized noise matrix $\mathbf{N}$ can be written as $\mathbf{N} = \mathbf{G} \text{diag}(1/\sqrt{n})$, where $\mathbf{G} \in \mathbb{R}^{n \times p}$ has entries $G_{ij} \overset{iid}{\sim} \mathcal{N}(0, 1)$ and the empirical distribution function of $(v_1, \ldots, v_p)$ converges to $H$. Thus, as is well known, the empirical singular value distribution of $\mathbf{N}/\sqrt{n}$ converges to the generalized Marčenko-Pastur distribution defined by $H$ (see, e.g., Bai and Silverstein, 2010, Theorem 4.3). Namely, $\mathbf{NN}^\top/n = (1/n)\mathbf{G} \text{diag}(v)$ has a limiting spectral distribution defined by the unique Stieltjes transform $m(z)$ that satisfies the equation

$$z + \frac{1}{m(z)} = \frac{\gamma}{1 + \gamma tm(z)} \int \frac{tdH(t)}{1 + tm(z)}, \quad z \in \mathbb{C}^+.$$  

(35)

So, it remains to show that the empirical singular value distribution of $\mathbf{N}_\pi/\sqrt{n}$ also converges to the generalized Marčenko-Pastur distribution defined by $H$. Namely, we need to show that $\mathbf{N}_\pi \mathbf{N}_\pi^\top/n$ has a limiting spectral distribution defined by the unique Stieltjes transform $m(z)$ that satisfies (35). Since the random permutations $\pi_1, \ldots, \pi_p$ induce dependence among the entries of $\mathbf{N}_\pi$, doing so requires establishing the generalized Marčenko-Pastur law without assuming that the entries are independent.

The remainder of the proof consists of two parts. First, Appendix C.1 establishes general conditions under which random matrices with dependent entries still follow the generalized Marčenko-Pastur law. The conditions include settings beyond what is needed here and may be of independent interest. Then, Appendix C.2 completes the proof by showing that $\mathbf{N}_\pi^\top$ satisfies these conditions.

C.1 General conditions for the generalized Marčenko-Pastur law

This section proves the following lemma, which establishes the generalized Marčenko-Pastur law under relaxed independence conditions. Specifically, it allows for some dependence within each row in the case where the rows all have isotropic covariances. See Hui and Pan (2010); Wei et al. (2016); Bryson et al. (2021) for some related (but different) results.

**Lemma C.1** (Generalized Marčenko-Pastur law under relaxed independence conditions). Let $\mathbf{X} \in \mathbb{R}^{n \times p}$ have independent rows with zero mean entries, and suppose that $n, p \to \infty$ with $p/n \to \gamma > 0$. Suppose furthermore that

1. Each row $x_k \in \mathbb{R}^p$ of $\mathbf{X}$ has an isotropic covariance of $\mathbb{E}(x_k x_k^\top) = \eta_k^2 \mathbf{I}_p$.
2. The variances $\eta_1^2, \ldots, \eta_n^2$ are uniformly bounded with empirical distribution converging to some deterministic distribution $H$.
3. For any sequence of possibly complex-valued symmetric deterministic $p \times p$ matrices $(\mathbf{A}_p)_{p \geq 1}$ with uniformly bounded spectral norms, and for every row $x_k$, we have

$$\text{Var} (x_k^\top \mathbf{A}_p x_k) \leq C \|\mathbf{A}_p\|_F^2,$$

(36)

where $C$ does not depend on the sequence $(\mathbf{A}_p)_{p \geq 1}$, and $\text{Var}(Z) = \mathbb{E}|Z - \mathbb{E}Z|^2$ denotes the variance for a complex-valued random variable.

Then, with probability one, the empirical spectral distribution of $n^{-1}\mathbf{X}^\top \mathbf{X}$ converges weakly to the generalized Marčenko-Pastur distribution, whose Stieltjes transform $m(z)$ satisfies:

$$z + \frac{1}{m(z)} = \gamma \int \frac{tdH(t)}{1 + \gamma tm(z)}, \quad z \in \mathbb{C}^+.$$  

(37)

The next section (Appendix C.2) shows that $\mathbf{N}_\pi^\top$ satisfies these conditions. The remainder of this section proves Lemma C.1 by carefully combining techniques used in the proofs of (Bai and Zhou, 2008, Theorem 1.1) and (Bai and Silverstein, 2010, Theorem 4.3).
Proof of Lemma C.1. Let \( m_n(z) = p^{-1} \text{tr}(n^{-1} X^\top X - zI_p)^{-1} \) be the Stieltjes transform for the empirical spectral distribution of \( n^{-1} X^\top X \). Following the proof of Theorem 1.1 of Bai and Zhou (2008), we proceed in three steps:

1. \( m_n(z) - \text{Em}_n(z) \to 0, \ a.s. \)
2. \( \text{Em}_n(z) \to m(z) \), which satisfies (37).
3. (37) has a unique solution in \( \mathbb{C}^+ \).

Note that \( m_n(z) = p^{-1} \text{tr}B_n^{-1} \) where

\[
B_n := B_n - zI_p \in \mathbb{C}^{p \times p}, \quad B_n := \frac{1}{n} \sum_{i=1}^{n} x_ix_i^\top \in \mathbb{C}^{p \times p}.
\]

For any \( k \in \{1, \ldots, n\} \), we also define

\[
B_{k,n} := B_{k,n} - zI_p \in \mathbb{C}^{p \times p}, \quad B_{k,n} := \frac{1}{n} \sum_{i \neq k} x_ix_i^\top \in \mathbb{C}^{p \times p}.
\]

Throughout the proof, for fixed \( z \in \mathbb{C}^+ \), we will write \( z = \Re(z) + i\Im(z) = u + iv \), where \( u \in \mathbb{R}, v > 0 \) are the real and imaginary parts of \( z \). Also, we consider a constant \( L > 0 \) such that for all \( n, \eta_k^2 \leq L, k = 1, \ldots, n \).

**Step 1.** \( m_n(z) - \text{Em}_n(z) \to_{a.s.} 0 \).

Using the notation \( E_k(z) = \mathbb{E}(\text{tr} x_{k+1} \ldots x_n) \), we have

\[
m_n(z) - \text{Em}_n(z) = E_0m_n(z) - \text{Em}_n(z) = \sum_{k=1}^{n} (E_{k-1}m_n(z) - E_km_n(z)) = \frac{1}{p} \sum_{k=1}^{n} (E_{k-1} - E_k)(\text{tr} B_n^{-1} - \text{tr} B_{k,n}^{-1}) = \frac{1}{p} \sum_{k=1}^{n} (E_{k-1} - E_k)\nu_k
\]

where \( \nu_k := \text{tr} B_n^{-1} - \text{tr} B_{k,n}^{-1} \). By using Lemma 2.6 of Silverstein and Bai (1995), we have \( |\nu_k| \leq v^{-1} \). Thus, \( (E_{k-1} - E_k)\nu_k \) forms a bounded martingale difference sequence and applying the Burkholder inequality (Bai and Silverstein, 2010, Lemma 2.12) yields, for any \( q \geq 2 \) and for some \( K_q > 0 \) depending only on \( q \),

\[
\mathbb{E}|m_n(z) - \text{Em}_n(z)|^q \leq K_q p^{-q} \mathbb{E} \left( \sum_{k=1}^{n} |(E_{k-1} - E_k)\nu_k|^2 \right)^{q/2} \leq K_q \left( \frac{2}{v} \right)^q p^{-n/2} \left( \frac{p}{n} \right)^{-q/2}.
\]

By choosing \( q > 2 \), this implies \( m_n(z) - \text{Em}_n(z) \to_{a.s.} 0 \) due to the Borel-Cantelli lemma.

**Step 2.** \( \text{Em}_n(z) \to m(z) \), which satisfies (37).

We define the scalars \( K, \hat{K} \) by

\[
K = \frac{1}{n} \sum_{k=1}^{n} \frac{\eta_k^2}{1 + n^{-1} \text{tr} B_{k,n}^{-1} \eta_k^2}, \quad \hat{K} = \frac{1}{n} \sum_{k=1}^{n} \frac{\eta_k^2}{1 + n^{-1} \text{tr} B_{k,n}^{-1} \eta_k^2}.
\]

Since \( v > 0 \), it directly follows that \( \exists K, \exists \hat{K} < 0 \), hence \( |(K - z)^{-1}| \leq 1/v \) and \( |(\hat{K} - z)^{-1}| \leq 1/v \).

Now, by using the resolvent identity \( A^{-1} - B^{-1} = -A^{-1}(A - B)B^{-1} \), holding for any two invertible square matrices of the same size, we have

\[
(K - z)^{-1} I_p - (B_n - zI_p)^{-1} = \left\{ \frac{1}{n} \sum_{k=1}^{n} (K - z)^{-1} x_k x_k^\top (B_n - zI_p)^{-1} \right\} - (K - z)^{-1} K (B_n - zI_p)^{-1} = \left\{ \sum_{k=1}^{n} \frac{(K - z)^{-1} n^{-1} x_k x_k^\top B_{k,n}^{-1}}{1 + n^{-1} x_k B_{k,n}^{-1} x_k} \right\} - (K - z)^{-1} K (B_n - zI_p)^{-1}
\]

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where the last line uses that

\[
x_k^\top B_k^{-1} = x_k^\top B_k^{-1,n} - \frac{x_k^\top B_k^{-1,n}(n^{-1}x_k x_k^\top) B_k^{-1,n}}{1 + n^{-1} x_k^\top B_k^{-1,n} x_k} = \frac{x_k^\top B_k^{-1,n}}{1 + n^{-1} x_k^\top B_k^{-1,n} x_k}.
\]

Taking the trace and dividing by \( p \) yields

\[
(K - z)^{-1} - \frac{1}{p} \text{tr} B_k^{-1} = \frac{1}{p} \left\{ \sum_{k=1}^{n} \frac{n^{-1}(K - z)^{-1} x_k^\top B_k^{-1,n} x_k}{1 + n^{-1} x_k^\top B_k^{-1,n} x_k} \right\} - \frac{1}{p} (K - z)^{-1} K \text{tr}[B_k^{-1}]
\]

\[
= \frac{1}{p} \left\{ \sum_{k=1}^{n} \frac{n^{-1}(K - z)^{-1} x_k^\top B_k^{-1,n} x_k}{1 + n^{-1} x_k^\top B_k^{-1,n} x_k} \right\} - \frac{1}{p} \left\{ \sum_{k=1}^{n} \frac{n^{-1} \eta_k^2 (K - z)^{-1} \text{tr}[B_k^{-1,n}]}{1 + n^{-1} \text{tr} B_k^{-1,n} \eta_k^2} \right\}
\]

\[
= \frac{1}{p} \sum_{k=1}^{n} \frac{d_k}{1 + n^{-1} x_k^\top B_k^{-1,n} x_k},
\]

where for \( k \in \{1, \ldots, n\},

\[
d_k := n^{-1}(K - z)^{-1} x_k^\top B_k^{-1,n} x_k - n^{-1} \eta_k^2 (K - z)^{-1} \text{tr}[B_k^{-1,n}]
\]

\[
= d_{k1} + d_{k2} + d_{k3},
\]

with

\[
d_{k1} := n^{-1} \eta_k^2 (K - z)^{-1} \text{tr}[B_k^{-1,n}] - n^{-1} \eta_k^2 (K - z)^{-1} \text{tr}[B_k^{-1,n}],
\]

\[
d_{k2} := n^{-1}(K - z)^{-1} x_k^\top B_k^{-1,n} x_k - n^{-1} \eta_k^2 (K - z)^{-1} \text{tr}[B_k^{-1,n}],
\]

\[
d_{k3} := n^{-1}(K - z)^{-1} \text{tr}[B_k^{-1,n}] \cdot \eta_k^2 \left( 1 - \frac{1 + n^{-1} x_k^\top B_k^{-1,n} x_k}{1 + n^{-1} \text{tr} B_k^{-1,n} \eta_k^2} \right).
\]

By using Lemma 2.6 of Silverstein and Bai (1995) and the fact that \(|(K - z)^{-1}| \leq 1/v\), we have

\[
|d_{k1}| \leq \frac{\eta_k^2 |(K - z)^{-1}|}{nv} \leq \frac{L}{nv^2}.
\]

Further, we have \(|d_{k2}| \leq \frac{1}{nv^2} \left| x_k^\top B_k^{-1,n} x_k - \eta_k^2 \text{tr} B_k^{-1,n} \right|\). Thus, from \( E(x_k x_k^\top) = \eta_k^2 I_p \), (36) by using that all singular values of \( B_k^{-1,n} \) are bounded by \( 1/v \),

\[
E[d_{k2}]^2 \leq \frac{1}{nv^2} E \left| x_k^\top B_k^{-1,n} x_k - \eta_k^2 \text{tr} B_k^{-1,n} \right|^2
\]

\[
= \frac{1}{nv^2} \text{Var}(x_k^\top B_k^{-1,n} x_k) = \frac{O(||B_k^{-1,n}||^2)}{n^2 v^4} = O(p) \frac{O(1)}{n^2 v^4} = O(1) \frac{O(1)}{nv^4}.
\]

Now recall from (Couillet and Debbah, 2011, Corollary 3.1), that if \( m \) is the Stieltjes transform of a measure on \( \mathbb{R} \), then for any \( z \in \mathbb{C}^+ \), we have

\[
\left| \frac{1}{1 + m(z)} \right| \leq |z| \left[ \arg(z) \right]^{-1}.
\]

For \( d_{k3} \), by using \(|(K - z)^{-1}| \leq 1/v\), \(|\text{tr} B_k^{-1,n}| \leq p/v\), \( \eta_k^2 \leq L \), and that (41) holds for \( n^{-1} \eta_k^2 \text{tr} B_k^{-1,n} \) as it is a Stieltjes transform, we have

\[
|d_{k3}| \leq \frac{m\eta_k^2}{n^2 v^2} \left| x_k^\top B_k^{-1,n} x_k - \eta_k^2 \text{tr} B_k^{-1,n} \right| \leq \frac{p|z|L}{n^2 v^4} \left| x_k^\top B_k^{-1,n} x_k - \eta_k^2 \text{tr} B_k^{-1,n} \right|.
\]
Thus,
\[
\mathbb{E}[d_{k,j}]^2 \leq \frac{p^2|z|^2L^2}{n^4v^6}\mathbb{E}\left[x_k^\top B_{k,n}^{-1}x_k - \eta_k^2\text{tr} B_{k,n}^{-1}\right]^2 = O\left(\frac{|z|^2L^2}{nv^6}\right). \tag{42}
\]

From (39), (40), and (42), since \(z, L\) are fixed, we have, uniformly over \(k \in \{1, \ldots, n\},\)
\[
|\mathbb{E}d_k|^2 = |\mathbb{E}d_{k1} + \mathbb{E}d_{k2} + \mathbb{E}d_{k3}|^2 \leq 3(\mathbb{E}|d_{k1}|^2 + \mathbb{E}|d_{k2}|^2 + \mathbb{E}|d_{k3}|^2) = O(1/n).
\]

Hence, from (38), by using that (41) holds for \(n^{-1}x_k^\top B_{k,n}^{-1}x_k\), as it is a Stieltjes transform, and since the bound for \(d_k\) is uniform over \(k\),
\[
\left|\mathbb{E}\left[(K - z)^{-1} - \frac{1}{p} \text{tr} B_{n}^{-1}\right]\right| = \frac{1}{\sum_{k=1}^{n} \mathbb{E} \left|\text{tr} B_{k,n}^{-1} - \text{tr} B_{n}^{-1}\right|}
\leq \frac{|z|^2L^4}{n^2v^4} \sum_{k=1}^{n} \mathbb{E} \left|\text{tr} B_{k,n}^{-1} - \text{tr} B_{n}^{-1}\right| \rightarrow 0.
\tag{43}
\]

Next, we have
\[
\left|\mathbb{E}[(K - z)^{-1} - (K - z)^{-1}]\right| \leq \frac{|\hat{K} - K|}{u^2} = \frac{1}{\sum_{k=1}^{n} \mathbb{E} \left|\text{tr} B_{k,n}^{-1} - \text{tr} B_{n}^{-1}\right|}
\leq \frac{|z|^2L^4}{n^2v^4} \sum_{k=1}^{n} \left(\mathbb{E} \left|\text{tr} B_{k,n}^{-1} - \text{tr} B_{n}^{-1}\right| + \mathbb{E} \left|\text{tr} B_{k,n}^{-1} - \text{tr} B_{n}^{-1}\right|\right) \rightarrow 0.
\]

Thus, from (43), we reach
\[
\mathbb{E}\left[(K - z)^{-1} - \frac{1}{p} \text{tr} B_{n}^{-1}\right] = \left(\frac{1}{n} \sum_{k=1}^{n} \frac{\eta_k^2}{1 + n^{-1}\eta_k^2\mathbb{E} \text{tr} B_{n}^{-1}} - z\right)^{-1} - \frac{1}{p} \mathbb{E} \text{tr} B_{n}^{-1} \rightarrow 0. \tag{44}
\]

For each fixed \(z \in \mathbb{C}^+\), \(\mathbb{E}_{m_n}(z) = p^{-1}\mathbb{E} \text{tr} B_{n}^{-1}\) is a bounded sequence. Thus, for any subsequence \(\{n'(a)\}_{a \geq 1}\) of the values taken by \(n\), there is a subsequence \(\{n''(b)\}_{b \geq 1}\) of \(\{n'(a)\}_{a \geq 1}\), such that \(\mathbb{E}_{m_{n''}(b)}(z)\) converges to a limit \(m(z)\) as \(b \rightarrow \infty\).

Now, for all \(t \in [0, L]\) and \(n\)
\[
\left|\frac{t}{1 + n^{-1}t^2\mathbb{E} \text{tr} B_{n}^{-1}} - \frac{t}{1 + \gamma tm}\right| = \left|\frac{\gamma t^2(m - \mathbb{E}_{m_n}(z))}{(1 + n^{-1}tm_n(z))(1 + \gamma tm)}\right| \leq \frac{\gamma L^2|z|^2|m - \mathbb{E}_{m_n}(z)|}{v^2}.
\]

and thus the functions \(f_n(t) = t/(1 + \gamma tm_n(z))\) converge to \(f(t) = t/(1 + \gamma tm(z))\) uniformly over \(t \in [0, L]\), and over the sequence \(\{n'(a)\}_{b \geq 1}\). Then, from (44), by using that the empirical distribution of \((\eta_k^2)_{k=1,\ldots,n}\) converges to the distribution \(H\) on \([0, L]\) (on any sequence, in particular on \(\{n''(b)\}_{b \geq 1}\)), we have, on the sequence \(\{n''(b)\}_{b \geq 1}\)
\[
\frac{1}{n} \sum_{k=1}^{n} \frac{\eta_k^2}{1 + n^{-1}\eta_k^2\mathbb{E} \text{tr} B_{n}^{-1}} \rightarrow \int \frac{t}{1 + \gamma tm} dH(t).
\]

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Further, we have $\exists(\int_1^t \frac{t}{1+\gamma t} \cdot dH(t)) \leq 0$ and $\exists(z) > 0$. Hence $m$ satisfies the equation

$$
\left( \int_1^t \frac{t}{1+\gamma t} \cdot dH(t) - z \right)^{-1} = m.
$$

(45)

We will show in the next step that the solution to (45) is unique. Thus, $E_{m_a}(z)$ converges to a limit which is the unique solution to (45). Combining Step 1, we have $m_a(z) \to_a s.m. \ m(z)$ for any fixed $z \in \mathbb{C}^+$. Finally, applying a standard argument based on Vitali’s convergence theorem (e.g., see the proof of Theorem 2.9 of Bai and Silverstein (2010)) yields $m_a(z) \to_a s.m. \ m(z)$ for all $z \in \mathbb{C}^+$, where for all $z \in \mathbb{C}^+$, $m(z)$ is the unique solution to (45).

**Step 3.** Show (37) has a unique solution in $\mathbb{C}^+$. This step follows immediately as a special case of (Bai and Silverstein, 2010, Proof of Theorem 4.3, Step 3).

C.2 Showing that $N_{\pi}^\top$ satisfies the conditions of Lemma C.1

This section completes the proof of Theorem 3.7 by applying Lemma C.1. Since $N_{\pi}$ has independent columns, we apply the lemma to $N_{\pi}^\top$, which has independent rows. For this, we must show that $N_{\pi}^\top$ satisfies the three conditions of Lemma C.1. The first two conditions are straightforward to verify in this case:

1. The covariance matrix of the $j$-th row of $N_{\pi}^\top$ (i.e., the $j$-th column of $N_{\pi}$) is 

$$
E \left[ (N_{\pi})_j (N_{\pi})_j^\top \right] = E \left[ (\pi_j N_j)(\pi_j N_j)^\top \right] = E \left[ \pi_j N_j N_j^\top \pi_j^\top \right].
$$

Since $\pi_j$ and $N_j$ are independent and $E \left[ N_j N_j^\top \right] = \text{diag} \left( E \left[ |N_{1j}|^2 \right], \ldots, E \left[ |N_{nj}|^2 \right] \right)$, we have

$$
E \left[ \pi_j N_j N_j^\top \pi_j^\top \right] = \left[ \pi_j \text{diag} \left( E \left[ |N_{1j}|^2 \right], \ldots, E \left[ |N_{nj}|^2 \right] \right) \pi_j^\top \right]
$$

$$
= E \left[ \sum_{m=1}^n E \left( |N_{mj}|^2 \right) \cdot (\pi_j)_{m}(\pi_j)_{m}^\top \right] = \sum_{m=1}^n E \left( |N_{mj}|^2 \right) \cdot E \left[ (\pi_j)_{m}(\pi_j)_{m}^\top \right].
$$

Finally, $E \left[ (\pi_j)_{m}(\pi_j)_{m}^\top \right] = (1/n) I_n$ since $\pi_j$ is uniform over all permutations, so we have

$$
E \left[ (N_{\pi})_j (N_{\pi})_j^\top \right] = \sum_{m=1}^n E \left( |N_{mj}|^2 \right) \cdot E \left[ (\pi_j)_{m}(\pi_j)_{m}^\top \right] = \sum_{m=1}^n E \left( |N_{mj}|^2 \right) \cdot \frac{1}{n} I_n = v_j I_n.
$$

2. The row variances $v_1, \ldots, v_p$ have an empirical distribution converging to $H$ by assumption. Moreover, since the entries of $N$ have uniformly bounded fourth moments, it follows that

$$
\max_{j=1,\ldots,p} v_j = \max_{j=1,\ldots,p} \left[ \frac{1}{n} \sum_{m=1}^n E |N_{mj}|^2 \right] \leq \max_{j=1,\ldots,p} E |N_{mj}|^2 \leq \max_{j=1,\ldots,p} \frac{1}{n} \sum_{m=1}^n E |N_{mj}|^4,
$$

is also uniformly bounded, i.e., $v_1, \ldots, v_p$ are uniformly bounded.

It now remains to establish the third condition, i.e., to bound the variance of the quadratic form (36). This condition controls the amount of dependence and is more involved.

3. For convenience, let $x_k = (N_{\pi})_k \in \mathbb{R}^n$ denote the $k$-th row of $N_{\pi}^\top$, let $T_{ik} = \sqrt{E|N_{ik}|^2}$ denote the standard deviation of $N_{ik}$, and let $\eta_k = \sqrt{\eta}$ denote the standard deviation for the $k$-th row of $N_{\pi}^\top$. Now, note that

$$
\text{Var}(x_k^\top A x_k) = E (x_k^\top A x_k - E x_k^\top A x_k)^2 = E (x_k^\top A x_k - E x_k^\top A x_k)(x_k^\top A x_k - E x_k^\top A x_k)^* = E (x_k^\top A x_k x_k^* x_k - E x_k^\top A x_k \cdot E x_k^\top A^* x_k).
$$

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where these expectations are all with respect to both the randomness in the noise \(N\) and the random permutations \(\pi\). By using the independence of the coordinates of \(x_k\), as well as the symmetry of \(A\), we find

\[
E[x_k^\top Ax_k x_k^\top A^* x_k] = \sum_{i,j,l,m} A_{ij} A_{lm}^* E(x_{ki} x_{kj} x_{lk} x_{km})
\]

\[
= \left( \sum_{i=j=l=m} + \sum_{i=j \neq l=m} + \sum_{i=l \neq j=m} + \sum_{i=m \neq j=l} \right) A_{ij} A_{lm}^* E(x_{ki} x_{kj} x_{lk} x_{km})
\]

\[
= \sum_{i} |A_{ii}|^2 E(x_{ki}^4) + \sum_{i \neq l} (A_{ii} A_{ll}^* + 2|A_{il}|^2) E(x_{ki}^2 x_{kl}^2).
\]

For \(i \neq l\), we have

\[
E(x_{ki}^2 x_{kl}^2) = \frac{\sum_{i \neq j} T_{ik}^2 T_{lk}^2}{n(n-1)} = \frac{(\sum_i T_{ik}^2)^2 - \sum_i T_{ik}^4}{n(n-1)} = \frac{n^2 \eta_k^4 - \sum_i T_{ik}^4}{n(n-1)} =: M.
\]

Thus,

\[
E \left[ |x_k^\top Ax_k|^2 \right] = \sum_i |A_{ii}|^2 E(x_{ki}^4) + \sum_{i \neq l} (A_{ii} A_{ll}^* + 2|A_{il}|^2) M
\]

\[
= \sum_i |A_{ii}|^2 (E(x_{ki}^4) - M) + \left( \sum_i |A_{ii}|^2 + \sum_{i \neq l} 2|A_{il}|^2 \right) M.
\]

Similarly, by using \(E(x_{ki}^2) = n^{-1} \sum_i T_{ik}^2 = \eta_k^2\) we have

\[
E x_k^\top A x_k \cdot E x_k^\top A^* x_k = \sum_i |A_{ii}|^2 \left[ E(x_{ki}^2) \right]^2 + \sum_{i \neq l} A_{ii} A_{ll}^* E(x_{ki}^2) E(x_{kl}^2)
\]

\[
= \sum_i \eta_k^4 |A_{ii}|^2 + \sum_{i \neq l} \eta_k^4 A_{ii} A_{ll}^* = \eta_k^4 \sum_i |A_{ii}|^2.
\]

By putting these together, we have

\[
\text{Var}(x_k^\top Ax_k) = \sum_i |A_{ii}|^2 \left[ E(x_{ki}^4) - \eta_k^4 - M \right] + \sum_i |A_{ii}|^2 \left[ M - \eta_k^4 \right] + \sum_{i \neq j} 2|A_{ij}|^2 M.
\]

For the first term, by using the assumptions that the entries of \(N\) have uniformly bounded fourth moments and the entries of \(\eta\) are uniformly bounded, we have

\[
\sum_i |A_{ii}|^2 \left[ E(x_{ki}^4) - \eta_k^4 - M \right] \lesssim \sum_i |A_{ii}|^2.
\]

For the second and last terms,

\[
|M - \eta_k^4| = \left| \frac{\eta_k^4 - \sum_i T_{ik}^4}{n(n-1)} \right| = O(1/n), \quad \left| \sum_{i \neq j} 2|A_{ij}|^2 M \right| \lesssim \sum_{i \neq j} |A_{ij}|^2.
\]

Thus,

\[
\text{Var}(x_k^\top Ax_k) \lesssim \sum_i |A_{ii}|^2 + \frac{1}{n} \sum_i |A_{ii}|^2 + \sum_{i \neq j} |A_{ij}|^2 = \|A\|^2_F + \|A\|^2_F/2.
\]

Moreover, \(|\text{tr} A|^2 = \|A\|^2_F \leq n \sum_{i=1}^n |a_{ii}|^2 \leq n \sum_{i=1}^n |a_{ii}|^2 \leq n\|A\|^2_F\). Hence, \(\text{Var}(x_k^\top Ax_k) \lesssim \|A\|^2_F\).
Thus, we have shown that $\mathbf{N}_\pi^T$ satisfies all the conditions of Lemma C.1 and so we have from Lemma C.1 that $p^{-1}\mathbf{N}_\pi^T\mathbf{N}_\pi^T$ has a limiting spectral distribution defined by the unique Stieltjes transform that satisfies (37). From properties of the Stieltjes transform, it follows that $\mathbf{N}_\pi^T\mathbf{N}_\pi^T/n$ has a limiting spectral distribution defined by the unique Stieltjes transform that satisfies (35). Namely, the empirical singular value distributions of $\mathbf{N}_\pi/\sqrt{n}$ and $\mathbf{N}$ both converge to the same generalized Marčenko-Pastur distribution. This finishes the proof.

D Simulations with $n \ll p$

This section repeats the experiments from Sections 4.1 to 4.3 for a higher dimensional setting with $n \ll p$, specifically with $n = 60$ and $p = 5000$. We consider the same methods as before, with the exception of BEMA, which took too long to run.

Fig. 11 provides the analogue of Fig. 5 from Section 4.1. PermPA, BEMA0, Biwhitening, and FlipPA were again highly effective once $\theta$ was large enough, i.e., once the signal rose above the noise, and they estimated the rank correctly in most of the runs. BCF, GIC, and ACT dramatically over-estimated the rank across the entire range in this experiment; they selected all or nearly all the components. For $\theta = 0$, BEMA0 rejected the pure noise null hypothesis in 4 of the 100 trials (achieving an empirical type I error rate of 4%); Biwhitening rejected the null in 3 of the 100 trials (achieving an empirical type I error rate of 3%); PermPA and FlipPA both rejected the null in 1 of the 100 trials (achieving empirical type I error rates of 1%); and the remaining methods (BCF, GIC, and ACT) all rejected the null in all of the 100 trials (achieving empirical type I error rates of 100%).

Fig. 12 provides the analogue of Fig. 6 from Section 4.2, where here $\theta = 12$, $n_1 = n_2 = 30$, $p_1 = 4000$, and $p_2 = 1000$. With the exceptions of BCF, GIC, and ACT (all of which dramatically over-estimated the rank again), the remaining methods (PermPA, BEMA0, Biwhitening, and FlipPA) performed similarly to the lower dimensional setting in Fig. 6. They were highly effective when $\Delta$ was small, but only FlipPA and Biwhitening remained effective as $\Delta$ grew and the noise became more heteroscedastic. PermPA and BEMA0 again overestimated the rank as $\Delta$ grew; notably, their performance degraded more rapidly here than in Fig. 6.

Fig. 13 provides the analogue of Fig. 7 from Section 4.3, where here $\theta = 48$, $n_1 = n_2 = 30$, $p_1 = 4000$, $p_2 = 1000$, $b_1 = 3$, and $b_2 = 250$. As in the lower dimensional setting of Fig. 7, a few methods (PermPA,
Figure 12: Higher-dimensional analogue of Fig. 6 from Section 4.2, where here $n = 60$ and $p = 5000$. Performance across 100 runs is shown for each method for a rank-one signal in noise having a block-structured noise variance profile (7), where the amount of heteroscedasticity increases as $\Delta$ increases from zero (homoscedastic noise) to one (maximal heteroscedasticity). The left plot shows the average selected rank across the runs $E[\hat{k}]$; the second column of plots shows what proportion of runs resulted in over-estimation $Pr[\hat{k} > 1]$, correct estimation $Pr[\hat{k} = 1]$, and under-estimation $Pr[\hat{k} < 1]$. BCF, GIC, and ACT do not appear in the left plot because their averages are close to 60 for the entire sweep.

Figure 13: Higher-dimensional analogue of Fig. 7 from Section 4.3, where here $n = 60$ and $p = 5000$. Performance across 100 runs is shown for each method for a rank-one signal in noise having a block-structured noise variance profile with blockwise dependence, where the amount of dependence increases as $\gamma$ increases from zero (independent entries) to $1/2$ (increasing blockwise dependence). The left plot shows the average selected rank across the runs $E[\hat{k}]$; the second column of plots shows what proportion of runs resulted in over-estimation $Pr[\hat{k} > 1]$, correct estimation $Pr[\hat{k} = 1]$, and under-estimation $Pr[\hat{k} < 1]$. BCF, GIC, and ACT do not appear in the left plot because their averages are all above 35 for the entire sweep; in fact BCF and GIC are close to 60 for the entire sweep.
Figure 14: Higher-dimensional analogue of Fig. 8 from Section 4.3, where here \( n = 60 \) and \( p = 5000 \). Performance is shown for the same setting as Fig. 13 across 100 runs of each method with prewhitening using the estimates \( \hat{\Sigma}_1, \hat{\Sigma}_2 \). The left plot shows the average selected rank across the runs \( E[\hat{k}] \); the second column of plots shows what proportion of runs resulted in over-estimation \( \Pr[\hat{k} > 1] \), correct estimation \( \Pr[\hat{k} = 1] \), and under-estimation \( \Pr[\hat{k} < 1] \). BCF and GIC do not appear in the left plot because their averages are close to 60 for the entire sweep.

Biwhitening, FlipPA, and BlockFlipPA) were effective when \( \gamma \) was small, but only BlockFlipPA remained effective across the entire sweep. The rest dramatically over-estimated the rank across the entire sweep. Interestingly, FlipPA was significantly more robust to the growing dependence here than it was in the lower dimensional setting in Fig. 7.

Fig. 14 provides the analogue of Fig. 8 from Section 4.3, where here \( \theta = 48 \), \( n_1 = n_2 = 30 \), \( p_1 = 4000 \), \( p_2 = 1000 \), \( b_1 = 3 \), and \( b_2 = 250 \). In contrast to the lower dimensional setting of Fig. 7, prewhitening did not significantly improve the performance of most of the methods. BCF, GIC, ACT, and BEMA0 continued to dramatically over-estimate the rank. Biwhitening actually performed worse with prewhitening than without, perhaps due to poor estimation of the prewhitening matrices in this higher dimensional setting. Interestingly, the performance of PermPA and FlipPA improved with prewhitening for large values of \( \gamma \), but FlipPA performed worse with prewhitening for small values of \( \gamma \). Only BlockFlipPA was effective across the sweep.

E Selection and preprocessing for astronomy data

Here we describe the selection and preprocessing steps taken to produce the dataset used in Section 5 and illustrated in Fig. 9a; it is essentially the same as the steps in (Hong et al., 2023, Section SM5) except that here we do not remove spectra with highly heterogeneous variances. Specifically, the dataset was formed as follows:

1. Select spectra from DR16Q that satisfy the following conditions:
   - SURVEY = "eboss",
   - PLATEQUALITY = "good",
   - redshift: \( 2.0 < Z < 2.1 \),
   - BAL_PROB < 0.2,
   - the rest frame wavelengths measured cover the range 1280–1820 without missing entries (i.e., without entries for which IVAR = 0).
2. Form a data vector $\mathbf{y}_i \in \mathbb{R}^p$ and an associated variance vector $\mathbf{v}_i \in \mathbb{R}^p$ for each of the $\tilde{n} = 10052$ selected spectra by linearly interpolating FLUX and $1 \odot$ IVAR to obtain entries for the $p = 1080$ rest frame wavelengths $\text{LAMREST} = (1280, 1280.5, \ldots, 1820) \in \mathbb{R}^p$.

3. Center each spectrum, i.e., $\mathbf{y}_i \leftarrow \mathbf{y}_i - \frac{1}{n} \mathbf{1}_p \mathbf{y}_i$ for $i = 1, \ldots, \tilde{n}$.

4. Normalize each spectrum so that its average value for rest frame wavelengths inside the range $1525$–$1575$ is $\pm 1$, i.e., for $i = 1, \ldots, \tilde{n}$,
   
   (a) $\sigma_i \leftarrow |\text{mean}(\mathbf{y}_i(1525 < \text{LAMREST} < 1575))|$,  
   
   (b) $\mathbf{y}_i \leftarrow \mathbf{y}_i / \sigma_i$,  
   
   (c) $\mathbf{v}_i \leftarrow \mathbf{v}_i / \sigma_i^2$.

5. Sort the spectra in increasing order of their average noise variance profiles $(\frac{1}{n}) \mathbf{v}_i$.

6. Select the $n = 5000$ final (i.e., noisiest) spectra that remain after first dropping the 80 final (i.e., noisiest) spectra.

7. Stack the selected vectors: $\mathbf{Y} = [\mathbf{y}_1^\top; \ldots; \mathbf{y}_n^\top] \in \mathbb{R}^{n \times p}$, $\mathbf{V} = [\mathbf{v}_1^\top; \ldots; \mathbf{v}_n^\top] \in \mathbb{R}^{n \times p}$. 

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