De-biased sparse PCA: Inference and testing for eigenstructure of large covariance matrices

Jana Janková  Sara van de Geer

Seminar for Statistics
ETH Zürich

Abstract

Sparse principal component analysis (sPCA) has become one of the most widely used techniques for dimensionality reduction in high-dimensional datasets. The main challenge underlying sPCA is to estimate the first vector of loadings of the population covariance matrix, provided that only a certain number of loadings are non-zero. In this paper, we propose confidence intervals for individual loadings and for the largest eigenvalue of the population covariance matrix. Given an independent sample $X^i \in \mathbb{R}^p, i = 1, \ldots, n$, generated from an unknown distribution with an unknown covariance matrix $\Sigma_0$, we study estimation of the first vector of loadings in a setting where $p \gg n$. Next to the high-dimensionality, another challenge lies in the inherent non-convexity of the problem. We base our methodology on a Lasso-penalized M-estimator which, despite non-convexity, may be solved by a polynomial-time algorithm such as coordinate or gradient descent. We show that our estimator achieves the minimax optimal rates in $\ell_1$ and $\ell_2$-norm. We identify the bias in the Lasso-based estimator and propose a de-biased sparse PCA estimator for the vector of loadings and for the largest eigenvalue of the covariance matrix $\Sigma_0$. Our main results provide theoretical guarantees for asymptotic normality of the de-biased estimator. The major conditions we impose are sparsity in the first eigenvector of small order $\sqrt{n}/\log p$ and sparsity of the same order in the columns of the inverse Hessian matrix of the population risk.

Keywords: covariance matrix, eigenvectors, eigenvalues, PCA, high-dimensional model, sparsity, Lasso, asymptotic normality, confidence intervals.
1 Introduction

1.1 Background and problem

Principal component analysis (PCA) is a fundamental technique employed for a multitude of tasks including dimension reduction, data visualization and clustering. The applications of PCA range from genomics to image recognition, data compression and financial econometrics. While in low-dimensional settings, PCA is generally well-understood (see e.g. Anderson [1963]), estimation of eigenstructure in high-dimensional settings has opened many intriguing questions. Consequently, the problem has attracted substantial interest in the recent decades, see, for example Baik and Silverstein [2006]; Paul [2007]; Johnstone and Lu [2009]; Amini and Wainwright [2009]; Vu and Lei [2012]; Birnbaum et al. [2013]; Berthet and Rigollet [2013]; Cai et al. [2013].

The key challenge underlying the principal component analysis is to estimate the eigenstructure of an unknown population covariance matrix. In a typical setting, we observe a data matrix $X$ with independent rows $X_i \in \mathbb{R}^p, i = 1, \ldots, n$, generated from a $p$-dimensional distribution. Without loss of generality, we assume that $E X_i = 0$. The population covariance matrix will be denoted by $\Sigma_0 := E X^i (X^i)^T \in \mathbb{R}^{p \times p}$. In this paper, we study estimation and inference for the first loadings vector of the population covariance matrix $\Sigma_0$, defined by

$$\beta_0 := \argmin_{\beta \in \mathbb{R}^p} \frac{1}{4} \left\| \Sigma_0 - \beta \beta^T \right\|_F^2,$$

where $\| \cdot \|_F$ is the Frobenius norm of a matrix. The loadings vector $\beta_0$ is an eigenvector of $\Sigma_0$ that satisfies $\| \beta_0 \|_2^2 = \Lambda_{\text{max}}(\Sigma_0)$, where $\Lambda_{\text{max}}(\Sigma)$ denotes the largest eigenvalue of a real symmetric matrix $\Sigma$ and $\| \cdot \|_2$ the Euclidean norm. It defines the best rank-one approximation $\beta_0 \beta_0^T$ to the matrix $\Sigma_0$. We remark that $\beta_0$ is only identifiable up to a sign (meaning that $-\beta_0$ is also a global minimizer), thus we may choose this sign arbitrarily.

The eigenstructure of the population covariance matrix can be naturally estimated by the eigenstructure of the sample covariance matrix

$$\hat{\Sigma} := \frac{1}{n} \sum_{i=1}^{n} X_i (X_i)^T.$$

When the dimension $p$ of the observations is fixed, distributional properties of eigenvalues and eigenvectors of the sample covariance matrix are well understood: they are consistent estimators of their population counterparts and have a Gaussian limiting distribution (Anderson [1963], Kollo and Neudecker [1997]). If $\hat{\beta}_{\text{PCA}}$ is the first eigenvector of $\hat{\Sigma}$ rescaled such that $\| \hat{\beta}_{\text{PCA}} \|_2^2 = \Lambda_{\text{max}}(\hat{\Sigma})$, then under certain regularity conditions on the eigenvalues of $\Sigma_0$

$$\sqrt{n}(\hat{\beta}_{\text{PCA}} - \beta_0) \Rightarrow \mathcal{N}_p(0, V),$$

$$\sqrt{n}(\Lambda_{\text{max}}(\hat{\Sigma}) - \Lambda_{\text{max}}(\Sigma_0)) \Rightarrow \mathcal{N}(0, \sigma^2 \Lambda),$$
where \( V \) and \( \sigma^2 \) are certain asymptotic variances depending on the distribution of \( X \).

In a high-dimensional regime, when \( p \) is allowed to grow with the sample size, the sample covariance matrix exhibits poor behaviour: Bai and Yin [1993] show that the eigenvalues of \( \hat{\Sigma} \) are inconsistent estimators of their population counterparts. Namely if \( p/n \to \alpha \in (0, \infty) \), then, almost surely

\[
\lim_{n \to \infty} \Lambda_{\text{max}}(\hat{\Sigma}) = \Lambda_{\text{max}}(\Sigma_0)(1 + \sqrt{\alpha})^2.
\]

In the same regime, Johnstone [2001] shows an analogous statement for the sample eigenvectors. In particular, even in a simple model known as the spiked covariance model (studied in numerous works including Johnstone and Lu [2009], Amini and Wainwright [2009], Deshpande and Montanari [2014]) the sample eigenvectors can be asymptotically perpendicular to the population eigenvectors with high probability. More precisely, if \( \Sigma_0 = I + (\Lambda - 1)uu^T \), with \( u^Tu = 1 \), \( \Lambda \geq 1 \) and under technical conditions, as \( p/n \to \alpha > 0 \), then almost surely,

\[
\frac{\hat{u}^Tu_1}{\|\hat{u}\|_2\|u_1\|_2} \to \begin{cases} 
0 & \text{if } \Lambda - 1 \leq \sqrt{\alpha} \\
\frac{1-\alpha/(\Lambda-1)^2}{1+\alpha/(\Lambda-1)^2} & \text{if } \Lambda - 1 > \sqrt{\alpha},
\end{cases}
\] (1)

where \( \hat{u} \) is the first eigenvector of \( \hat{\Sigma} \) and \( u_1 \) is the first eigenvector of \( \hat{u} \). These results show the inconsistency of \( \hat{u} \), however, note that they also suggest that consistent estimation might be possible if \( \alpha/(\Lambda - 1)^2 \to 0 \), that is if the gap between the largest and second largest eigenvalue of \( \Sigma_0 \), \( \Lambda - 1 \), grows at least as fast as \( \sqrt{p/n} \). This special but interesting setting has recently attracted substantial interest and we will remark on it in Section 1.3 on related literature.

The above results show that consistent estimation of eigenstructure in high-dimensional settings is not possible without further structural assumptions. However, in many applications, it is inevitable that the number of variables \( p \) is of the same order or even much larger than the sample size \( n \). This motivated research in sparse settings, where the first few population eigenvectors are assumed to only have a certain number of entries non-zero. Examples of settings where sparse representations are relevant include micro-array studies in genetics or EEG studies of the heart, where the heart-beat cycle may be expressed in a sparse wavelet basis (see Johnstone and Lu [2009]). Under sparsity conditions, consistent estimation of the eigenstructure becomes possible. A large body of literature studies methodology and lower bounds for estimation of the population eigenstructure. A simple and popular methodology is based on thresholding of the sample covariance matrix, which was investigated mostly within the spiked covariance model [Johnstone and Lu, 2009; Amini and Wainwright, 2009; Deshpande and Montanari, 2014]. Methods exploiting Lasso penalization were studied among others in Jolliffe et al. [2003] and Zou et al. [2006]; these however lead to non-convex problems which pose computational difficulties. The paper d’Aspremont et al. [2007] addresses the non-convexity problem by deriving a semidefinite programming-based relaxation for the Lasso-penalized principal component analysis, which was later extended by Vu et al.
Important work on lower bounds for estimation of eigenstructure includes Vu and Lei [2012], Berthet and Rigollet [2013] and Cai et al. [2013]. In particular, Vu and Lei [2012] propose an estimator \( \hat{Z} \) of \( u_1 u_1^T \) which achieves the minimax rate, namely, with probability tending to one,

\[
\| \hat{Z} - u_1 u_1^T \|_F^2 \leq \frac{C}{(\Lambda_1 - \Lambda_2)^2} s \lambda^2.
\]  

(2)

where \( s := \|u_1\|_0 \) is the sparsity of the first eigenvector, \( \lambda \approx \sqrt{\log p/n} \) and \( C \) is a universal constant. The estimator \( \hat{Z} \) is not computable in polynomial time, however, they propose a polynomial-time estimator which achieves a somewhat slower rate, namely \( s^2 \lambda^2 \). To achieve the minimax rate with a polynomial-time algorithm may be impossible, see Berthet and Rigollet [2013].

The literature on estimation of eigenstructure in high-dimensional settings is vast and provides a wide variety of sparsity-inducing estimators. However, these methods do not lead to methodology for inference such as confidence intervals and tests. To the best of our knowledge, asymptotically normal estimation of eigenstructure has yet not been investigated in sparse high-dimensional regimes. We aim to contribute to filling this practical and theoretical gap, in particular, we address construction of confidence intervals for entries of the first loadings vector \( \beta_0 \) and the largest eigenvalue of \( \Sigma_0 \).

1.2 Outline of methodology, results and contributions

We briefly summarize the main contributions of this paper. We base our construction of asymptotically normal estimators of \( \beta_0 \) on a Lasso-regularized M-estimation procedure of type

\[
\hat{\beta} \in \arg\min_{\beta \in B} \frac{1}{4} \| \hat{\Sigma} - \beta \beta^T \|_F^2 + \lambda \| \beta \|_1,
\]

(3)

where \( \| \cdot \|_1 \) is the \( \ell_1 \)-norm and \( B \) is a certain local set that guarantees convexity of the population loss function. The local set will be obtained from an initial rough estimator. We will then show in Theorem 1 that any stationary point of the program (3) is a near-oracle estimator of \( \beta_0 \) and that it achieves near-oracle rates in \( \ell_2 \)-norm, namely \( \| \hat{\beta} - \beta_0 \|_2^2 = O_P(s \log p/n) \). Since we use localization first, we are able to achieve the minimax rates (2) even with a polynomial-time algorithm.

The estimator \( \hat{\beta} \) is asymptotically biased; consequently, we identify the bias term and propose methodology to estimate it, which leads to a de-biased estimator. Our main theoretical results in Theorem 2 show that a de-biased sparse PCA estimator leads to asymptotically normal estimators for the entries of the first loadings vector \( \beta_0 \). We also propose an estimator for the largest eigenvalue of \( \Sigma_0 \) and provide theoretical guarantees on the limiting distribution in Theorem 3. Moreover, the asymptotic variance of the Gaussian limiting distribution corresponds to the asymptotic variance of asymptotically efficient estimation in the low-dimensional setting. An implication of our work is that we require the
sparsity condition is \( s = o(\sqrt{n}/\log p) \) in \( \beta_0 \) and sparsity in the inverse Hessian matrix of the population risk at \( \beta_0 \).

In an empirical study, we show that our method performs well even when the classical PCA fails, the gain is especially visible in regimes when \( p \) is of the same order as \( n \) and the eigenvalue gap is relatively small.

### 1.3 Related literature

In this section, we discuss prior related work and outline the differences to our settings and results. The recent papers Fan and Wang [2015] and the line of papers Koltchinskii et al. [2016], Koltchinskii et al. [2017], Koltchinskii and Lounici [2017] and Koltchinskii et al. [2017], study asymptotically normal estimation of eigenstructure in high-dimensional settings. However, their setting and results substantially differs from ours. Their setting essentially requires that the maximum eigenvalue or the eigenvalue gap diverges (see the comment following equation (1) above). Therefore, thanks to this structural assumption, the papers Koltchinskii et al. [2016] and Fan and Wang [2015] manage to study the high-dimensional setting \( p \gg n \) and do not require any sparsity conditions. We study the setting where the eigenvalue gap may be even very small, thus our situation becomes more difficult, which requires that we impose sparsity conditions.

We briefly discuss their contributions below. The paper Koltchinskii et al. [2016] derives the asymptotic distribution of the leading sample eigenvector of the sample covariance matrix in a setting where \( p \) is allowed to grow with the sample size. This is established under the “effective rank” condition \( \Lambda_{\text{max}}(\Sigma_0) \gg \text{tr}(\Sigma_0)/n \), where \( \Lambda_{\text{max}}(\Sigma_0) \) is the maximum eigenvalue of \( \Sigma_0 \) and under a Gaussianity assumption. They show that in this setting the leading eigenvector is biased. The paper then proposes a way of estimating this bias via sample splitting and constructs a de-biased estimator which is asymptotically normal. Interestingly, their results imply that in special high-dimensional settings where the effective rank condition holds, consistent estimation is possible even if \( p/n \to \infty \), without imposing sparsity assumptions.

The paper Fan and Wang [2015] (see also a related paper Shen et al. [2013]) provides similar results as Koltchinskii et al. [2016], but considers the spiked covariance model. In particular, it is required that the first \( d \) eigenvalues of \( \Sigma_0 \) diverge to infinity (denoting the eigenvalues by \( \Lambda_j, j = 1, \ldots, d \), they must satisfy the condition \( \Lambda_j \geq \sqrt{p/n} \)) and the non-spiked eigenvalues are assumed to be bounded. This means that the eigenvalue gap (the difference between the smallest eigenvalue in the spiked part and the largest eigenvalue in the non-spiked part) must grow at least at the rate \( \sqrt{p/n} \). Under this condition and a sub-Gaussianity condition, they derive the asymptotic distribution of the first \( d \) eigenvalues and the corresponding eigenvectors of the sample covariance matrix. Similarly as in Koltchinskii et al. [2016], their results reveal a bias in the asymptotic distribution, in particular the spiked eigenvalues \( \Lambda_j(\hat{\Sigma}) \) of \( \hat{\Sigma} \) satisfy,
for \( j = 1, \ldots, d, \)

\[
\sqrt{n} \left[ \frac{\Lambda_j(\hat{\Sigma})}{\Lambda_j} - 1 - \left( \frac{C_p}{n \Lambda_j} + O_P \left( \frac{1}{n} \right) \right) \right] \xrightarrow{\Pr} N(0, \kappa_j - 1), \quad (4)
\]

where \( \kappa_j \) is a certain measure of kurtosis. The asymptotic bias term is \( \frac{C_p}{n \Lambda_j} \), where the constant \( C \) is unknown. The authors propose a shrinkage estimator based on soft-thresholding which also involves a bias correction based on equation (4), and the unknown \( C \) is replaced by a consistent estimator.

1.4 Organization of the paper

We discuss the properties and non-convexity of the population risk function in Section 2 a propose a first-step estimator which is guaranteed to reach a local neighbourhood of the true underlying parameter where the population risk function is convex. In Section 3, we provide the main methodology for an oracle estimator of the first loadings vector and asymptotically normal estimators of the loadings vector and the maximum eigenvalue of \( \Sigma_0 \), and establish our main theoretical results. In Section 4, we investigate the performance of our methodology in an empirical study. Section 5 discusses conclusions and implications and the proofs are deferred to Section 6.

1.5 Notation

For a vector \( x \in \mathbb{R}^d \), we let \( x_j \) denote its \( j \)-th entry. For a matrix \( A \in \mathbb{R}^{m \times d} \) we use the notation \( A_{ij} \) or \((A)_{ij}\) for its \((i,j)\)-th entry and \( A_j \) to denote its \( j \)-th column. We let \( \|A\|_\infty = \max_i \|e_i^T A\|_1 \), where \( e_i \) is the \( i \)-th unit vector, \( \|A\|_1 = \|A^T\|_\infty \), \( \|A\|_\infty = \max_{i,j} |A_{ij}| \) and the Frobenius norm is denoted by \( \|A\|_F = (\sum_{i,j} A_{ij}^2)^{1/2} \). By \( \Lambda_{\min}(A) \) and \( \Lambda_{\max}(A) \) we denote the minimum and maximum eigenvalue of \( A \), respectively. For sequences of random variables \( X_n, Y_n \), we write \( X_n = O_P(Y_n) \) if \( X_n/Y_n \) is bounded in probability. We write \( X_n = o_P(1) \) if \( X_n \) converges to zero in probability and we use \( \sim \) to denote convergence in distribution.

2 Preliminaries

2.1 Landscape of population risk and non-convexity

In this section, we introduce the setup and develop methodology to obtain an initial estimator of the vector of loadings \( \beta_0 \) in a high-dimensional setting, under a sparsity assumption on the entries of \( \beta_0 \). The main methodology for construction of an asymptotically normal estimator is given in Section 3.

The spectral decomposition of \( \Sigma_0 \) is given by

\[
\Sigma_0 = U^T \Phi^2 U,
\]
where $\Phi := \text{diag}(\phi_1, \ldots, \phi_p)$ and we assume that

$$\phi_1 > \phi_2 \quad \text{and} \quad \phi_2 \geq \cdots \geq \phi_p \geq 0,$$

and $U = (u_1, \ldots, u_p)$ is such that $UU^T = I$. Note that while $\Phi$ is unique, the matrix $U$ is in general not unique if the eigenvalues have multiplicities. We do not require that $U$ is unique, however, we require that the first eigenvector $u_1$ is unique (up to a sign): this is the case if $\phi_1 > \phi_2$. The eigenvalues of $\Sigma_0$ will be denoted by $\Lambda_j := \phi_j^2$ for $j = 1, \ldots, p$. We also use the alternative notations $\phi_{\text{max}} := \phi_1$ and $\Lambda_{\text{max}} := \Lambda_1$. The gap between the square-root of the largest and second largest eigenvalue of $\Sigma_0$ will be denoted by

$$\rho := \phi_1 - \phi_2.$$

Note that this definition also implies that $\Lambda_1 - \Lambda_2 = (\phi_1 - \phi_2)(\phi_1 + \phi_2) = \rho^2 + 2\rho\phi_2 \geq \rho^2$. We will refer to both $\rho$ and $\Lambda_1 - \Lambda_2$ as the “eigenvalue gap”, depending on the context. The eigenvalue gap determines the curvature of the population risk and thus naturally plays an intrinsic role in estimation of the related eigenspaces: if the eigenvalue gap vanishes too fast, consistent estimation of the first eigenvector becomes impossible.

Our main methodologies are based on the (regularized) M-estimation framework. To this end, we consider the theoretical risk function

$$R(\beta) := \frac{1}{4} \|\Sigma_0 - \beta \beta^T\|^2_F = \frac{1}{4} \text{tr}(\Sigma_0) - \frac{1}{2} \beta^T \Sigma_0 \beta + \frac{1}{4} \|\beta\|_2^4.$$

The risk function is plotted in Figure 1 for the simple case $p = 2$.

![Figure 1: A toy example: the graph (left) and contours (right) of the population risk for $p = 2$. The two global minima are labeled by red points, the two saddle points by blue points. The blue circles in the contour plot show the convex local neighbourhood from Lemma 1 below.](image)

The gradient $\hat{R}(\beta)$ and the Hessian $\hat{\hat{R}}(\beta)$ of $R(\beta)$ are given by

$$\hat{R}(\beta) = -\Sigma_0 \beta + \|\beta\|_2^2 \beta,$$

and $\hat{\hat{R}}(\beta)$ is given by

$$\hat{\hat{R}}(\beta) = -\Sigma_0 + \|\beta\|_2^2 I.$$
\[ \tilde{R}(\beta) = -\Sigma_0 + \|\beta\|^2 I + 2\beta\beta^T. \]

We consider the empirical analogue of \( R(\beta) \), the empirical risk function

\[ R_n(\beta) = \frac{1}{4}\|\tilde{\Sigma} - \beta\beta^T\|_F. \]

The gradient and Hessian of \( R_n \) will be denoted by \( \dot{R}_n(\beta) \) and \( \ddot{R}_n(\beta) \), respectively. This choice of a risk function allows us to formulate estimation of \( \beta_0 \) in the M-estimation framework. However, a simple naive approach via minimizing the empirical risk \( R_n(\beta) \) is plagued by non-convexity: even the population risk \( R(\beta) \) itself is a non-convex function on \( \mathbb{R}^p \). If \( \phi_1 > \phi_2 \), the population risk has a unique (up to sign) global minimizer \( \phi_1 u_1 = \beta_0 \), however, it is well known that computing the global minimizer of a non-convex function is a difficult problem. It is easy to deduce that the population risk has stationary points which are given by \( \pm \phi_j u_j \), \( j = 1, \ldots, p \), where \( u_j \) is any normalized eigenvector corresponding to \( \phi_j \) or \( u_j \) is the zero vector. Thus, the population risk might have a continuum of stationary points (consider e.g. the degenerate case \( \Sigma_0 = \mathbb{I} \): the stationary points form a sphere if we disregard the zero vector). In the simple case when there are no eigenvalue multiplicities, there are \( 2p + 1 \) stationary points: the points \( \pm \phi_1 u_1 \) are the global minimizers and one can easily deduce that the remaining stationary points (except zero) are all saddle points by inspecting the Hessian matrix

\[ \ddot{R}(\phi_j u_j) = \sum_{i=1}^p (\Lambda_j - \Lambda_i) u_i u_i^T + 2\Lambda_j u_j u_j^T. \]

The strategy we will employ to overcome the non-convexity of the population risk is based on the observation that locally around the true \( \beta_0 \), the population risk function \( R(\beta) \) is convex, as illustrated in Figure 1. Lemma 1 below relates the eigenvalue gap \( \rho \) to the convexity of the population risk function: in an \( \ell_2 \)-ball around \( \beta_0 \) whose radius is small enough compared to the eigenvalue gap, the population risk is convex.

**Lemma 1** (Lemma 12.7 in van de Geer [2016]). *Suppose that \( 3\eta < \rho \). Then for all \( \beta \in \mathbb{R}^p \) satisfying \( \|\beta - \beta_0\|_2 \leq \eta \) we have

\[ \Lambda_{\min}(\ddot{R}(\beta)) \geq 2(\rho - 3\eta). \]

However, note that the statement of Lemma 1 is not necessarily true for the empirical risk \( R_n(\beta) \). In high-dimensional settings, the empirical risk might be non-convex even in the local neighbourhood from Lemma 1, because it depends on the sample covariance matrix \( \tilde{\Sigma} \) whose eigenvalues are inconsistent estimators of the population eigenvalues and might even diverge to infinity in the regime \( p \gg n \); for illustration of the empirical risk function, see Figure 2.

Following the idea of Lemma 1, our strategy is to estimate the loadings vector \( \beta_0 \) using a two step procedure. In the first step, we localize to an \( \ell_2 \)-ball around \( \beta_0 \), which is small enough such that \( \rho - 3\eta > 0 \). In the second step, we make use of the locality to obtain a near-oracle estimator.
2.2 Localization: first step estimator

We base our first-step estimator on a convex program originally proposed in d’Aspremont et al. [2007] (and later studied by Vu et al. [2013]),

\[ \hat{Z} := \arg\max_{\text{tr}(Z)=1, \ 0 \leq Z \leq I} \text{tr}(\hat{\Sigma}Z) - \lambda \|Z\|_1. \]  

The feasible set is a convex relaxation of the set of positive definite rank-one matrices and the \(\ell_1\)-norm of a matrix is the \(\ell_1\)-norm of its vectorized version. Note that due to the relaxation, \(\hat{Z}\) is not necessarily of rank one. However, we show that the normalized eigenvector of \(\hat{Z}\) corresponding to its largest eigenvalue, denote it by \(\hat{u}_1\), may be used to estimate the corresponding population eigenvector \(u_1\) (up to a sign). We then define an initial estimator of \(\beta_0\) as a properly scaled version of \(\hat{u}_1\),

\[ \hat{\beta}_{\text{init}} := \text{tr}(\hat{\Sigma}\hat{Z})^{1/2} \hat{u}_1. \]  

Lemma 2 below provides guarantees for the estimator \(\hat{\beta}_{\text{init}}\) under mild conditions. To this end, we recall Theorem 3.3 in Vu et al. [2013] which derives the bound for \(\hat{Z}\) in Frobenius norm. By the standard arguments for deriving oracle inequalities for \(\ell_1\)-penalized M-estimators (see e.g. Bühlmann and van de Geer [2011]) the bound from Theorem 3.3 in Vu et al. [2013] can be easily extended to the \(\ell_1\)-norm error. Recall that \(u_1\) is the eigenvector of \(\Sigma_0\) corresponding to its largest eigenvalue. Then for \(\lambda \geq 2\|\Sigma - \Sigma_0\|_\infty\), it holds

\[ \|\hat{Z} - u_1 u_1^T\|_F + \lambda \|\hat{Z} - u_1 u_1^T\|_1 \leq \frac{C s^2 \lambda^2}{(\Lambda_1 - \Lambda_2)^2} =: \epsilon^2, \]  

Figure 2: A toy example: the graph (left) and contours (right) of the empirical risk for \(p = 2\) and a randomly generated sample of size \(n = 4\) (the observations are normally distributed in this example). The blue circles in the contour plot show the convex local neighbourhood from Lemma 1 (around the true \(\beta_0\)).
where $s$ is the number of non-zero entries in $\beta_0$ and $C > 0$ is a universal constant.

**Lemma 2.** Let $\hat{Z}$ be the estimator defined in (5), with $\lambda \geq 2\|\hat{\Sigma} - \Sigma_0\|_\infty$. Letting $\hat{u}_1$ denote the normalized eigenvector of $\hat{Z}$ corresponding to its largest eigenvalue and assuming $\hat{u}_1^T u_1 \geq 0$, it holds

$$\|\hat{u}_1 - u_1\|_2^2 \leq 4\epsilon,$$

where $\epsilon$ is defined in (7), and

$$\|\hat{\beta}_{\text{init}} - \beta_0\|_2 \leq \frac{\zeta}{4\sqrt{\|\beta_0\|_2^2 - \zeta}} + 2\|\beta_0\|_2\sqrt{\epsilon},$$

where

$$\zeta := s\lambda + \epsilon^2 + 6\|\beta_0\|_2^2\epsilon + 4\|\beta_0\|_2\sqrt{\epsilon},$$

provided that we assume $\|\beta_0\|_2^2 - \zeta > 0$.

Under a sub-Gaussianity condition on the design (as will be assumed below in Section 3.2), Lemma 2 implies that with $\lambda \approx \sqrt{\log p/n}$, it holds that

$$\|\hat{\beta}_{\text{init}} - \beta_0\|_2 = O_P(\sqrt{s\lambda}),$$

provided that $\|\beta_0\|_2 = O(1), 1/(\Lambda_1 - \Lambda_2) = O(1)$ and $s\lambda \to 0$.

### 3 Main results

#### 3.1 Methodology and de-biasing

In this section, we define the second step estimator and propose methodology for asymptotically normal estimation of loadings and the maximum eigenvalue of $\Sigma_0$.

We aim to define the second-step estimator localized in an $\ell_2$-neighbourhood of the initial estimator $\hat{\beta}_{\text{init}}$. However, for simplicity of presentation, we will define the local neighbourhood around $\beta_0$ instead of $\hat{\beta}_{\text{init}}$ as follows,

$$B := \{\beta \in \mathbb{R}^p : \|\beta - \beta_0\|_2 \leq \eta\},$$

where $\eta$ is some suitable positive constant. In practice we replace $\beta_0$ in the above definition by $\hat{\beta}_{\text{init}}$; then Lemma 2 provides guarantees that for $n$ sufficiently large, a small $\ell_2$-neighbourhood around $\hat{\beta}_{\text{init}}$ will contain $\beta_0$ with high probability. We define the program

$$\hat{\beta} \in \arg\min_{\beta \in B, \|\beta\| \leq T} R_n(\beta) + \lambda\|\beta\|_1,$$

where $(\lambda, T)$ is a pair of positive tuning parameters. We include the constraint $\|\beta\|_1 \leq T$ due to non-convexity of $R_n(\beta)$. This will be necessary for deriving theoretical guarantees for $\hat{\beta}$, namely for bounding the probabilistic error term.
This constraint is not restrictive, but requires to provide a value for the tuning parameter $T$. Asymptotically, $T \approx 1/\lambda \approx \sqrt{n}/\log p$. Similar constraints were studied e.g. in Loh and Wainwright [2014].

As pointed out previously, the optimized function (8) may be non-convex even over the local set $B$. Hence it may possess stationary points that are not global optima. Iterative methods such as gradient or coordinate descent are guaranteed to eventually converge to a stationary point, regardless of convexity, but this point could be a local minimum, saddle point or even a local maximum. Otherwise computing global optima of non-convex functions in an efficient manner may be very difficult in practice. To overcome this difficulty, we provide statistical guarantees for any stationary point of the program (8), not only for the global minimizer. Similar statistical guarantees providing oracle inequalities for non-convex regularized M-estimators were studied e.g. in Loh and Wainwright [2014] or van de Geer [2016].

A stationary point $\hat{\beta}$ of the program (8) is any point of the feasible set where

$$(R_n(\hat{\beta}) + \lambda \partial \|\hat{\beta}\|_1)^T (\beta - \hat{\beta}) \geq 0, \quad \text{for all } \beta \in B, \|\beta\|_1 \leq T,$$

(9)

where $\partial \|\hat{\beta}\|_1$ denotes the sub-differential of $\|\hat{\beta}\|_1$ evaluated at $\hat{\beta}$. This definition accounts also for local minima at the boundary; if the stationary point lies in the interior of the feasible set, then (9) reduces to the Karush-Kuhn-Tucker (KKT) conditions $R_n(\hat{\beta}) + \lambda \partial \|\hat{\beta}\|_1 = 0$.

In the next section, we show that any stationary point $\hat{\beta}$ is a near-oracle estimator of $\beta_0$. However, it is asymptotically biased as will be shown in the sequel, but we can employ de-biasing (or de-sparsifying) techniques studied in van de Geer et al. [2014]. If $\hat{\beta}$ is a stationary point defined as in (9), the de-sparsifying approach suggests to take the bias-corrected “estimator”

$$\tilde{b} := \hat{\beta} - \Theta_0(\|\hat{\beta}\|_2^2, \hat{\Sigma} \hat{\beta}),$$

where $\Theta_0$ is the inverse Hessian matrix of the population risk, $\Theta_0 := R(\beta_0)^{-1}$. The $p \times p$ matrix $\Theta_0$ is not known and needs to be replaced by a consistent estimator as will be proposed below.

Furthermore, we aim to construct an asymptotically normal estimator for the maximum eigenvalue, which is a quadratic function of $\beta_0$. This estimation problem was not considered in van de Geer et al. [2014], but similar ideas may be applied. We will show that the estimator $\|\hat{\beta}\|_2^2$ is biased for $\Lambda_{\max}$, but may be de-biased by defining

$$\tilde{\Lambda} := \|\hat{\beta}\|_2^2 - 2\hat{\beta}^T \Theta_0^T(\|\hat{\beta}\|_2^2 \hat{\beta} - \hat{\Sigma} \hat{\beta}).$$

An estimator of $\Theta_0$ may be constructed in a similar spirit as in van de Geer et al. [2014] using nodewise regression. Nodewise regression was studied in van de Geer et al. [2014] for generalized linear models which have a special structure in the Hessian matrix of the empirical risk and the empirical Hessian matrix is positive semi-definite. We however aim to apply nodewise regression to approximately invert the Hessian matrix

$$R_n(\hat{\beta}) := -\hat{\Sigma} + \|\hat{\beta}\|_2^2 I + 2\hat{\beta} \hat{\beta}^T,$$
where the special structure from generalized semi-linear models is not present and moreover, the empirical Hessian is not necessarily positive definite. To deal with the non-convexity which arises due to absence of positive semi-definiteness, we modify the nodewise regression program from van de Geer et al. [2014] by adding an extra constraint \( \| \cdot \|_1 \leq T \) with a tuning parameter \( T > 0 \). Moreover, due to non-convexity, we need to derive oracle inequalities for any stationary point instead of only the global minimum.

In Algorithm 1 below we formulate the modified version of the nodewise regression program for an arbitrary input matrix \( A \). Recall that for a matrix \( A \in \mathbb{R}^{p \times p} \), we let \( A_j \) denote its \( j \)-th column, \( A_{-j} \in \mathbb{R}^{(p-1) \times p} \) the matrix \( A \) without its \( j \)-th column, \( A_j,_{-j} \in \mathbb{R}^{(p-1) \times 1} \) denote the column vector obtained by selecting the \( j \)-th row of \( A \) and removing its \( j \)-th entry, and by \( A_{-j},_{-j} \in \mathbb{R}^{(p-1) \times (p-1)} \) we denote the matrix \( A \) without its \( j \)-th column and the \( j \)-th row.

### Algorithm 1. Non-convex Nodewise Lasso

**Input:** \( A \in \mathbb{R}^{p \times p} \), positive tuning parameters \((\lambda_j, T_j)\), \( j = 1, \ldots, p \)

**for** \( j = 1, \ldots, p \):

1. Compute any stationary point \( \hat{\gamma}_j \) of the program

   \[
   \min_{\gamma_j \in \mathbb{R}^{p-1}: \|\gamma_j\|_1 \leq T_j} \Gamma_j^T A \Gamma_j + \lambda_j \|\gamma_j\|_1, \tag{10}
   \]

   where

   \[
   \Gamma_j := (-\gamma_{j,1}, \ldots, -\gamma_{j,j-1}, 1, -\gamma_{j,j+1}, \ldots, -\gamma_{j,p}). \tag{11}
   \]

2. Define \( \hat{\Gamma}_j \) via the relation (11) with \( \hat{\gamma}_j \) and compute the estimator of the noise level \( \hat{\tau}_j^2 := \hat{\Gamma}_j A \hat{\Gamma}_j + \frac{1}{2} \lambda_j \|\hat{\gamma}_j\|_1 \).

3. Compute the nodewise Lasso estimator defined by \( \hat{\Theta}_j := \hat{\Gamma}_j / \hat{\tau}_j^2 \).

Stack \( \hat{\Theta}_j, j = 1, \ldots, p \) into the columns of \( \hat{\Theta} := [\hat{\Theta}_1, \ldots, \hat{\Theta}_p] \).

**Output:** \( \hat{\Theta} \)

We remark that a stationary point \( \hat{\gamma}_j \) is defined analogously as in (9), that is, \( \hat{\gamma}_j \) is a stationary point of the program (10) if it lies in the feasible set and for all \( \gamma_j \in \mathbb{R}^{p-1} \) in the feasible set it holds

\[
(-2A_{-j,-j} + 2A_{-j,j} \hat{\gamma}_j + \lambda_j \partial \|\hat{\gamma}_j\|_1)^T (\gamma_j - \hat{\gamma}_j) \geq 0,
\]

where \( \partial \|\hat{\gamma}_j\|_1 \) is the sub-differential of the \( \ell_1 \)-norm evaluated at \( \hat{\gamma}_j \). If \( \hat{\gamma}_j \) is a stationary point of the program (10) which lies in the interior of the feasible set, then

\[
-2A_{-j,-j} + 2A_{-j,j} \hat{\gamma}_j + \lambda_j \partial \|\hat{\gamma}_j\|_1 = 0. \tag{12}
\]

In this case, using the KKT conditions (12), one can show that

\[
A_j^T \hat{\Gamma}_j = \hat{\tau}_j^2 \quad \text{and} \quad \|A_j^T \hat{\Gamma}_j\|_\infty \leq \lambda_j/2.
\]
which implies
\[ \| A^T \hat{\Theta} - I \|_\infty = \mathcal{O}( \max_{j=1,\ldots,p} \lambda_j / T_j^2 ). \]

We aim to apply the nodewise Lasso with \( A := \hat{R}_n(\hat{\beta}) \) and for this choice, we show in the following section that we can obtain an oracle inequality for \( \hat{\Theta} \). Our theoretical results also identify the (asymptotically) correct choice of the tuning parameters \( \lambda \asymp 1/T \asymp \sqrt{\log p/n} \). From a computational viewpoint, calculating any stationary point of the Lasso-type program (10) can be achieved by a polynomial time algorithm (such as the gradient or coordinate descent).

We collect the full procedure for obtaining the de-biased estimator in the scheme below.

**Algorithm 2. De-biased sparse PCA**

**Input:** \( n \times p \) data matrix \( X \), positive tuning parameters \( \lambda_{\text{init}}, (\lambda, T), (\lambda_j, T_j) \), \( j = 1, \ldots, p \)

1: Compute the initial estimator \( \hat{\beta}_{\text{init}} \) defined in (6) with the tuning parameter \( \lambda_{\text{init}} \)

2: Compute any stationary point \( \hat{\beta} \) of the following program, with tuning parameters \( (\lambda, T) \)

\[
\arg\min_{\beta \in \mathbb{R}^p : \|\beta\|_1 \leq T; \|\beta - \hat{\beta}_{\text{init}}\|_2 \leq \eta} \left( \frac{1}{2} \beta^T \hat{\Sigma} \beta + \|\beta\|_2^4 + \lambda \|\beta\|_1 \right). \tag{13}
\]

3: Run the nodewise Lasso in Algorithm 1 with input matrix

\[ \hat{R}_n(\hat{\beta}) = -\hat{\Sigma} + \|\hat{\beta}\|_2^2 I + 2\hat{\beta} \hat{\beta}^T, \]

with tuning parameters \( (\lambda_j, T_j) \), \( j = 1, \ldots, p \) and output \( \hat{\Theta} \)

4: Compute the de-sparsified estimator and the eigenvalue estimator:

\[
\hat{b} := \hat{\beta} - \hat{\Theta}^T (\|\hat{\beta}\|_2^2 \hat{\beta} - \hat{\Sigma} \hat{\beta}), \tag{14}
\]

\[
\hat{\Lambda} := \|\hat{\beta}\|_2^2 - 2 \hat{\beta}^T \hat{\Theta}^T (\|\hat{\beta}\|_2^2 \hat{\beta} - \hat{\Sigma} \hat{\beta}). \tag{15}
\]

**Output:** \( \hat{b}, \hat{\Lambda} \)

The tuning parameters in Algorithm 2 have to be chosen of order \( \lambda_{\text{init}} \asymp \lambda \asymp 1/T \asymp \lambda_j \asymp 1/T_j \asymp \sqrt{\log p/n} \) and the constant \( \eta \) in program (13) must be chosen sufficiently small.

### 3.2 Theoretical results

In this section, we derive the main theoretical results: firstly we provide oracle inequalities for \( \hat{\beta} \) and the nodewise Lasso \( \hat{\Theta} \) (thoughout this section, \( \hat{\beta} \) is the estimator defined in (8), where we assume we are already in the neighbourhood
around $\beta_0$ and $\hat{\Theta}$ is based on $\hat{\beta}$); secondly we provide results on asymptotic normality of the bias-corrected estimators based on $\hat{\beta}$ and $\hat{\Theta}$. We discuss how these results may be used to construct confidence intervals and support recovery.

To bound the terms arising from the probabilistic analysis of the estimators, we assume sub-Gaussian design, but we remark that similar results could be obtained under bounded design using the concentration results derived in van de Geer [2014].

**Definition 1.** We say that a vector $Y \in \mathbb{R}^p$ is sub-Gaussian with a parameter $\sigma$ if for all vectors $\alpha \in \mathbb{R}^p$ such that $\|\alpha\|_2 = 1$, it holds
\[
E|\alpha^T Y|^2 / \sigma^2 \leq 2.
\]

**Condition 1 (Sub-Gaussian design).** Assume that the $n \times p$ random matrix $X$ has independent rows, which are sampled from a zero-mean distribution with a covariance matrix $\Sigma_0$ and are sub-Gaussian vectors with a parameter $\sigma$. We say that $X$ is a sub-Gaussian matrix with a parameter $\sigma$.

The following lemma derives an oracle inequality for the second step estimator $\hat{\beta}$. Recall that $\eta$ is the size of the neighbourhood in the definition of $\hat{\beta}$, $\rho = \phi_{\max} - \phi_2$ is the eigenvalue gap and the sparsity in $\beta_0$ is denoted by $s := \|\beta_0\|_0$.

**Theorem 1.** Assume that Condition 1 is satisfied with a parameter $\sigma$, let $\lambda_0 = \sqrt{2 \log(2p)/n}$, $\lambda_1 = 4\sigma^2(\|\beta_0\|_2 + 1)[\lambda_0 + \lambda_0^2]$ and $\rho - 3\eta \geq c_0\sigma^2 C_T[3C_T + \sqrt{6}]$, where $c_0$ is a suitable universal constant. Let the tuning parameters $(\lambda, T)$ of the program (8) satisfy
\[
\lambda \geq 2\lambda_1, \quad (16)
\]
\[
T \leq C_T / (2\lambda_0), \text{ and } \|\beta_0\|_1 \leq T. \text{ Then any stationary point } \hat{\beta} \text{ as defined in (9) satisfies with probability at least } 1 - 2(J + 2)e^{-\log(2p)} \text{ where } J = \lceil \log T \rceil \text{ the error bound}
\]
\[
\|\hat{\beta} - \beta_0\|_2^2 + \lambda\|\hat{\beta} - \beta_0\|_1 \leq \frac{C_2s\lambda^2}{(\rho - 3\eta)^2}, \quad (17)
\]
where $C_2$ is a universal constant.

In an asymptotic formulation, we require that $\|\beta_0\|_1 = O(\sqrt{n} / \log p)$ and $\|\beta_0\|_2 = \phi_{\max} = O(1)$. Then for $\lambda \asymp \sqrt{\log p / n}$ and $T \asymp \sqrt{n / \log p}$, we obtain rates of order $s \log p / n$, provided that $\rho - 3\eta$ is lower bounded by a universal constant. The tuning parameter $T$ must be chosen large enough to guarantee that $\beta_0$ lies in the feasible set. The above result essentially requires that $\lambda_0\|\beta_0\|_1$ is bounded by a universal constant for $\hat{\beta}$ to achieve the oracle rates $s \log p / n$. 

14
Similar oracle inequalities may be derived for the nodewise Lasso estimators; but due to high-dimensionality, sparsity conditions on the columns of $\Theta_0$ are necessary. Sparsity conditions on the inverse population Hessian have appeared in literature on linear regression (Zhang and Zhang [2014]; van de Geer et al. [2014]; Javanmard and Montanari [2014]) and generalized linear models (van de Geer et al. [2014]; Belloni et al. [2015]; Chernozhukov et al. [2015]). For $j = 1, \ldots, p$, we define the population parameters

$$ \gamma_j^0 := \arg \min_{\gamma \in \mathbb{R}^{p-1}} \Gamma_j^T \tilde{R}(\beta_0) \Gamma_j, \quad (18) $$

where $\Gamma_j$ is defined in (11) and we define the corresponding sparsity parameters

$$ s_j := \|\gamma_j^0\|_0, \quad \text{for } j = 1, \ldots, p. $$

These sparsity parameters as well correspond to the sparsity in the columns of $\Theta_0$. To keep the presentation simpler, in the results that follow, we assume that the maximum eigenvalue of $\Sigma_0$ is bounded ($\phi_{\max} = O(1)$) and that there exists a constant $c > 0$ such that $\rho - 3\eta \geq c$. A more refined result might allow the quantities $\phi_{\max}$ and $1/(\rho - 3\eta)$ to grow, although their growth cannot be faster than (a certain power of) $\sqrt{n}/(\max(s, \max_j s_j) \log p)$.

Lemma 3. Assume Condition 1 with a universal parameter $\sigma > 0$, suppose that $\rho - 3\eta \geq c$, $\phi_{\max} \leq C_{\max}$, for some universal constants $c, C_{\max}$ and $\max_j s_j = o(\sqrt{n}/\log p)$. Let $\tilde{\Theta}$ be defined by the nodewise Lasso in Algorithm 1 with input matrix $\tilde{R}_n(\hat{\beta})$, where $\hat{\beta}$ is defined in (9) with suitable tuning parameters

$$ \lambda \asymp \sqrt{\log(2p)/n}, \quad \|\beta_0\|_1 \leq T \leq C_T \sqrt{n/\log(2p)}, $$

and for $j = 1, \ldots, p$,

$$ \lambda_j \asymp \sqrt{\log(2p)/n} \quad \text{and} \quad \|\gamma_j^0\|_1 \leq T_j \leq \tilde{C}_T \sqrt{n/\log(2p)}, $$

where $C_T, \tilde{C}_T$ are suitable universal constants. Then it holds

$$ \max_{j=1,\ldots,p} \|\tilde{\Theta}_j - \Theta_j^0\|_1 = O_p(\max_{j=1,\ldots,p} s_j \lambda_j), $$

$$ \max_{j=1,\ldots,p} \|\tilde{\Theta}_j - \Theta_j^0\|_2 = O_p(\max_{j=1,\ldots,p} \sqrt{s_j} \lambda_j). $$

Our main results derive the asymptotic distribution of the entries $\hat{b}_j$ of $\hat{b}$ and the asymptotic distribution of $\hat{\Lambda}$.

Theorem 2. Assume Condition 1 holds with a universal parameter $\sigma$. Suppose that $\phi_{\max} \leq C_{\max}$ and $\rho - 3\eta \geq c$ for some universal constants $C_{\max}, c > 0$. Consider the estimator

$$ \hat{b} := \hat{\beta} - \tilde{\Theta}^T (\|\hat{\beta}\|_2^2 \hat{\beta} - \hat{\Sigma} \hat{\beta}), $$

where $\hat{\Sigma}$ is estimated by $\hat{\Sigma}^0$.
with \(\hat{\beta}\) and \(\hat{\Theta}\) as in Lemma 3 and with the same tuning parameters as in Lemma 3. Then, under the sparsity conditions
\[
s = o\left(\sqrt{n} / \log p\right) \quad \text{and} \quad \max_{j=1,\ldots,p} s_j = o\left(\sqrt{n} / \log p\right),
\]
the de-sparsified estimator satisfies
\[
\hat{b} - \beta_0 = -\Theta_0 \hat{R}_n(\beta_0) + \text{rem},
\]
where
\[
\|\text{rem}\|_\infty = O_P\left(\max_{j=1,\ldots,p} \max(s, s_j) \max\left(\lambda^2, \lambda_j^2, \frac{\log(2p)}{n}\right)\right) = o_P\left(\frac{1}{\sqrt{n}}\right).
\]
Moreover, for \(j = 1,\ldots,p\), if \(1/\sigma^2_j = O(1)\), it follows that
\[
\sqrt{n}(\hat{b}_j - \beta^0_j)/\sigma_j \sim \mathcal{N}(0,1),
\]
where
\[
\sigma^2_j := n \text{var}((\Theta_0^j)^T \hat{\Sigma} \beta_0).
\]

We require sparsity of small order \(\sqrt{n} / \log p\) in both \(\beta_0\) and in the columns of \(\Theta_0\). We remark that for estimation of a single entry \(\beta^0_j\), it is enough to assume sparsity in \(\beta_0\) and in the corresponding column \(\Theta_0^j\). The sparsity requirement on \(\beta_0\) is in line with literature on asymptotically normal estimation in sparse high-dimensional settings. In particular, for linear regression, the same sparsity condition on the high-dimensional vector of regression coefficients is required. For linear regression, this condition was shown to be necessary for construction of confidence intervals (see Cai and Guo [2015]). A sparsity condition on the columns of the inverse Hessian of the population risk (here \(\Theta_0\)) also arises as a requirement for asymptotically normal estimation, see e.g. Zhang and Zhang [2014], van de Geer et al. [2014], Javanmard and Montanari [2014], Chernozhukov et al. [2015]. Sparsity in the columns of \(\Theta_0\) is for instance satisfied in the popular “spiked covariance model” (see e.g. Johnstone and Lu [2009], Deshpande and Montanari [2014]) as discussed in the example below.

**Example 1.** In the spiked covariance model, the covariance matrix has the special form
\[
\Sigma_0 = I + \sum_{i=1}^r \omega_i u_i u_i^T,
\]
for \(u_i, i = 1,\ldots,r\) being orthonormal vectors and \(\omega_i\) positive numbers. Then one can easily deduce that the vectors \(u_i\) are the first \(r\) eigenvectors of \(\Sigma_0\) with corresponding eigenvalues \(\Lambda_i = 1 + \omega_i, i = 1,\ldots,r\). We denote the remaining \(p-r\) eigenvectors by \(u_i, i = r+1,\ldots,p\), and their eigenvalues are \(\Lambda_i = 1\) for \(i = r+1,\ldots,p\). Assuming \(\omega_1 > \omega_2\), we have \(\beta_0 = \sqrt{1 + \omega_1} u_1\) and one can also deduce that the eigendecomposition of \(\Theta_0\) is given by \(U^T D U\), where \(U\) has rows \(u_i, i =

1, \ldots, p \text{ and } D := \text{diag}(2(1 + \omega_1), (\omega_1 - \omega_2), \ldots, (\omega_1 - \omega_r))(\omega_1, \ldots, \omega_1)^{-1}. \text{ Then one can show that}

\[
\Theta_0 = \sum_{i \leq r} D_{ii}u_i u_i^T + \frac{1}{\omega_1}(I - \sum_{i \leq r} u_i u_i^T)
\]

\[
= \sum_{i \leq r} (D_{ii} - 1/\omega_1)u_i u_i^T + \frac{1}{\omega_1}I.
\]

If we assume that each of the first \( r \) eigenvectors, \( u_i, i = 1, \ldots, r, \) has sparsity at most \( s \), then each row of \( \Theta_0 \) has sparsity at most \( rs + 1 \).

For asymptotically normal estimation of the maximum eigenvalue, which is a quadratic function of \( \beta_0 \), we need to assume a somewhat stronger sparsity condition.

**Theorem 3.** Assume the conditions of Theorem 2 and, in addition, assume that

\[
s^{3/2} = o(\sqrt{n}/\log p) \quad \text{and} \quad \max_{j=1, \ldots, p}s_j^{3/2} = o(\sqrt{n}/\log p).
\]

Recalling that

\[
\hat{\Lambda} = \|\hat{\beta}\|_2^2 - 2\hat{\beta}^T \hat{\Theta}^T \hat{R}_n(\beta),
\]

the following asymptotic expansion holds

\[
\hat{\Lambda} - \Lambda_{\text{max}} = -2\beta_0^T \Theta_0 \hat{R}_n(\beta) + \text{rem},
\]

where

\[
\|\text{rem}\|_\infty = O_P\left(\max_{j=1, \ldots, p}\max(s, s_j)^{3/2}\max(2, \lambda_j, \frac{\log(2p)}{\sqrt{n}})\right)
\]

\[
= O_P\left(\frac{1}{\sqrt{n}}\right).
\]

Denoting the variance of the pivot by

\[
\sigma^2_\Lambda := 4n\text{var}(\hat{\beta}_0^T \Theta_0 \hat{\Sigma} \beta_0),
\]

it follows

\[
\sqrt{n}\left(\hat{\Lambda} - \Lambda_{\text{max}}\right)/\sigma_\Lambda \rightsquigarrow N(0, 1).
\]

The asymptotic variances of the estimators in Theorems 2 and 3 correspond to the asymptotic variance of the loadings vector based on the sample covariance matrix from fixed-\( p \)-regime (see e.g. Kollo and Neudecker [1997]). For instance, if the observations are Gaussian \( N(0, \Sigma) \) and there are no eigenvalue multiplicities, then

\[
\sigma^2_\Lambda = 2\Lambda_{\text{max}}^2.
\]
\[
\sigma_j^2 = (\Theta_j^0)^T \Sigma_0 \Theta_j^0 \| \beta_0 \|^2_2 + \| \beta_0 \|^2_2 (\Theta_j^0)^T \beta_0)^2, \\
= \frac{\beta_j^0}{2} + \| \beta_0 \|^4_2 \sum_{i=1, i \neq j}^p u_{i,j}^2 \Lambda_i (\Lambda_{\text{max}} - \Lambda_i)^2, 
\]

where \( u_{i,j} \) is the \( j \)-th entry of the \( i \)-th eigenvector of \( \Sigma_0 \) (see Lemma 6 in Section 6.2.3 for the derivation). The asymptotic variance \( \sigma_j^2 \) can be easily estimated by \( \hat{\sigma}_j^2 := 2 \| \hat{\beta} \|^2_2 \). The asymptotic variances \( \sigma_j^2 \) however depend on all the eigenvectors \( u_i, i \neq j \). Simultaneous estimation of all the eigenvectors would in theory require \( p \ll n \) and is moreover impractical if we are only interested in inference about the first few loadings vectors. Therefore, we suggest to use an alternative procedure, which computes the natural estimator

\[
\hat{\sigma}_j^2 := \frac{1}{n} \sum_{i=1}^n (\hat{\Theta}_j^T X_i (X_i)^T \hat{\beta})^2 - (\hat{\Theta}_j^T \hat{\Sigma} \hat{\beta})^2. 
\]

This does not assume the knowledge of the distribution of \( X_i \) and is only based on the estimators \( \hat{\Sigma}, \hat{\Theta}_j \) and \( \hat{\beta} \). Analogously one can estimate the variance \( \sigma_\Lambda^2 \) in the non-Gaussian case. We omit the theoretical guarantees for these estimators, but point the reader to results of a similar flavour which are proved for estimation of asymptotic variance in Janková and van de Geer [2015] under sub-Gaussianity conditions on the design.

The result of Theorem 2 can be applied for support recovery of the entries of \( \beta_0 \) by thresholding the de-sparsified estimator at the level \( C \sqrt{\log p/n} \) for a suitable (possibly data-driven) \( C > 0 \). Define the thresholded estimator

\[
\hat{b}_{\text{thresh}, i} := \hat{b}_i 1_{\hat{b}_i > C \sqrt{\log p/n}},
\]

where \( \hat{b}_i \) is the \( i \)-th entry of \( \hat{b} \). Then \( \hat{b}_{\text{thresh}} := (\hat{b}_{\text{thresh}, 1}, \ldots, \hat{b}_{\text{thresh}, p}) \) recovers no false positives, i.e. the support \( \hat{S} \) of \( \hat{b}_{\text{thresh}} \) satisfies asymptotically, with probability tending to one,

\[
\hat{S} \subseteq S_0,
\]

where \( S_0 \) is the support of \( \beta_0 \). Moreover, if in addition the beta-min condition holds, i.e.

\[
\min_{j \in S_0} \beta_j^0 \geq 2C \sqrt{\frac{\log p}{n}},
\]

then we obtain exact support recovery, i.e. \( \hat{S} = S_0 \) (asymptotically, with probability tending to one). The problem of support recovery of the first eigenvector was studied in a number of papers, see e.g. Johnstone and Lu [2009], Amini and Wainwright [2009], Deshpande and Montanari [2014], under irrepresentability conditions or under the spiked covariance model. Our results do not need to assume the irrepresentability condition, but require a sparsity condition on \( \Theta_0 \), which may be viewed as a less stringent condition.
4 Empirical results

4.1 Setup

In this section, we demonstrate the performance of the de-biased sparse PCA in several models and different dimensionality regimes. We provide a comparison to the classical PCA.

We consider the spiked covariance model with a single spike,
\[
\Sigma_0 = I + \omega vv^T,
\]
where
\[
v = (1, 1, 1, 0, 1, 0, \ldots, 0) \in \mathbb{R}^p
\]
for two different spike sizes \( \omega \):

- **Model 1 (Small spike):** \( \omega = 1/5 \)
- **Model 2 (Large spike):** \( \omega = 1 \)

The observations \( X_1, \ldots, X_n \) are independent and \( \mathcal{N}(0, \Sigma_0) \)-distributed.

The more challenging model is arguably Model 1, where the eigenvalue gap is smaller. Indeed, one can easily check that for Model 1, \( \Lambda_{\text{max}} = 1.8 \), while for Model 2, \( \Lambda_{\text{max}} = 5 \). As we will see in the simulation study, classical PCA does not perform well in Model 1, while it does perform well in our Model 2. In terms of theoretical conditions such as sparsity, one can check that the vector \( \beta_0 = \sqrt{1 + \|v\|^2_2} v \) is the first loadings vector with sparsity \( s = 4 \) and the inverse Fisher information \( \bar{R}((\beta_0)^{-1} \) has sparsity 4.

We demonstrate the performance of the de-biased sparse PCA (and classical PCA) for construction of confidence intervals for individual entries of \( \beta_0 \). We first calculate the confidence intervals assuming the asymptotic variance from (19) is known. This gives a fairer comparison, otherwise for the classical PCA, we would observe that too large estimates of asymptotic variance lead to large confidence intervals and perfect coverage. We look at estimating the asymptotic variance separately.

The sparse PCA estimator (8) is calculated using gradient descent, with a tuning parameter \( \lambda = \sqrt{\log p/n} \) and the starting point of the algorithm is the initial estimator \( \hat{\beta}_{\text{init}} \). The constraint on the \( \ell_1 \)-norm turns out to be unnecessary in our simulations. We compute the non-convex nodewise Lasso estimator with tuning parameters \( \lambda_j = \sqrt{\log p/n}, j = 1, \ldots, p \).

For Model 1, we investigate the scenarios: \( (p = 200, n = 200) \) (Figure 3), \( (p = 200, n = 400) \) (Figure 4) and \( (p = 500, n = 800) \) (Figure 5). For Model 2, we consider the scenario \( (p = 200, n = 200) \) (Figure 6). The target coverage is 95% in all simulations. The average coverage is reported over the non-zero set \( S_0 := \{i : \beta_0^i \neq 0 \} \) and \( \bar{S}_0 \). The number of generated random samples is always \( N = 200 \).

We can observe that the classical PCA does not perform well in estimation of the non-zero entries of \( \beta_0 \) in Model 1, while the de-biased estimator per-
forms reasonably well. We also find that our theoretical condition requiring $s = o(\sqrt{n}/\log p)$ seems to be needed for our method to perform well in simulations. Namely, comparing Figures 3 and 4, we see that the performance of our estimator was substantially improved with the increased sample size. Note that in the setting in Figure 3 ($p = 200, n = 200$), we have sparsity $s = 4$ and $\sqrt{n}/\log p \approx 2.67$, while in Figure 4 ($p = 200, n = 400$), we still have sparsity $s = 4$ but due to a bigger sample size, we have $\sqrt{n}/\log p \approx 3.77$. This confirms our theoretical findings and we note that a similar phenomenon has also been observed in other settings: the generalized linear models in Janková and van de Geer [2016] and Gaussian graphical models (Janková and van de Geer [2015] and Janková and van de Geer [2016]).

Finally, we look at estimating the asymptotic variance, measured by the length of confidence intervals given by $\Phi^{-1}(0.95)\hat{\sigma}_j^2\sqrt{n}$, where $\hat{\sigma}_j^2$ is the estimator of asymptotic variance estimator as proposed in (20). For the de-biased sparse PCA, we use $\hat{\beta}$ and $\hat{\Theta}$ as defined in Section 3 to calculate the estimate of the asymptotic variance (20). For the classical PCA, we use $\hat{\beta} := \hat{\beta}_{PCA}$ and $\hat{\Theta} := \hat{\Sigma}^{-1}$ to calculate (20). The results are reported in Table 1. The average length of a confidence interval is calculated over $N = 100$ randomly generated samples. We also report the “Asymptotically efficient length”, which is the asymptotically optimal length of a confidence interval corresponding to the fixed-$p$ setting.

5 Discussion

We have proposed a computationally feasible methodology with theoretical guarantees for constructing confidence intervals for loadings and the maximum eigenvalue of the covariance matrix in a sparse high-dimensional regime. The results may also be applied for support recovery without requiring irrepresentability conditions, although we do require the (arguably weaker) sparsity condition on the columns of the inverse population Hessian matrix. We have shown that the de-biasing methodology which was studied in a line of papers (Zhang and Zhang [2014]; van de Geer et al. [2014]; Janková and van de Geer [2015, 2016]) may be used even in a non-convex setting. The challenge here lied especially in estimating the inverse Fisher information, which is not guaranteed to be positive definite under non-convexity of the loss function.

To position our research relative to the existing literature on asymptotic normality for principal component analysis in high dimensions, it is worth to point out that contrary to the papers Koltchinskii et al. [2016] and Fan and Wang [2015], our results do not study the special setting where the maximum eigenvalue diverges, or where the eigenvalue gap diverges. We allow the eigenvalue gap to be very small, what arguably presents a more challenging setting, requiring us to rely on sparsity conditions.
Model 1: \( p = 200, n = 200 \)

|                      | Average coverage |
|----------------------|------------------|
| **Method**           | \( S_0 \)    | \( S_{\hat{0}} \) |
| De-biased sparse PCA | 0.78           | 0.84              |
| Classical PCA        | 0.16           | 0.98              |

Figure 3: Histograms corresponding to (normalized) estimators of the first 9 entries of the loadings vector \( \beta_0 \). Left: de-biased sparse PCA estimator, right: classical PCA. The non-zero entries of \( \beta_0 \) are underlined.

Model 1: \( p = 200, n = 400 \)

|                      | Average coverage |
|----------------------|------------------|
| **Method**           | \( S_0 \)    | \( S_{\hat{0}} \) |
| De-biased sparse PCA | 0.95           | 0.97              |
| Classical PCA        | 0.24           | 0.96              |

Figure 4: Histograms corresponding to (normalized) estimators of \( \beta_0 \).
Model 1: $p = 500, n = 800$

De-biased sparse PCA

Classical PCA

| Average coverage | Method     | $S_0$ | $S_0^*$ |
|------------------|------------|-------|---------|
| De-biased sparse PCA | 0.78       | 0.77  |
| Classical PCA     | 0.00       | 0.89  |

Figure 5: Histograms corresponding to (normalized) estimators of the first 9 entries of $\beta_0$.

Model 2: $p = 200, n = 200$

De-biased sparse PCA

Classical PCA

| Average coverage | Method     | $S_0$ | $S_0^*$ |
|------------------|------------|-------|---------|
| De-biased sparse PCA | 0.96       | 0.93  |
| Classical PCA     | 0.94       | 0.95  |

Figure 6: Histograms corresponding to (normalized) estimators of the first 9 entries of $\beta_0$. 
Estimating the asymptotic variance

| Model 1: p = 200, n = 200 | Average length | \( S_0 \) | \( S_0^c \) |
|---------------------------|----------------|--------|--------|
| De-biased sparse PCA      | 0.406          | 0.319  |
| Classical PCA             | 3.327          | 3.496  |
| Asymptotically efficient length* | 0.278          | 0.312  |

| Model 2: p = 200, n = 200 | Average length | \( S_0 \) | \( S_0^c \) |
|---------------------------|----------------|--------|--------|
| De-biased sparse PCA      | 0.178          | 0.181  |
| Classical PCA             | 0.232          | 0.268  |
| Asymptotically efficient length* | 0.186          | 0.173  |

Table 1: Average length of confidence intervals.

* corresponding to the fixed-p regime (see Kollo and Neudecker [1997]).

6 Proofs

6.1 Proofs for Section 2: First step estimator

Proof of Lemma 2. Using the arguments of Theorem 3.3 in Vu et al. [2013], one can easily show (with the techniques used to prove oracle inequalities for \( \ell_1 \)-regularized estimators - see e.g. Bühlmann and van de Geer [2011]) that for \( \lambda \geq 2\|\Sigma - \Sigma_0\|_\infty \),

\[
\|\hat{Z} - u_1 u_1^T\|_F^2 + \lambda\|\hat{Z} - u_1 u_1^T\|_1 \leq \frac{C}{(A_1 - A_2)^2}\lambda^2,
\]

where \( C \) is a universal constant. Let \( \|A\| := \sqrt{\Lambda_{\max}(AA^T)} \) denote the spectral norm. Since for any square matrix \( A \) it holds \( \|A\| \leq \|A\|_F \), then

\[
\|\hat{Z} - u_1 u_1^T\| \leq \|\hat{Z} - u_1 u_1^T\|_F.
\]

Hence

\[
\|\hat{Z}\| \geq \|u_1 u_1^T\| - \epsilon = 1 - \epsilon.
\]

Write the eigendecomposition of \( \hat{Z} \) as

\[
\hat{Z} = \sum_{j=1}^p \hat{\phi}^2_j \hat{u}_j \hat{u}_j^T,
\]

where \( \hat{\phi}_1 \geq \cdots \geq \hat{\phi}_p \) and \( \hat{u}_j^T \hat{u}_j = 1 \). Since \( \hat{\phi}_1^2 = \|\hat{Z}\| \geq 1 - \epsilon \) and \( \text{tr}(\hat{Z}) = \sum_{j=1}^p \hat{\phi}_j^2 = 1 \), then

\[
\text{tr}(\hat{Z}^T \hat{Z}) = \text{tr}(\hat{Z}^2) = \sum_{j=1}^p \hat{\phi}_j^4 = \hat{\phi}_1^4 + \sum_{j=2}^p \hat{\phi}_j^4 \geq (1 - \epsilon)^2.
\]
Hence it follows
\[ \| \hat{Z} - u_1 u_1^T \|_F^2 = 2 \left( 1 - \text{tr}(\hat{Z} u_1 u_1^T) \right) + \text{tr}(\hat{Z}^T \hat{Z}) - 1 \]
\[ \geq 2 \left( 1 - \text{tr}(\hat{Z} u_1 u_1^T) \right) - 2\epsilon + \epsilon^2 \]
\[ = 2 \left( 1 - \sum_{j=1}^{p} \phi_j^2 (\hat{u}_1^T \hat{u}_j)^2 \right) - 2\epsilon + \epsilon^2. \]

Thus
\[ 2 \left( 1 - \sum_{j=1}^{p} \phi_j^2 (\hat{u}_1^T \hat{u}_j)^2 \right) \leq 2\epsilon. \]  

(21)

Moreover,
\[ \sum_{j=1}^{p} \phi_j^2 (u_1^T u_j)^2 \leq \phi_1^2 (u_1^T u_1)^2 + \sum_{j=2}^{p} \phi_j^2 \leq (u_1^T u_1)^2 + \epsilon. \]  

(22)

Then combining (21) and (22) it follows
\[ 2 \left( 1 - (u_1^T \hat{u}_1)^2 \right) \leq 4\epsilon. \]

Since we assume without loss of generality that \( \hat{u}_1^T u_1 \geq 0 \),
\[ \| u_1 - \hat{u}_1 \|_2^2 = 2(1 - u_1^T \hat{u}_1) = 2(1 - (u_1^T \hat{u}_1)^2) \leq 4\epsilon. \]

Now we proceed to show the bound for \( \| \hat{\beta}_{\text{init}} - \beta_0 \|_2 \). Recall that \( \hat{\beta}_{\text{init}} = \text{tr}(\Sigma \hat{Z})^{1/2} \hat{u}_1 \). Using the eigendecomposition of \( \hat{Z} \), we can write
\[ \text{tr}(\hat{\Sigma} \hat{Z}) - \text{tr}(\Sigma_0 u_1 u_1^T) \leq \left| \text{tr}(\hat{\Sigma} - \Sigma_0) \hat{Z} \right| + \sum_{j=2}^{p} \phi_j^2 (\hat{u}_1^T \hat{u}_j)^2 \]
\[ \leq \sum_{j=1}^{p} \phi_j^2 \left( \hat{u}_j^T \Sigma_0 \hat{u}_j - u_1^T u_1^T \right) \leq \lambda \max \sum_{j=2}^{p} \phi_j^2 \leq \Lambda_{\max} \epsilon. \]

Firstly, since \( \| u_1 u_1^T \|_1 \leq s \| u_1 u_1^T \|_F \leq s \) and \( \| \hat{Z} - u_1 u_1^T \|_1 \leq \epsilon^2 / \lambda \), it follows
\[ i_1 \leq \| \Sigma - \Sigma_0 \|_\infty \| \hat{Z} \|_1 \leq \lambda / 2(s + \epsilon^2 / \lambda). \]

Secondly,
\[ i_2 = \text{tr}(\Sigma_0 (\sum_{j=2}^{p} \phi_j^2 \hat{u}_j \hat{u}_j^T)) \leq \sum_{j=2}^{p} \phi_j^2 \hat{u}_j \Sigma_0 \hat{u}_j \leq \Lambda_{\max} \sum_{j=2}^{p} \phi_j^2 \leq \Lambda_{\max} \epsilon. \]
Thirdly,
\[ i_3 = |\text{tr}(\Sigma_0(\hat{\phi}_1^2\hat{u}_1\hat{u}_1^T - u_1u_1^T))| \leq |\text{tr}(\Sigma_0(\hat{\phi}_1^2 - 1)\hat{u}_1\hat{u}_1^T)| \\
+ |\text{tr}(\Sigma_0(\hat{u}_1\hat{u}_1^T - u_1u_1^T))| \leq \epsilon\|\hat{u}_1\|_2\Lambda_{\text{max}} + |(\hat{u}_1 - u_1)^T\Sigma_0(\hat{u}_1 - u_1)| \\
+ 2|u_1^T\Sigma_0(\hat{u}_1 - u_1)| \leq \epsilon\Lambda_{\text{max}} + \Lambda_{\text{max}}\|\hat{u}_1 - u_1\|^2 \\
+ 2\Lambda_{\text{max}}\|\hat{u}_1 - u_1\|_2 \leq 5\epsilon\Lambda_{\text{max}} + 4\sqrt{\epsilon}\Lambda_{\text{max}}^{1/2}.
\]

Hence, collecting the bounds,
\[ |\text{tr}(\hat{\Sigma}\hat{Z}) - \text{tr}(\Sigma_0u_1u_1^T)| \leq \lambda/2(s + \epsilon^2/\lambda) + 2\left(3\Lambda_{\text{max}}\epsilon + 2\Lambda_{\text{max}}^{1/2}\sqrt{\epsilon}\right) : = \zeta.
\]

But then, assuming \(\Lambda_{\text{max}} - \zeta > 0\),
\[ \|\hat{\beta}_{\text{init}} - \beta_0\|_2 \leq |\text{tr}(\hat{\Sigma}\hat{Z})^{1/2} - \text{tr}(\Sigma_0u_1u_1^T)^{1/2}|\|\hat{u}_1\|_2 \\
+ \text{tr}(\Sigma_0u_1u_1^T)^{1/2}\|\hat{u}_1 - u_1\|_2 = \frac{1}{2\sqrt{\Lambda_{\text{max}} - \zeta}} \zeta + 2\sqrt{\epsilon}\Lambda_{\text{max}}^{1/2}.
\]

\[\Box\]

### 6.2 Proofs for Section 3.2

#### 6.2.1 Oracle inequalities for the second step estimator

**Proof of Theorem 1.** The definition of a stationary point \(\hat{\beta}\) in particular implies
\[ (\hat{\beta}, \lambda\hat{Z})^T(\beta_0 - \hat{\beta}) \geq 0, \] (23)

where \(\hat{Z}\) is the sub-differential of the \(\ell_1\)-norm of \(\beta\) evaluated at \(\hat{\beta}\). By Taylor expansion of the population loss, we obtain
\[ R(\beta_0) - R(\hat{\beta}) = \hat{\beta}(\beta_0 - \hat{\beta}) + \frac{1}{2}(\beta_0 - \hat{\beta})^T\hat{R}(\beta_0 - \hat{\beta}), \]

for an intermediate point \(\hat{\beta} = \alpha\hat{\beta} + (1 - \alpha)\beta_0\), for some \(\alpha \in [0, 1]\).

Since \(\|\beta - \beta_0\|_2 \leq \eta\), Lemma 1 implies \(\Lambda_{\text{min}}(\hat{R}(\hat{\beta})) \geq 2(\rho - 3\eta) > 0\). Thus, combining (23) and (24) and rearranging yields
\[ R(\hat{\beta}) - R(\beta_0) + (\hat{\beta}(\beta_0 - \hat{\beta}) - \lambda\hat{Z}^T(\beta_0 - \hat{\beta}) \leq 0.
\]

Using that \(\hat{\beta}\) and \(\hat{Z}\) satisfies
\[ \hat{Z}^T\hat{\beta} = \|\hat{\beta}\|_1 \quad \text{and} \quad \|\hat{Z}\|_\infty\|\beta_0\|_1 \leq \|\beta_0\|_1.
\]

\[ \]
it follows
\[ R(\hat{\beta}) - R(\beta_0) + \lambda \|\hat{\beta}\|_1 \leq \lambda \|\beta_0\|_1 + \mathcal{E}(\hat{\beta}), \]
where we denoted the empirical process term by
\[ \mathcal{E}(\beta) := |(R_n(\beta) - \hat{R}(\beta))^T (\hat{\beta}_0 - \beta)|. \]

It remains to bound the random term \( \mathcal{E}(\hat{\beta}) \). Note that
\[ \mathcal{E}(\hat{\beta}) = - (\hat{\beta} - \beta_0)^T W(\hat{\beta} - \beta_0) + \beta_0^T W(\beta_0 - \hat{\beta}), \]
where we denote \( W := \tilde{\Sigma} - \Sigma_0 \). First note that for \( \lambda_0 = 4\sigma^2 \|\beta_0\|_2 (\lambda_0 + \lambda_0^2) \), by Lemma 7 it follows that with probability at least \( 1 - \alpha \), where \( \alpha := 2e^{-\log(2p)} \)
\[ \|W\beta_0\|_\infty \leq \lambda_1. \]
Hence
\[ \|\beta_0^T W(\beta_0 - \hat{\beta})\|_\infty \leq \lambda_1 \|\beta_0 - \hat{\beta}\|_1. \] (25)

By Lemma 10 with \( \lambda_0 = \sqrt{\frac{\log(2p)}{n}} \), by (25) and using Hölder’s inequality, with probability at least \( 1 - 2(J + 2)e^{-\log(2p)} \),
\[ \mathcal{E}(\hat{\beta}) \leq \lambda_0 \|\hat{\beta} - \beta_0\|_1 + \lambda_2 \|\hat{\beta} - \beta_0\|_1 + 4 \times 27\sigma^2 \left[ 3 \|\hat{\beta} - \beta_0\|_1^2 \lambda_0^2 + \sqrt{6} \|\hat{\beta} - \beta_0\|_1 \lambda_0 \right] \|\hat{\beta} - \beta_0\|_2^2, \]
where \( \lambda_2 = 4\sigma^2 (\lambda_0 + \lambda_0^2) \). Next by the triangle inequality and by the definition of the tuning parameter \( T \),
\[ \lambda_0 \|\beta_0 - \hat{\beta}\|_1 \leq \lambda_0 \|\beta_0\|_1 + \lambda_0 T \leq C_T. \]
Then it follows
\[ 3 \|\hat{\beta} - \beta_0\|_1 \lambda_0^2 + \sqrt{6} \|\hat{\beta} - \beta_0\|_1 \lambda_0 \leq \|\hat{\beta} - \beta_0\|_1 \lambda_0 (3C_T + \sqrt{6}). \]
But then
\[ \mathcal{E}(\hat{\beta}) \leq 4 \times 27\sigma^2 C_T (3C_T + \sqrt{6}) \|\hat{\beta} - \beta_0\|_2^2 + (\lambda_2 + \lambda_0^2) \|\hat{\beta} - \beta_0\|_1. \]

By the condition on the tuning parameter \( \lambda \), we have \( \lambda \geq 2(\lambda_2 + \lambda_0^2) \), hence
\[ \mathcal{E}(\hat{\beta}) \leq 4 \times 27\sigma^2 C_T (3C_T + \sqrt{6}) \|\hat{\beta} - \beta_0\|_2^2 + \lambda / 2 \|\hat{\beta} - \beta_0\|_1. \]
Returning to the oracle inequality, by the condition \( \rho - 3\eta \geq c_0 \sigma^2 C_T (3C_T + \sqrt{6}) \), where we take \( c_0 := 2 \times 4 \times 27 \), we obtain
\[ R(\hat{\beta}) - R(\beta_0) + \lambda \|\hat{\beta}\|_1 \leq \lambda \|\beta_0\|_1 + (\rho - 3\eta)/2 \|\beta_0 - \hat{\beta}\|_2^2 + \lambda / 2 \|\beta_0 - \hat{\beta}\|_1. \] (26)
The oracle inequalities then follow by the usual techniques (see e.g. Bühlmann and van de Geer [2011]), since the population risk satisfies \( R(\hat{\beta}) - R(\beta_0) \geq (3\rho - \eta) \|\hat{\beta} - \beta_0\|_2^2 \) as already derived above.

\[ \square \]
6.2.2 Oracle inequalities for nodewise regression

In this section, we derive the rates of convergence for the estimator \( \hat{\Theta} \) defined in Algorithm 1. These results are contained in Lemmas 4 and 5 below. Recall the definition of the population parameters \( \gamma_j^0 \) from (18) and define

\[
\tau_j^2 = \mathbb{E} \hat{R}_n(\beta_0)_{j,j} - \hat{R}_n(\beta_0)_{j,-j} \gamma_j^0. 
\]

We now summarize several relationships that will be used throughout the proofs without further reference. One can easily check that the definition of \( \gamma_j^0 \) implies

\[
\gamma_j^0 = (\hat{R}(\beta_0)_{-j,-j})^{-1}\hat{R}(\beta_0)_{j,-j},
\]

provided that the matrix is \( \hat{R}(\beta_0)_{-j,-j} \) is invertible. One can also verify that \( \tau_j^2 \) satisfies

\[
\frac{1}{\tau_j^2} = \Theta_0^0.
\]

It is moreover not difficult to calculate the following relations, which will be used throughout the proofs:

\[
\Lambda_{\min}(\hat{R}(\beta_0)) = \phi_\max^2 - \phi_2^2,
\]

\[
\Lambda_{\max}(\hat{R}(\beta_0)) = 2\phi_\max^2,
\]

\[
\Lambda_{\min}(\Theta_0) = 1/(2\phi_\max^2),
\]

\[
\Lambda_{\max}(\Theta_0) = 1/(\phi_\max^2 - \phi_2^2).
\]

This also implies \( 1/\tau_j^2 \leq \Lambda_{\max}(\Theta_0) \leq 1/(\phi_\max^2 - \phi_2^2) \) and hence \( \tau_j^2 \geq \phi_\max^2 - \phi_2^2 \).

To simplify notation, in this section we denote \( \alpha := \phi_\max^2 - \phi_2^2 \).

**Lemma 4.** Assume Condition 1 with parameter \( \sigma \), let

\[
\lambda_0 = \sqrt{\log(2p)/n},
\]

\[
\bar{\lambda}_1 \geq 16\sigma^2(||\gamma_j^0||_2 + 1)[\lambda_0 + \lambda_0^2]
\]

\[
\rho - 3\eta \geq c_0\sigma^2 C_T[3C_T + \sqrt{6}],
\]

where \( c_0 \) is a suitable universal constant. Let the tuning parameters \( \lambda_j, T_j, j = 1, \ldots, p \) of the program (8) satisfy

\[
\lambda_j \geq 2\bar{\lambda}_1,
\]

\[
T_j \leq C_T/(2\lambda_0) \text{ and } ||\gamma_j^0||_1 \leq T_j.
\]

Then any stationary point \( \hat{\gamma}_j \) as defined in (9) satisfies with probability at least \( 1 - 2(J + 1)e^{-2\log(2p)} \), where \( J = \left\lfloor \log T \right\rfloor \),

\[
\max_{j=1,\ldots,p} ||\hat{\gamma}_j - \gamma_j^0||_2 + \lambda_j ||\hat{\gamma}_j - \gamma_j^0||_1 \leq \max_{j=1,\ldots,p} \frac{C_1 s_j \lambda_j^2}{(\rho - 3\eta)^2},
\]

where \( s_j = ||\gamma_j^0||_0 \) and \( C_1 \) is a universal constant.
Proof of Lemma 4. The proof is similar to the proof of Lemma 1. For simplicity, we denote the loss function by $L_n(\gamma_j) := \Gamma_j^T \tilde{R}_n(\beta) \Gamma_j$ where the notation is as in (10). Define $L(\gamma_j) := \Gamma_j^T \tilde{R}(\beta) \Gamma_j$. The derivatives are denoted by dots. The definition of the stationary point $\hat{\gamma}_j$ implies

$$(\hat{L}_n(\hat{\gamma}_j) + \lambda \hat{Z})^T (\gamma^0_j - \hat{\gamma}_j) \geq 0,$$  
(30)

where $\hat{Z}$ is the sub-differential of the $\ell_1$-norm evaluated at $\hat{\gamma}_j$. By Taylor expansion of the population loss, we obtain

$$L(\gamma^0_j) - L(\hat{\gamma}_j) = \hat{L}(\hat{\gamma}_j) + (\hat{\gamma}_j - \gamma^0_j)^T (\gamma^0_j - \hat{\gamma}_j) - \lambda_j \hat{Z}^T (\gamma^0_j - \hat{\gamma}_j).$$  
(31)

We have $\Lambda_{\text{min}}(\tilde{R}(\beta)) \geq 2(\rho - 3\eta)$ by Lemma 1. Thus, combining (30) and (31) and rearranging yields

$$L(\hat{\gamma}_j) - L(\gamma^0_j) + (\hat{L}_n(\hat{\gamma}_j) - \hat{L}(\hat{\gamma}_j)) (\gamma^0_j - \hat{\gamma}_j) - \lambda_j \hat{Z}^T (\gamma^0_j - \hat{\gamma}_j) \leq 0.$$  
(32)

Then it follows (using that $\hat{Z}^T \hat{\gamma}_j = \|\hat{\gamma}_j\|_1$ and $|\hat{Z}^T \gamma^0_j| \leq \|\hat{Z}\|_\infty \|\gamma^0_j\|_1 \leq \|\gamma^0_j\|_1$)

$$L(\hat{\gamma}_j) - L(\gamma^0_j) + \lambda_j \|\hat{\gamma}_j\|_1 \leq \lambda_j \|\gamma^0_j\|_1 + |(\hat{L}_n(\hat{\gamma}_j) - \hat{L}(\hat{\gamma}_j)) (\gamma^0_j - \hat{\gamma}_j)|.$$  
(33)

It remains to bound the term

$$(\hat{L}_n(\hat{\gamma}_j) - \hat{L}(\hat{\gamma}_j))^T (\gamma^0_j - \hat{\gamma}_j) = 2(\Sigma_{j,-j} - \Sigma^0_{j,-j})^T (\gamma^0_j - \hat{\gamma}_j) + 2\hat{\gamma}_j^T (\Sigma_{j,-j} - \Sigma^0_{j,-j}) (\gamma^0_j - \hat{\gamma}_j).$$

We may use the same bounds as in Lemma 1, only now we need to consider maximum over all $j = 1, \ldots, p$. Hence by union bound, we obtain with probability at least $1 - 2(J + 1)e^{-\log(2p)/n}$, with $\lambda_0 = \sqrt{\frac{2 \log(2p)}{n}}$, and

$$\bar{\lambda}_1 \geq 16\sigma^2(\|\gamma^0\|_2 + 1)(\lambda_0 + \lambda_0^2),$$

and by the definition of tuning parameters $T_j$,

$$|(\hat{L}_n(\hat{\gamma}_j) - \hat{L}(\hat{\gamma}_j))^T (\gamma^0_j - \hat{\gamma}_j)| \leq 4 \times 27\sigma^2 C_T (3C_T + \sqrt{6}) \|\hat{\gamma}_j - \gamma^0_j\|_2^2 + \lambda_j / \|\beta - \beta_0\|_1.$$  
(34)

Returning to the oracle inequality, we have

$$L(\hat{\gamma}_j) - L(\gamma^0_j) + \lambda_j \|\hat{\gamma}_j\|_1 \leq \lambda_j \|\gamma^0_j\|_1 + (\rho - 3\eta)/2 \|\gamma^0_j - \hat{\gamma}_j\|_2^2 + \lambda_j / 2 \|\gamma^0_j - \hat{\gamma}_j\|_1.$$  
(34)

By the usual techniques (see e.g. Bühlmann and van de Geer [2011]), we obtain the oracle inequalities.

\[\square\]
Lemma 5. Suppose that conditions of Lemma 4 are satisfied and denote $\mu := \|\hat{\beta} - \beta_0\|_2$ and $\hat{c}_j := \hat{\gamma}_j - \gamma_0^j$. Then for $\lambda_0 \geq \|\hat{\Sigma} - \Sigma_0\|_\infty$, it holds

$$|\hat{\tau}^2_j - \tau^2_j| \leq r_{\tau,j},$$

where

$$r_{\tau,j} := \lambda_0 (\|\hat{c}_j\|_1 + \sqrt{s_j + \phi^2_{\text{max}}}/\alpha) + 2\phi^2_{\text{max}}\|\hat{c}_j\|_2 + 2\mu(\mu + 2\phi_{\text{max}})(\|\hat{c}_j\|_2 + \phi^2_{\text{max}}/\alpha).$$

Moreover, if $\alpha - r_{\tau,j} > 0$,

$$\|\hat{\Theta}_j - \Theta^0_j\|_1 \leq \frac{1}{\alpha} \|\hat{c}_j\|_1 + \left(1 + \sqrt{s_j + \phi^2_{\text{max}}}/\alpha\right) \frac{r_{\tau,j}}{\alpha - r_{\tau,j}},$$

$$\|\hat{\Theta}_j - \Theta^0_j\|_2 \leq \frac{1}{\alpha} \|\hat{c}_j\|_2 + \left(1 + \phi^2_{\text{max}}/\alpha\right) \frac{r_{\tau,j}}{\alpha - r_{\tau,j}},$$

where $\alpha = \Lambda_1 - \Lambda_2$.

Proof of Lemma 5. First, one can easily show from the KKT conditions for the nodewise Lasso that $\hat{\tau}^2_j = \hat{R}_n(\hat{\beta})_j^T \hat{\Gamma}_j$. Consider the decomposition

$$\hat{\tau}^2_j - \tau^2_j = \underbrace{(\hat{R}_n(\hat{\beta})_j - \hat{R}(\hat{\beta}_0)_j)^T \hat{\Gamma}_j}_{i} + \underbrace{(\hat{R}(\hat{\beta})_j - \hat{R}(\beta)_j)^T \hat{\Gamma}_j}_{ii} + \underbrace{\hat{R}(\beta)_j^T (\hat{\Gamma}_j - \Gamma^0_j)}_{iii}.$$

We need to bound the terms $i$, $ii$, $iii$. Before doing so, we prepare a few preliminary results. Firstly,

$$\|\Gamma^0_j\|_2 = ((\Theta^0_j)^T (\Theta^0_j))^{1/2}/\Theta^0_j \leq \Lambda_{\text{max}}(\Theta_0)/\Lambda_{\text{min}}(\Theta_0) \leq 2\phi^2_{\text{max}}/\alpha.$$  

Next observe,

$$\|\|\hat{\beta}\|_2^2 - \|\beta_0\|_2^2\| \leq \|\beta_0 - \beta_0\|_2^2 + 2\|\beta_0\|_2 \|\hat{\beta} - \beta_0\|_2 \leq \mu^2 + 2\phi_{\text{max}}\mu.$$  

(35)
Hence,
\[
\| (\hat{R}(\hat{\beta}) - \hat{R}(\beta_0)) e_j \|_2 = \| (\| \hat{\beta} \|_2^2 - \| \beta_0 \|_2^2) e_j + \hat{\beta}_j - \beta_0^j \|_2 \\
\leq \| \| \hat{\beta} \|_2^2 - \| \beta_0 \|_2^2 \| + \| \hat{\beta}_j - \beta_0^j \|_2 \\
+ \| \beta_0^j \|_2^2 \| \hat{\beta}_j - \beta_0^j \|_2 \\
\leq \| \| \hat{\beta} \|_2^2 - \| \beta_0 \|_2^2 \| + \| \hat{\beta}_j \|_2 \| \hat{\beta}_j - \beta_0^j \|_2 \\
+ \| \beta_0^j \|_2^2 \| \hat{\beta}_j - \beta_0^j \|_2 \\
\leq 2\mu^2 + 2\phi_{\max} \mu.
\]

Now using the above preliminaries, we obtain the bounds for \( i, ii, iii \). Firstly, observing that
\[
\| \hat{\Gamma}_0 \|_1 \leq \sqrt{s_j + 1} \| \hat{\Gamma}_0 \|_2,
\]
where \( \| \hat{\Sigma} - \Sigma_0 \|_\infty \leq \lambda_0 \). Moreover,
\[
| ii | \leq \| \hat{R}(\hat{\beta}_j) - \hat{R}(\beta_0) \|_2 \| \hat{\Gamma}_j \|_2 \\
\leq 2\mu(\mu + \phi_{\max})(\| \hat{\epsilon}_j \|_2 + 2\phi_{\max}^2/\alpha).
\]

Next
\[
| iii | \leq \| \hat{R}(\beta_0) \|_2 \| \hat{\epsilon}_j \|_2 \\
= 2\phi_{\max}^2 \| \hat{\epsilon}_j \|_2.
\]

Thus collecting the results above,
\[
| \hat{\tau}_j^2 - \tau_j^2 | \leq r_{\tau,j},
\]
where
\[
r_{\tau,j} := \lambda_0(\| \hat{\epsilon}_j \|_1 + \sqrt{s_j + 1} \phi_{\max}^2/\alpha) \\
+ 2\phi_{\max}^2 \| \hat{\epsilon}_j \|_2 \\
+ 2\mu(\mu + 2\phi_{\max})(\| \hat{\epsilon}_j \|_2 + \phi_{\max}^2/\alpha).
\]
By the mean value theorem,
\[
| \frac{1}{\hat{\tau}_j^2} - \frac{1}{\tau_j^2} | \leq \frac{1}{\hat{\tau}_j^2} | \hat{\tau}_j^2 - \tau_j^2 |,
\]
for some intermediate point \( \hat{\tau}_j^2 \). But we have
\[
\hat{\tau}_j^2 \geq \tau_j^2 - | \hat{\tau}_j^2 - \tau_j^2 | \geq 1/\Theta_{jj}^0 - | \hat{\tau}_j^2 - \tau_j^2 | \geq \alpha - r_{\tau,j},
\]
Hence, assuming that \( \alpha - r_{\tau,j} > 0 \),
\[
| \frac{1}{\hat{\tau}_j^2} - \frac{1}{\tau_j^2} | \leq \frac{r_{\tau,j}}{\alpha - r_{\tau,j}}.
\]
Then we can easily obtain the rates of convergence for \( \hat{\Theta}_j \) using the bound

\[
\| \hat{\Theta}_j - \Theta_0 \|_1 \leq \frac{1}{\alpha} \| \hat{\gamma}_j \|_1 + \left( 1 + 2\sqrt{s_j} + \frac{\phi^2_{\text{max}}}{\alpha} \right) \frac{r_{\tau,j}}{\alpha - r_{\tau,j}}.
\]

Hence

\[
\| \hat{\Theta}_j - \Theta_0 \|_1 \leq \frac{1}{\alpha} \| \hat{\gamma}_j \|_1 + \left( 1 + 2\sqrt{s_j} + \frac{\phi^2_{\text{max}}}{\alpha} \right) \frac{r_{\tau,j}}{\alpha - r_{\tau,j}}.
\]

Similarly follow the rates for \( \| \hat{\Theta}_j - \Theta_0 \|_2 \).

**Proof of Lemma 3.** Follows from Lemmas 4 and 5 by noting that \( \alpha = \phi_1^2 - \phi_2^2 \geq \rho^2 \geq \phi_0^2 \) for a universal constant, and \( \phi_{\text{max}} \leq C_{\text{max}} \). Then by Lemma 4 it follows \( \max_{j=1,...,p} \| \hat{\gamma}_j - \gamma_j \|_2 = O_P(\text{max}_j s_j \lambda_j^2) \) and \( \max_{j=1,...,p} \| \hat{\gamma}_j - \gamma_j \|_1 = O_P(\text{max}_j s_j \lambda_j) \). By Lemma 5 (since \( \| \hat{\Sigma} - \Sigma_0 \|_\infty = O_P(\sqrt{\log p/n}) \)), it then follows \( \max_{j=1,...,p} \| \hat{\Theta}_j - \Theta_j \|_2 = O_P(\text{max}_j s_j \lambda_j^2) \),

and

\[
\max_{j=1,...,p} \| \hat{\Theta}_j - \Theta_j \|_1 = O_P(\text{max}_j s_j \lambda_j).
\]



\[\]

**6.2.3 Asymptotic normality**

**Proof of Theorem 2.** Using Taylor expansion of the function \( \beta \mapsto \hat{\Theta}_j^T \hat{R}_n(\beta) \) around \( \beta_0 \) we obtain:

\[
\hat{\Theta}_j^T \hat{R}_n(\hat{\beta}) = \hat{\Theta}_j^T \hat{R}_n(\beta_0) + \hat{\Theta}_j^T \hat{R}_n(\hat{\beta})(\hat{\beta} - \beta_0),
\]

where \( \hat{\beta} = \alpha \hat{\beta} + (1 - \alpha) \beta_0 \) for some \( \alpha \in [0, 1] \). Then for the de-sparsified estimator, we may write the decomposition

\[
\hat{b}_j - \beta_j^0 = \hat{\beta}_j - \beta_j^0 - \hat{\Theta}_j^T \hat{R}_n(\hat{\beta})
\]

\[
= - (\Theta_j^0)^T \hat{R}_n(\beta_0)
\]

\[
- (\hat{\Theta}_j - \Theta_j^0)^T \hat{R}_n(\beta_0)
\]

\[
+ \hat{\beta}_j - \beta_j^0 - \Theta_j^T \hat{R}_n(\hat{\beta})(\hat{\beta} - \beta_0)
\]

\[
- \hat{\Theta}_j^T (\hat{R}_n(\hat{\beta}) - \hat{R}_n(\hat{\beta}))(\hat{\beta} - \beta_0),
\]

We first bound \( ii \) using Hölder’s inequality and the KKT conditions for nodewise Lasso for inversion of \( \hat{R}_n(\hat{\beta}) \). The estimator \( \hat{\gamma}_j \) is defined as any stationary
point of the program (10), but as we have shown oracle inequalities for \( \hat{\gamma}_j \), for 
\( n \) sufficiently large, \( \hat{\gamma}_j \) must lie in the interior of the feasible set and hence the 
KKT conditions \(-2\bar{R}_n(\hat{\beta})_\cdot - \gamma_j + 2\bar{R}_n(\hat{\beta})_\cdot - \gamma_j + \lambda_j \partial |\hat{\gamma}_j|_1 = 0\), are satisfied 
with high probability. The KKT conditions for nodewise regression imply that 
\[ \|\bar{R}_n(\hat{\beta})_j - e_j\|_\infty = O(\lambda_j^{1/2}) \] (see e.g. van de Geer et al. [2014]). Hence 
\[
|ii| = \|\hat{\beta} - \beta_0\|_\infty \|e_j - \hat{\Theta}_j^T \bar{R}_n(\hat{\beta})\|_\infty \leq \|\hat{\beta} - \beta_0\|_1 \|e_j - \hat{\Theta}_j^T \bar{R}_n(\hat{\beta})\|_\infty \\
\leq \|\hat{\beta} - \beta_0\|_1 \lambda_j^{1/2} \frac{\gamma_j}{\hat{\gamma}_j^2}.
\]
Next we bound \( iii \) using the Cauchy-Schwarz inequality 
\[
|iii| \leq \|\hat{\beta} - \beta_0\|_2 |\hat{\Theta}_j^T (\bar{R}_n(\hat{\beta}) - \bar{R}_n(\beta_0))|_2.
\]
By the definition of \( \hat{\beta} \) it follows that \( \|\hat{\beta} - \beta_0\|_2 \leq \|\hat{\beta} - \beta_0\|_2. \) But then 
\[
\|\hat{\Theta}_j^T (\bar{R}_n(\hat{\beta}) - \bar{R}_n(\beta_0))\|_2 \\
\leq \|\hat{\Theta}_j^T (\bar{R}_n(\hat{\beta}) - \bar{R}_n(\beta_0))\|_2 + \|\hat{\Theta}_j^T (\bar{R}_n(\hat{\beta}) - \bar{R}_n(\beta_0))\|_2 \\
\leq \|\hat{\Theta}_j\|_2 \|\|\hat{\beta}\|_2 - \|\beta_0\|_2\|_2 + \|\hat{\Theta}_j\|_2 \|\|\hat{\beta}\|_2 - \|\beta_0\|_2\|_2 + \|\|\hat{\beta}\|_2 - \|\beta_0\|_2\|_2 \\
\leq \|\hat{\Theta}_j\|_2 \left( \|\|\hat{\beta}\|_2 - \|\beta_0\|_2\|_2 + \|\|\hat{\beta}\|_2 - \|\beta_0\|_2\|_2 \right) \\
\leq \|\hat{\Theta}_j\|_2 (2\mu^2 + 2\phi_{\max} \mu) \\
\leq (\|\hat{\Theta}_j - \Theta_0\|_2 + 1/\alpha)(2\mu^2 + 2\phi_{\max} \mu).
\]
where we used the bound (35) from the proof of Lemma 5. Therefore, 
\[
|iii| \leq (\|\hat{\Theta}_j - \Theta_0\|_2 + 1/\alpha)(2\mu^2 + 2\phi_{\max} \mu) \mu.
\]
Finally, 
\[
|i| \leq \|\hat{\Theta}_j - \Theta_0\|_1 \|\bar{R}_n(\beta_0)\|_\infty \\
= \|\hat{\Theta}_j - \Theta_0\|_1 \|\bar{R}_n(\beta_0) - \bar{R}(\hat{\beta}_0)\|_\infty \\
= \|\hat{\Theta}_j - \Theta_0\|_1 \|\bar{R}_n(\beta_0) - \bar{R}(\hat{\beta}_0)\|_\infty \\
\leq \lambda_0 \|\hat{\Theta}_j - \Theta_0\|_1,
\]
for \( \lambda_0 \geq \|\|\Sigma - \Sigma_0\|\beta_0\|_\infty \). Hence the bound for the remainder is 
\[
\begin{align*}
\max_{j=1,\ldots,p} |\text{rem}_j| \\
:= \max_{j=1,\ldots,p} |i| + |ii| + |iii| \\
\leq \max_{j=1,\ldots,p} \|\hat{\beta} - \beta_0\|_1 \lambda_j^{1/2} \frac{\gamma_j}{\hat{\gamma}_j^2} \\
+ (\|\hat{\Theta}_j - \Theta_0\|_2 + 1/\alpha)(2\|\hat{\beta} - \beta_0\|_2 + 2\phi_{\max} \|\hat{\beta} - \beta_0\|_2) \|\hat{\beta} - \beta_0\|_2 \\
+ \|\hat{\Theta}_j - \Theta_0\|_1 \lambda_0.
\end{align*}
\]
We now combine the last bound with the result of Lemma 5 and probability results from Section 6.3. In particular, under the Condition 1 and the assumptions \( \phi_{\max} \leq C_{\max}, \rho - 3\eta \geq c > 0 \) and the assumed sparsity conditions, it follows that

\[
\max_{j=1,\ldots,p} |\text{rem}_j| = O_P \left( \max_{j=1,\ldots,p} \max(s, s_j) \max \left( \lambda^2, \lambda_j^2, \log(2p) \right) \right) = o_p \left( \frac{1}{\sqrt{n}} \right).
\]

Thus we conclude that

\[
\hat{\beta} - \beta - \hat{\Theta} \hat{R}_n(\hat{\beta}) = -\Theta_0 \hat{R}_n(\beta_0) + o_p(1/\sqrt{n}).
\]

Finally, one can easily check that the random variable \((\Theta_0^T X^i (X^i)^T \beta_0)\) has bounded fourth moments under Condition 1 with \(\sigma\) is a universal constant and if \(\phi_{\max} \leq C_{\max}, \rho \geq c > 0\). Hence we may use the Lindeberg central limit theorem on the term \((\Theta_0^T \hat{R}_n(\beta_0) / \sigma_j \rightarrow N(0, 1)\)

This then implies

\[
\sqrt{n}(\hat{\beta}_j - \beta_{0j}) / \sigma_j = \sqrt{n}(\Theta_0^T \hat{R}_n(\beta_0) / \sigma_j + o_p \left( \frac{1}{\sigma_j} \right) \rightarrow N(0, 1).
\]

\[
\square
\]

**Proof of Theorem 3.** By Theorem 2, we have the asymptotic expansion

\[
\hat{b} - \beta_0 = -\Theta_0 \hat{R}_n(\beta_0) + \text{rem},
\]

with \(\|\text{rem}\|_{\infty} = O_p(s \max(\lambda^2, \max_{j=1,\ldots,p} \lambda_j^2, \log p / n))\). Hence

\[
\|\hat{\beta}\|_2^2 - \|\beta_0\|_2^2 = 2 \beta_0^T (\hat{\beta} - \beta_0) + (\hat{\beta} - \beta_0)^T (\hat{\beta} - \beta_0) = 2 \beta_0^T (\hat{\beta} - \beta_0 - \hat{\Theta} \hat{R}_n(\beta)) + 2 \beta_0^T \hat{\Theta}^T \hat{R}_n(\beta) + \|\hat{\beta} - \beta_0\|_2^2 = 2 \beta_0^T (\hat{b} - \beta_0) + \|\hat{\beta} - \beta_0\|_2^2 = -2 \beta_0^T \Theta_0 \hat{R}_n(\beta_0) + 2 \beta_0^T \hat{\Theta}^T \hat{R}_n(\beta) + \text{rem}_2,
\]

where the remainder \(\text{rem}_2\) can be bounded

\[
|\text{rem}_2| := 2 \beta_0^T \text{rem} + 2(\beta_0 - \hat{\beta})^T \hat{\Theta}^T \hat{R}_n(\hat{\beta}) + \|\hat{\beta} - \beta_0\|_2^2 \leq 2 \|\beta_0\|_1 \|\text{rem}\|_{\infty} + 2 \|\beta_0 - \hat{\beta}\|_1 \left\| \hat{\Theta}^T \right\|_1 \|\hat{R}_n(\hat{\beta})\|_{\infty} + \|\hat{\beta} - \beta_0\|_2^2 \leq O_p(\sqrt{n} \max(s, s_j) \max(\lambda^2, \max_{j=1,\ldots,p} \lambda_j^2, \log p / n)) + O_p(\sqrt{n} \max(s, s_j) \lambda^2) + O_p(s \lambda^2) = O_p(\max(s, s_j) 3/2 \max(\lambda^2, \max_{j=1,\ldots,p} \lambda_j^2, \log p / n)).
\]
Hence, under the sparsity conditions, we obtain
\[ \|\hat{\beta} - \beta_0\|_2^2 - 2\hat{\beta}^T \hat{\Theta} \hat{R}_n(\hat{\beta}) = -2\beta_0^T \Theta_0 \hat{R}_n(\beta_0) + o_P(1/\sqrt{n}). \]
As in the proof of Theorem 2, it follows that the zero-mean random variable $2\hat{\beta}^T \Theta_0 \hat{R}_n(\beta_0)$ has bounded fourth moments. Asymptotic normality then follows by an application of the Lindeberg central limit theorem.

Lemma 6. If $X_i \sim \mathcal{N}(0, \Sigma_0), i = 1, \ldots, n$ and $\rho > 0$, then it holds that
\[ \sigma^2 = \text{var}(\Theta_0^T \hat{\Sigma} \beta_0) = \frac{\beta_0^2}{2} + \|\beta_0\|_2^4 \sum_{i=1, i \neq j}^p u_{i,j}^2 \frac{\Lambda_i}{(\Lambda_i - \Lambda_{\text{max}})^2}, \]
and
\[ \sigma^2 = 4\text{var}(\Theta_0^T \hat{\Sigma} \beta_0) = 2\Lambda_{\text{max}}. \]

Proof of Lemma 6. First under normality, it is well-known that
\[ \sigma^2 = (\Theta_0^T \Sigma_0 \Theta_0 \beta_0)^2 = \|\beta_0\|_2^4 \sum_{i=1, i \neq j}^p u_{i,j}^2 \frac{\Lambda_i}{(\Lambda_i - \Lambda_{\text{max}})^2}, \]
and
\[ \sigma^2 = 4\beta_0^2 \Theta_0 \Sigma_0 \Theta_0 \beta_0 = 4(\|\beta_0\|_2^4 \beta_0^T \Theta_0 \beta_0)^2. \]
We first calculate $\Theta_0 := \hat{R}(\beta_0)^{-1}$. We write the eigendecomposition of $\Sigma_0$ as $\Sigma_0 = U^T \Lambda U$, for some $U$ such that $U^T U = 1$. By the condition $\rho > 0$, the first column of $U$ is $u_1 = \beta_0/\|\beta_0\|_2$. Then we may write
\[ \hat{R}(\beta_0) = U^T (-\Lambda + \|\beta_0\|_2^2 + 2U \beta_0 \beta_0^T U^T) U = U^T (-\Lambda + \|\beta_0\|_2^2 + 2\|\beta_0\|_2^2 e_1 e_1^T) U, \]
which can be easily inverted
\[ \Theta_0 = \hat{R}(\beta_0)^{-1} = U^T DU, \]
where
\[ D := \text{diag} \left( \frac{1}{2\|\beta_0\|_2^2}, \frac{1}{\|\beta_0\|_2^2 - \Lambda_2(S_0)}, \ldots, \frac{1}{\|\beta_0\|_2^2 - \Lambda_p(S_0)} \right). \]
Then we have
\[ \Theta_0 \beta_0 = U^T DU \beta_0 = U^T \frac{1}{2\|\beta_0\|_2^2} \|\beta_0\|_2^2 e_1 = \beta_0/(2\|\beta_0\|_2^2), \]
and
\[ \Theta_0 \Sigma_0 \Theta_0 = U^T DADU. \]
Finally, we conclude
\[ \sigma^2 = 4\beta_0^2 \Theta_0 \Sigma_0 \Theta_0 \beta_0 + 4(\beta_0^T \Theta_0 \Sigma_0 \beta_0)^2 \]
\[ = 4 \frac{1}{4} \|\beta_0\|_2^4 + \frac{1}{2} \|\beta_0\|_2^4 = 2\|\beta_0\|_2^2 = 2\Lambda_{\text{max}}, \]
34
and
\[
\sigma_j^2 := (\Theta_j^0)^T \Sigma_0 \Theta_j^0 \beta_0 + ((\Theta_j^0)^T \Sigma_0 \beta_0)^2
\]
\[
= (\Theta_j^0)^T \Sigma_0 \Theta_j^0 \beta_0 \Sigma_0 \beta_0 + ((\Theta_j^0)^T \Sigma_0 \beta_0)^2
\]
\[
= \|\beta_0\|_2^2 U^T \Lambda^{1/2} D^{1/2} U + \frac{\beta_j^0}{4}
\]
\[
= \frac{\beta_j^0}{4} + \beta_j^0 + \|\beta_0\|_2^2 \sum_{i=1, i \neq j}^p u_{i,j}^2 (\Lambda_i - \Lambda_{\text{max}}^2).
\]

6.3 Probabilistic bounds for the empirical process

We collect probabilistic results needed to bound the empirical process part related to the estimators \( \hat{\beta}, \hat{\gamma}_j \). Recall the definition of a sub-Gaussian matrix from Condition 1.

**Lemma 7.** If \( X \in \mathbb{R}^{n \times p} \) is a sub-Gaussian matrix with parameter \( \sigma \), then for any fixed vector \( \beta \), with probability at least \( 1 - 2e^{-\log(2p)} \) it holds

\[
\| (\hat{\Sigma} - \Sigma_0) \beta \|_{\infty} \leq 4\|\beta\|_2 \sigma^2 \left( \sqrt{\frac{2\log(2p)}{n}} + \frac{2\log(2p)}{n} \right).
\]

**Proof of Lemma 7.** The result follows from Lemma 14.13 in Bühlmann and van de Geer [2011].

**Lemma 8.** If \( X \in \mathbb{R}^{n \times p} \) is a sub-Gaussian matrix with parameter \( \sigma \), then for all \( t > 0 \)

\[
P \left( \sup_{\theta \in \mathbb{R}^p : \| \theta \|_2 = 1, \| \theta \|_r \leq M} \left| \frac{\|X\theta\|_2^2}{n} - \mathbb{E} \frac{\|X\theta\|_2^2}{n} \right| \geq 2\sigma^2 (t + \sqrt{2t}) \right)
\]
\[
\leq 2 \exp \left( -nt + 2M\log(2p) \right)
\]

**Proof of Lemma 8.** This lemma is essentially Lemma 15 in Loh and Wainwright [2012], but we apply a slightly different version of Bernstein’s inequality, namely Lemma 14.9 in Bühlmann and van de Geer [2011].

Denote \( \mathbb{B}_r(M) = \{ \theta \in \mathbb{R}^p : \| \theta \|_r \leq M \} \) for \( r \geq 0 \).

**Lemma 9** (Lemma 11 in Loh and Wainwright [2012]). For any constant \( s \geq 1 \), it holds

\[
\mathbb{B}_1(\sqrt{s}) \cap \mathbb{B}_2(1) \subseteq 3\text{cl}(\text{conv}(\mathbb{B}_0(s) \cap \mathbb{B}_2(1))),
\]
where \( \text{cl}(\cdot) \) denotes the topological closure of a set and \( \text{conv}(\cdot) \) denotes the convex hull.
Lemma 10. Suppose that $X \in \mathbb{R}^{n \times p}$ is a sub-Gaussian matrix with parameter $\sigma$. Let $J := \lceil \log_2(T) \rceil$, and

$$\lambda_0 = \sqrt{\frac{2 \log(2p)}{n}},$$

$$\lambda_1 = 4\sigma^2(\lambda_0 + \lambda_0^2).$$

Then with probability at least $1 - 2(J + 1)2e^{-\log(2p)}$, it holds

$$\forall \theta \in B, \|\theta\|_1 \leq T :$$

$$|\theta^T W \theta| \leq \lambda_1 \|\theta\|_1 + \delta \|\theta\|_2^2,$$

where

$$\delta_M := 4 \times 2\sigma^2 \left[ 3M^2 \lambda_0^2 + \sqrt{6}M \lambda_0 \right].$$

Proof. Consider the set

$$A := \{ \theta \in B : \|\theta\|_1 \leq T \},$$

and the decomposition

$$A = A_0 \cup A_0^c,$$

where

$$A_0 := \{ \theta \in A : \|\theta\|_1 \leq 1 \}.$$

We denote $W := \hat{\Sigma} - \Sigma_0$. First note that for $\lambda_1 = 4\sigma^2(\lambda_0 + \lambda_0^2)$, by Lemma 7 it follows that with probability at least $1 - \alpha_1$, where $\alpha_1 := 2e^{-\log(2p)}$

$$\|W\|_\infty \leq \lambda_1.$$  \(36\)

If we are on the set $A_0$ and then by Hölder’s inequality and bound (36), with probability at least $1 - \alpha_1$, for all $\theta \in A$

$$|\theta^T W \theta| \leq \|W\|_\infty \|\theta\|_1^2 \leq \|W\|_\infty \|\theta\|_1 \leq \lambda_1 \|\theta\|_1.$$  \(37\)

To treat the complementary set, $A_0^c$, we use the peeling device (van de Geer [2000]). Let $M_j := 2^j$ and let $J$ be the smallest integer such that $2^J \geq T$. Consider partitioning of the set $A_0^c$

$$A_0^c = \bigcup_{j=1}^{J} A_j$$

where

$$A_j := \{ \theta \in A : M_{j-1} \leq \|\theta\|_1 \leq M_j \}.$$

Using the union bound and the definition of $A_j$ we obtain the sequence of upper bounds in the display below. Note that in the inequality (39) below, we used that $4\delta_{M_{j-1}}^2 \geq \delta_{M_j^2}^2$.  

36
We now show that if 

\[ \sup_{v: \|v\|_2 = 1, \|v\|_0 \leq M} |v^T Wv| \leq \delta, \]  

then

\[ |\theta^T W\theta| \leq 27\delta, \quad \forall \theta \in \text{cl(conv}(\mathbb{B}_2(3) \cap \mathbb{B}_0(M^2_j))). \]  

(42)

First if \( \theta \in \text{conv}(\mathbb{B}_2(3) \cap \mathbb{B}_0(M^2_j)) \), then we can write \( \theta = \sum_i v_i \alpha_i \), where \( v_i \in \mathbb{B}_2(3) \cap \mathbb{B}_0(M^2_j) \). For each \( i, j \) it holds

\[
|v_i^T Wv_j| = \frac{1}{2} |(v_i + v_j)^T W(v_i + v_j) - v_i^T Wv_i - v_j^T Wv_j| \\
\leq \frac{1}{2} (36\delta + 9\delta + 9\delta) = 27\delta.
\]

Hence

\[
|\theta^T W\theta| = |\sum_{i,j} v_i^T Wv_j| \leq \sum_{i,j} 27\delta \alpha_i \alpha_j = 27\delta.
\]

If \( \theta \) is in the closure of the set \( \text{conv}(\mathbb{B}_2(3) \cap \mathbb{B}_0(M^2_j)) \), we can obtain an analogous implication as \( (41) \Rightarrow (42) \) by continuity arguments. Therefore, we can continue...
the chain of bounds

\[
\sum_{j=1}^{J} P \left( \exists \theta \in \text{cl}(\text{conv}(B_2(3) \cap B_0(M_j^2))) : |\theta^T W \theta| \geq 27\delta M_j^2 \right) \quad (43)
\]

\[
\leq \sum_{j=1}^{J} P \left( \sup_{v: \|v\|_2=1, \|v\|_0 \leq M_j} |v^T W v| \geq \delta M_j^2 \right) \\
\leq \sum_{j=1}^{J} 2e^{-M_j^2 \log(2p)} \\
\text{(Lemma 8)} \leq 2Je^{-\log(2p)}.
\]

Therefore we conclude from (37) and (44) that

\[
P(\exists \theta \in A : |\theta^T W \theta| \geq \lambda_1 \|\theta\|_1 + 4\delta \|\theta\|_1^2 \|\theta\|_2^2) \\
\leq P(\exists \theta \in A_0 : |\theta^T W \theta| \geq \lambda_1 \|\theta\|_1) \\
+ P(\exists \theta \in A_0^c : |\theta^T W \theta| \geq 4\delta \|\theta\|_1^2 \|\theta\|_2^2) \\
\leq 2(J + 1)e^{-\log(2p)}.
\]

\[
\square
\]

References

Amini, A. and Wainwright, M. (2009). High-dimensional analysis of semidefinite relaxations for sparse principal components. *Annals of Statistics*, 37(5b):2877–2921.

Anderson, T. W. (1963). Asymptotic theory for principal component analysis. *Annals of Mathematical Statistics*, 34(1):122–148.

Bai, Z. D. and Yin, Y. Q. (1993). Limit of the smallest eigenvalue of large dimensional covariance. *Annals of Probability*, 21(3):1275–1294.

Baik, J. and Silverstein, J. W. (2006). Eigenvalues of large sample covariance matrices of spiked population models. *Journal of Multivariate Analysis*, 97:1382–1408.

Belloni, A., Chernozhukov, V., and Kato, K. (2015). Uniform post selection inference for LAD regression and other Z-estimation problems. *Biometrika*, 102(1):77–94.

Berthet, Q. and Rigollet, P. (2013). Optimal detection of sparse principal components in high dimension. *Annals of Statistics*, 41(4):1780–1815.
Birnbaum, A., Johnstone, I. M., Nadler, B., and Paul, D. (2013). Minimax bounds for sparse pca with noisy high-dimensional data. *The Annals of Statistics*, 41:1055–1084.

Bühlmann, P. and van de Geer, S. (2011). Statistics for high-dimensional data. *Springer*.

Cai, T. and Guo, Z. (2015). Confidence intervals for high-dimensional linear regression: Minimax rates and adaptivity. *ArXiv: 1506.05539*.

Cai, T., Ma, Z., and Wu, Y. (2013). Sparse PCA: Optimal rates and adaptive estimation. *Annals of Statistics*, 41(6):3074–3110.

Chernozhukov, V., Hansen, C., and Spindler, M. (2015). Valid post-selection and post-regularization inference: An elementary, general approach. *Annual Review of Economics*, 7(1):649–688.

d’Aspremont, A., El Ghaoui, L., Jordan, M., and Lanckriet, G. (2007). A Direct Formulation for Sparse PCA Using Semidefinite Programming. *SIAM Review*, 49(3):434–448.

Deshpande, Y. and Montanari, A. (2014). Sparse PCA via covariance thresholding. In *Advances in Neural Information Processing Systems*, pages 334–342.

Fan, J. and Wang, W. (2015). Asymptotics of Empirical Eigen-structure for Ultra-high Dimensional Spiked Covariance Model. *ArXiv:1502.04733*.

Janková, J. and van de Geer, S. (2015). Confidence intervals for high-dimensional inverse covariance estimation. *Electronic Journal of Statistics*, 9(1):1205–1229.

Janková, J. and van de Geer, S. (2016). Confidence regions for generalized linear models under sparsity. *ArXiv: 1610.01353*.

Janková, J. and van de Geer, S. (2016). Honest confidence regions and optimality for high-dimensional precision matrix estimation. *TEST*, 26(1):143–162.

Javanmard, A. and Montanari, A. (2014). Confidence intervals and hypothesis testing for high-dimensional regression. *Journal of Machine Learning Research*, 15(1):2869–2909.

Johnstone, I. M. (2001). On the distribution of the largest eigenvalue in principal components analysis. *Annals of Statistics*, 29(2):295–327.

Johnstone, I. M. and Lu, A. Y. (2009). On consistency and sparsity for principal components analysis in high dimensions. *Journal of the American Statistical Association*, 104(486):682–693.

Jolliffe, I. T., Trendafilov, N. T., and Uddin, M. (2003). A modified principal component technique based on the lasso. *Journal of Computational and Graphical Statistics*, 12(3):531–547.
Kollo, T. and Neudecker, H. (1997). Asymptotics of Pearson-Hotelling principal-component vectors of sample variance and correlation matrices. *Behaviorometrika*, 24(1):51–69.

Koltchinskii, V., Löffler, M., and Nickl, R. (2017). Efficient Estimation of Linear Functionals of Principal Components. *ArXiv e-prints*.

Koltchinskii, V. and Lounici, K. (2017). New asymptotic results in principal component analysis. *Sankhya A*, 79(254).

Koltchinskii, V., Lounici, K., et al. (2016). Asymptotics and concentration bounds for bilinear forms of spectral projectors of sample covariance. In *Annales de l’Institut Henri Poincaré, Probabilités et Statistiques*, volume 52, pages 1976–2013. Institut Henri Poincaré.

Koltchinskii, V., Lounici, K., et al. (2017). Normal approximation and concentration of spectral projectors of sample covariance. *The Annals of Statistics*, 45(1):121–157.

Loh, P. and Wainwright, M. (2014). Regularized M-estimators with nonconvexity: Statistical and algorithmic theory for local optima. *Journal of Machine Learning Research*, 1:1–56.

Loh, P.-L. and Wainwright, M. J. (2012). High-dimensional regression with noisy and missing data: Provable guarantees with nonconvexity. *Annals of Statistics*, 40(3):1637–1664.

Paul, D. (2007). Asymptotics of sample eigenstructure for a large dimensional spiked covariance model. *Statistica Sinica*, 17:1617–1642.

Shen, D., Shen, H., Zhu, H., and Marron, J. (2013). Surprising asymptotic conical structure in critical sample eigen-directions. *ArXiv:1303.6171*.

van de Geer, S. (2000). *Empirical processes in M-estimation*. Springer.

van de Geer, S. (2014). On the uniform convergence of empirical norms and inner products, with application to causal inference. *Electronic Journal of Statistics*, 8(1):543–574.

van de Geer, S. (2016). *Estimation and Testing under Sparsity: École d’Été de Saint-Flour XLV*. Springer.

van de Geer, S., Bühlmann, P., Ritov, Y., and Dezeure, R. (2014). On asymptotically optimal confidence regions and tests for high-dimensional models. *Annals of Statistics*, 42(3):1166–1202.

Vu, V., Cho, J., Lei, J., and Rohe, K. (2013). Fantope Projection and Selection: A near-optimal convex relaxation of Sparse PCA. *Advances in Neural Information Processing Systems (NIPS)*, 26.
Vu, V. and Lei, J. (2012). Minimax rates of estimation for sparse PCA in high dimensions. *Journal of Machine Learning Research*, 22:1278–1286.

Zhang, C.-H. and Zhang, S. S. (2014). Confidence intervals for low-dimensional parameters in high-dimensional linear models. *Journal of the Royal Statistical Society: Series B*, 76:217–242.

Zou, H., Hastie, T., and Tibshirani, R. (2006). Sparse principal component analysis. *Journal of Computational and Graphical Statistics*, 15:265–286.