# Principal Components Analysis in high dimensions

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#### Overview

- Motivation and PCA
  - Dimension reduction
  - Perturbations
- 2 Bounds for generic eigenvectors
  - General result
  - Spiked ensemble
- Sparse PCA
  - General result
  - Spiked model with sparsity

#### **Overview**

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#### Motivations

We consider  $\Sigma \in \mathcal{S}_+^{d \times d}$  which is a positive semidefinite matrix with an ordered eigenvalues  $\gamma_1(\Sigma) \geq \gamma_2(\Sigma) \geq \cdots \gamma_d(\Sigma) \geq 0$  and denote  $\mathcal{S}_{d-1}$  as the unit sphere. Assuming random variable  $\boldsymbol{X}$  with  $\mathbb{E}\boldsymbol{X}=0$ , then we obtain the maximal eigenvector as

$$\textbf{v}^* = \arg\max_{\textbf{v} \in \mathcal{S}_{d-1}} \mathrm{var}(\textbf{v}^\top \textbf{\textit{X}}) = \arg\max_{\textbf{v} \in \mathcal{S}_{d-1}} \textbf{v}^\top \boldsymbol{\Sigma} \textbf{v}.$$

More generally, we seek orthonormal matrix  $V \in \mathbb{R}^{d imes r}$  satisfying

$$V = \arg \max_{\mathcal{V}} \mathbb{E} ||V^{\top} \mathbf{X}||_2^2 = \arg \max_{\mathcal{V}} tr(V^{\top} \Sigma V).$$

By variational representation :

$$\sum_{i=1}^{k} \gamma_k(\Sigma) = \max\{tr(V^{\top}XV) : V \in \mathbb{R}^{n \times k}, V^{\top}V = I\}$$

, we know that  $V=(v_1,\cdots,v_r)$  where  $v_1,\cdots,v_r$  are first r eigenvectors of  $\Sigma$  with  $v_i^\top v_i=\delta_{ii}$ .

#### Uses of PCA

#### 1 Low-rank Approximation:

$$Z^* = \arg\min_{r(Z) \le r} (\|\Sigma - Z\|^2) = \sum_{j=1}^r \gamma_j(\Sigma) v_j v_j^\top,$$

where the matrix norm is invariant under orthonormal transformation. The solution can be derived by spectral decomposition of  $\Sigma = PDP^{\top}$  and let  $\tilde{Z} = P^{\top}ZP$ , laeding to  $r(Z) = r(\tilde{Z})$ . Under the Frobenius norm, we conclude  $\tilde{Z}$  has to be diagonal to achieve the minimum  $\tilde{Z} = diag(\gamma_1, \cdots, \gamma_r, 0, \cdots, 0)$ . So that  $Z^* = P\tilde{Z}P^{\top} = \sum_{i=1}^r \gamma_i(\Sigma)v_iv_i^{\top}$ . And our approximated arror is

$$\|Z^* - \Sigma\|_F^2 = \sum_{j=r+1}^d \gamma_j^2(\Sigma).$$

#### Uses of PCA

#### 2 Data Compression:

Given a zero-mean random variable  $X \in \mathbb{R}^d$ , we consider a projection to a subspace  $\mathbb{V}$  of dimension r.

$$\mathbb{V}^* = \arg\min_{\mathbb{V}} \mathbb{E} \left[ \| \textbf{\textit{X}} - \Pi_{\mathbb{V}}(\textbf{\textit{X}}) \|_2^2 \right].$$

We assume that the subspace  $\mathbb{V}^*$  is spanned by orthonormal vectors, i.e., its matrix expression is  $V_r$ , so that  $\Pi_{\mathbb{V}^*}(\mathbf{X}) = V_r V_r^{\top} \mathbf{X}$ .

$$\mathbb{E}\left[\|\boldsymbol{X} - V_r V_r^{\top} \boldsymbol{X}\|_2^2\right] = \mathbb{E}\left[\boldsymbol{X}^{\top} (I - V_r V_r^{\top}) \boldsymbol{X}\right] = tr((I - V_r V_r^{\top}) \Sigma)$$
$$= \sum_{i=1}^{d} \gamma_j(\Sigma) - tr(V_r^{\top} \Sigma V_r),$$

so we should maximize  $tr(V_r^\top \Sigma V_r)$ . By variational representation we know that  $V_r = (v_1, \dots, v_r)$ , whose vectors are top r eigenvectors of  $\Sigma$ , and  $\mathbb{V}^*$  is spanned by those vectors.

# Approximation and Perturbation

In practice, we do not know the covariance matrix  $\Sigma$  of the population  $\boldsymbol{X}$ . Instead, we make estimation by  $\hat{\Sigma} = \frac{1}{n} \sum_{i=1}^{n} \boldsymbol{x}_{i} \boldsymbol{x}_{i}^{\top}$ . Then a natural question rises: What is the gap between  $\Sigma$  and  $\hat{\Sigma}$ .

Given a symmetric matrix R, how does its eigenstructure relate to the perturbed matrix Q=R+P, where P is another symmetric matrix. In fact

$$\gamma_1(Q) \leq \max_{v \in \mathcal{S}_{d-1}} v^\top (R+P) v \leq \max_{v \in \mathcal{S}_{d-1}} v^\top R v + \max_{v \in \mathcal{S}_{d-1}} v^\top P v \leq \gamma_1(R) + \|P\|_2,$$

which means

$$|\gamma_1(Q) - \gamma_1(R)| \le ||Q - R||_2,$$

where  $\|\cdot\|_2$  denotes the operator norm of matrix.

# Weyl's Inequality

We claim that

$$\max_{j=1,\cdots,d} |\gamma_j(Q) - \gamma_j(R)| \le \|Q - R\|_2.$$

To prove this, we only need to prove

$$\gamma_j(Q) = \min_{\mathbb{V} \in \mathcal{V}_{j-1}} \max_{u \in \mathbb{V}^{\perp} \cap \mathcal{S}_{d-1}} u^{\top} Q u,$$

where  $V_{j-1}$  means all subspace of dimension j-1.

For all subspace of dimension k-1  $S_{k-1}$ , let  $S'=span\{u_1,\cdots,u_k\}$ , where eigenvectors of Q are  $\{u_1,\cdots,u_d\}$ . Then  $S'\cap S_{k-1}^{\perp}\neq 0$ . Thus, there exists  $x=\sum_{i=1}^k\alpha_iu_i\in S_{k-1}^{\perp}, \|x\|=1$ , satisfying  $x^{\top}Qx\geq \gamma_k$ , so that  $\max_{u\in \mathbb{V}^{\perp}\cap S_{d-1}}u^{\top}Qu\geq \gamma_k$ . Noting that, the process above is applied to all subspace of dimension k-1, then we have

$$\min_{\mathbb{V}\in\mathcal{V}_{j-1}}\max_{u\in\mathbb{V}^{\perp}\cap\mathcal{S}_{d-1}}u^{\top}Qu\geq\gamma_{k}.$$

Finally, we take  $S_{k-1} = span\{u_1, \dots, u_{k-1}\}$  to attain the equality.

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#### Notations

Given  $\Sigma \geq 0$  and  $\gamma_1(\Sigma) \geq \cdots \gamma_d(\Sigma) \geq 0$ , corresponding to its eigenvectors  $\{v_1, \cdots, v_d\}$ , let  $\theta^* \in \mathbb{R}^d$  be its (unique) maximal eigenvector. We have the perturbation as  $\hat{\Sigma} = \Sigma + P$ .

Define eigengap  $\nu = \gamma_1(\Sigma) - \gamma_2(\Sigma)$  assumed to be strictly positive. Define the transformed pertubation matrix

$$ilde{P} := U^{ op} P U = egin{pmatrix} ilde{p}_{11} & ilde{p}^{ op} \ ilde{p} & ilde{p}_{22} \end{pmatrix}$$

where  $\tilde{p}_{11} \in \mathbb{R}$ .

A direct observation is that  $|\tilde{p}_{11}| \leq ||\tilde{P}||_2$ , because  $|\tilde{p}_{11}| = e_1^\top \tilde{P} e_1 \leq ||\tilde{P}||_2$ .



#### Bound for maximal vector

#### Thereom 8.5

Given any  $P \in S^{d \times d}$  such that  $\|P\|_2 < \nu/2$ , the perturbed matrix  $\hat{\Sigma} = \Sigma + P$  has a unique maximal eigenvector  $\hat{\theta}$  satisfying the bound

$$\|\hat{\theta} - \theta^*\|_2 \le \frac{2\|\tilde{p}\|_2}{\nu - 2\|P\|_2}.$$

Define  $\hat{\Delta} = \hat{\theta} - \theta^*$  and the function

$$\psi(\Delta; P) = \Delta^{\top} P \Delta + 2 \Delta^{\top} P \theta^*.$$

Moreover, assume that  $\rho = \hat{\theta}^{\top} \theta^*$ , thus,  $\hat{\theta} = \rho \theta^* + \sqrt{1 - \rho^2} z$  where  $z \in \mathbb{R}^d$  which is orthogonal to  $\theta^*$ .

## Lemma 8.6 (PCA basic inequality)

$$\nu \left( 1 - \left( \hat{\theta}^{\top} \theta^* \right)^2 \right) \le |\psi(\hat{\Delta}; P)|. \tag{8.15}$$

Recall  $\tilde{P} = U^{T}PU$ , then we have

$$\psi(\Delta; P) = \hat{\Delta}^{\top} U \tilde{P} U^{\top} \hat{\Delta} + 2 \hat{\Delta}^{\top} U \tilde{P} U^{\top} \theta^*.$$
 (8.16)

Define  $U=(\theta^*,U_2)$  and  $\tilde{z}=U_2^\top z\in\mathbb{R}^{d-1}\Rightarrow \|\tilde{z}\|_2=\|z\|_2\leq 1$ . We can calculate that

$$\psi(\Delta; P) = (\rho^2 - 1)\tilde{p}_{11} + 2\rho\sqrt{1 - \rho^2}\tilde{z}^\top \tilde{p} + (1 - \rho^2)\tilde{z}^\top \tilde{P}_{22}\tilde{z}.$$

Thus,

$$\nu(1-\rho^2) \overset{8.15}{\leq} |\psi(\hat{\Delta}; P)| \leq 2(1-\rho^2) \|\tilde{P}\|_2 + 2\rho\sqrt{1-\rho^2} \|\tilde{p}\|_2,$$

## proof

which means  $\sqrt{1-\rho^2} \leq \frac{2\rho\|\tilde{p}\|_2}{\nu-2\|\tilde{P}\|_2}$ . Recall  $\|\hat{\Delta}\|_2 = \sqrt{2(1-\rho)}$ , we have

$$\|\hat{\Delta}\|_2 \leq \frac{\sqrt{2}}{\sqrt{1+\rho}} \sqrt{1-\rho^2} \leq \frac{\sqrt{2}}{\sqrt{1+\rho}} \frac{2\rho \|\tilde{p}\|_2}{\nu-2 \|\tilde{P}\|_2} \leq \frac{2 \|\tilde{p}\|_2}{\nu-2 \|\tilde{P}\|_2},$$

where the final inequality is because  $2\rho^2 \le 1 + \rho, \forall \rho \in [0, 1]$ .

Now we turn to the proof of 8.15: by definition we have  $(\theta^*)^{\top} \hat{\Sigma} \theta^* \leq (\hat{\theta})^{\top} \hat{\Sigma} \hat{\theta}$ . Under the defintion of  $P = \hat{\Sigma} - \Sigma$ , we have

$$tr\Big[\Sigma^{\top}\left(\theta^{*}(\theta^{*})^{\top}-\hat{\theta}(\hat{\theta})^{\top}\right)\Big] = tr\Big[\left(\Sigma-\hat{\Sigma}\right)\left(\theta^{*}(\theta^{*})^{\top}-\hat{\theta}(\hat{\theta})^{\top}\right)\Big]$$

$$+tr\Big[\hat{\Sigma}\left(\theta^{*}(\theta^{*})^{\top}-\hat{\theta}(\hat{\theta})^{\top}\right)\Big] \leq -tr\Big[P\left(\theta^{*}(\theta^{*})^{\top}-\hat{\theta}(\hat{\theta})^{\top}\right)\Big]$$

$$=-\left(\hat{\theta}^{\top}P\hat{\theta}-(\theta^{*})^{\top}P\theta^{*}\right) = -\psi(\hat{\Delta};P).$$
(\*)

Now we control the LHS in \*, by defining  $\Gamma = \Sigma - \gamma_1 \theta^*(\theta^*)^\top = \sum_{j=2}^d \gamma_j \theta_j \theta_j^\top \Rightarrow \Gamma \theta^* = 0. \text{ By considering } x = \sum_{j=1}^d x_j \theta_i \text{ with } \theta_1 = \theta^*, \text{ we have } x^\top \Gamma x \leq \gamma_2 \Rightarrow \|\Gamma\|_2 \leq \gamma_2. \text{ Then } x \leq \gamma_2 \Rightarrow \|\Gamma\|_2 \leq \gamma_2.$ 

$$tr\left[\Sigma^{\top}\left(\theta^*(\theta^*)^{\top} - \hat{\theta}(\hat{\theta})^{\top}\right)\right] = tr\left[\gamma_1(1-\rho^2)\right] - tr\left[\Gamma\hat{\theta}(\hat{\theta})^{\top}\right]$$
$$= (1-\rho^2)(\gamma_1 - z^{\top}\Gamma z) \ge (1-\rho^2)\nu.$$

Combining \*, we have

$$(1-\rho^2)\nu \leq -\psi(\hat{\Delta}; P)$$

which finishes the proof of Lemma.

# Spiked ensemble

A sample  $extbf{\emph{x}}_i \in \mathbb{R}^d$  from the spiked covariance ensemble takes the form

$$\mathbf{x}_{i} \stackrel{d}{=} \sqrt{\nu} \xi_{i} \theta^{*} + w_{i},$$

where  $\xi_i \in \mathbb{R}, \xi_i \sim (0,1), w_i \in \mathbb{R}^d, w_i \sim (0,I_d), \xi \perp w_i$  and  $\theta^* \in \mathcal{S}_{d-1}$ . It has a form similar to Factor anlysis

$$\mathbf{X} - \mu = \mathbf{LF} + \epsilon \Rightarrow \mathbf{\Sigma} = \mathbf{LL}^{\top} + \psi.$$

Under the spiked ensemble, we have the form of covariance as

$$\Sigma = \nu \theta^* (\theta^*)^\top + I_d.$$

By construction, if we take  $x \in \mathcal{S}_{d-1}$ , we have  $x^{\top} \Sigma x = \nu (x^{\top} \theta^*)^2 + 1 \leq \nu + 1$  by CS inequality. We achieve the equality when  $x = \theta^*$ , thus  $\gamma_1(\Sigma) = \nu + 1, \gamma_2(\Sigma) = \cdots = \gamma_d(\Sigma) = 1$ . Then  $\gamma_1(\Sigma) - \gamma_2(\Sigma) = \nu$ .

#### Error bounds

In the following result, we say that  $\mathbf{x}_i \in \mathbb{R}^d$  has sub-Gaussian tails if both  $\xi_i$ ,  $w_i$  are sub-Gaussian with parameter at most 1.

#### Corollary 8.7

Given i.i.d. sample  $\{ {m x}_i \}_{i=1}^n$  from the spiked covariance ensemble with sub-Gaussian tails, suppose that n>d and  $\sqrt{\frac{\nu+1}{\nu^2}}\sqrt{\frac{d}{n}} \leq \frac{1}{128}$ . Then, with probability at least  $1-c_1 exp(-c_2 n \min\{\sqrt{\nu}\delta,\nu\delta^2\})$ , there is a unique maximal eigenvector  $\hat{\theta}$  of the sample covariance matrix  $\hat{\Sigma} = \frac{1}{n} {m x}_i {m x}_i^{\top}$  such that

$$\left\|\hat{\theta} - \theta^*\right\|_2 \le c_0 \sqrt{\frac{\nu+1}{\nu^2}} \sqrt{\frac{d}{n}} + \delta.$$

In order to apply 9, we let  $P = \hat{\Sigma} - \Sigma$ ,  $\tilde{P} = U^{\top}PU$  and derive upper bound for  $\|P\|_2$  and  $\|\tilde{p}\|_2$ . Define  $\bar{w} = \frac{1}{n} \sum_{i=1}^n \xi_i w_i$ , then  $\hat{\Sigma} = \frac{1}{n} \sum_{i=1}^n (\sqrt{\nu} \xi_i \theta^* + w_i) (\sqrt{\nu} \xi_i \theta^* + w_i)^{\top}$ . We have the decomposition of P as

$$P = \underbrace{\nu\left(\frac{1}{n}\sum_{i=1}^{n}\xi_{i}^{2}-1\right)\theta^{*}(\theta^{*})^{\top}}_{P_{1}} + \underbrace{\sqrt{\nu}(\bar{w}(\theta^{*})^{\top}+\theta^{*}\bar{w}^{\top})}_{P_{2}} + \underbrace{\left(\frac{1}{n}\sum_{i=1}^{n}w_{i}w_{i}^{\top}-I_{d}\right)}_{P_{3}}$$

Therefore, we have the upper bound as

$$||P||_2 \le \nu \left| \frac{1}{n} \sum_{i=1}^n \xi_i^2 - 1 \right| + 2\sqrt{\nu} ||\bar{w}||_2 + \left| \left| \frac{1}{n} w_i w_i i^\top - I_d \right| \right|_2.$$
 (8.22a)

By the notation of  $U=(\theta^*,U_2)$ , we have  $\tilde{p}=\sqrt{\nu}U_2^{\top}\bar{w}+U_2^{\top}\left(\frac{1}{n}\sum_{i=1}^n w_iw_i^{\top}-I\right)\theta^*$ . Noting that  $\|U_2^{\top}\bar{w}\|_2\leq \|\bar{w}\|_2$  and also

$$\left\| \frac{1}{n} \sum_{i=1}^{n} U_{2}^{\top} w_{i} \langle w_{i}, \theta^{*} \rangle \right\|_{2} \stackrel{CS}{=} \sup_{v \in \mathcal{S}_{d-1}} \left| (U_{2}v)^{\top} \left( \frac{1}{n} \sum_{i=1}^{n} w_{i} w_{i}^{\top} - I \right) \theta^{*} \right|$$

$$\leq \sup_{v \in \mathcal{S}_{d-1}} \| U_{2}^{\top} v \|_{2} \left\| \frac{1}{n} \sum_{i=1}^{n} w_{i} w_{i}^{\top} - I \right\|_{2} \leq \left\| \frac{1}{n} \sum_{i=1}^{n} w_{i} w_{i}^{\top} - I \right\|_{2}$$

where the last inequality is because  $\|U_2^\top v\|_2 \le \|v\|_2$ . Therefore, we have

$$\|\tilde{p}\|_{2} \le \sqrt{\nu} \|\bar{w}\|_{2} + \left\| \frac{1}{n} \sum_{i=1}^{n} w_{i} w_{i}^{\top} - I \right\|_{2}.$$
 (8.22b)



#### Concentration Lemma

#### Lemma 8.8

Under the conditions of Corollary 8.7, we have

$$P\left(\left|\frac{1}{n}\sum_{i=1}^{n}\xi_{i}^{2}-1\right|\geq\delta_{1}\right)\leq2exp(-c_{2}n\min\{\delta_{1},\delta_{1}^{2}\}),\tag{8.23a}$$

$$P\left(\|\bar{w}\|_{2} \ge 2\sqrt{\frac{d}{n}} + \delta_{2}\right) \le 2exp(-c_{2}n\min\{\delta_{2}, \delta_{2}^{2}\}),$$
 (8.23b)

$$P\left(\left\|\frac{1}{n}\sum_{i=1}^{n}w_{i}w_{i}^{\top}-I\right\|_{2} \geq c_{3}\sqrt{\frac{d}{n}}+\delta_{3}\right) \leq 2\exp(-c_{2}n\min\{\delta_{3},\delta_{3}^{2}\}). \tag{8.23c}$$

8.23a is because product of sub-Gaussian is sub-Exponential; 8.23c is the result of Example 6.2 in Page 162.

We define

$$\begin{array}{l} \phi(\delta_1,\delta_2,\delta_3) = 2e^{-c_2n\min\{\delta_1,\delta_1^2\}} + 2e^{-c_2n\min\{\delta_2,\delta_2^2\}} + 2e^{-c_2n\min\{\delta_3,\delta_3^2\}}. \ \ \text{We} \\ \text{apply Lemma 8.8 with } \delta_1 = \frac{1}{16}, \delta_2 = \frac{\delta}{4\sqrt{\nu}}, \delta_3 = \delta/16 \in (0,1), \ \text{we have} \end{array}$$

$$||P||_2 \leq \frac{\nu}{16} + 8(\sqrt{\nu} + 1)\sqrt{\frac{d}{n}} + \delta \leq \frac{\nu}{16} + 16(\sqrt{\nu} + 1)\sqrt{\frac{d}{n}} + \delta.$$

As long as  $\sqrt{\frac{\nu+1}{\nu^2}}\sqrt{\frac{d}{n}} \leq \frac{1}{128}$ , we have

$$||P||_2 \le \frac{3}{16}\nu + \delta < \frac{\nu}{4} < \frac{\nu}{2} \quad \forall \delta \in (0, \frac{\nu}{16}).$$

Also, we have

$$\|\tilde{p}\|_2 \leq 2(\sqrt{\nu}+1)\sqrt{\frac{d}{n}} + \delta \leq 4\sqrt{\nu+1}\sqrt{\frac{d}{n}} + \delta.$$

Finally, by 9 we finish the proof.

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## Motivations

- Corollary 8.7 requires that the sample size *n* be larger than the dimension *d* in order for ordinary PCA to perform well.
- For any fixed signal-to-noise ratio, if the ratio d/n stays suitably bounded away from zero, then the eigenvectors of the sample covariance in a spiked covariance model become asymptotically orthogonal to their population analogs.
- Via the framework of minimax theory that no method can produce consistent estimators of the population eigenvectors when d/n stays bounded away from zero.
- So, the simplest such structure is that of sparsity in the eigenvectors, which allows for both effective estimation in high-dimensional settings.

#### General result

Consider the constrained problem

$$\widehat{\theta} \in \arg\max_{\|\theta\|_2 = 1} \{ \langle \theta, \widehat{\Sigma}\theta \rangle \} \quad \text{ such that } \|\theta\|_1 \le R, \tag{1}$$

as well as the penalized variant

$$\widehat{\theta} \in \arg\max_{\|\theta\|_2 = 1} \left\{ \langle \theta, \widehat{\mathbf{\Sigma}} \theta \rangle - \lambda_n \|\theta\|_1 \right\} \quad \text{ such that } \|\theta\|_1 \le \left(\frac{n}{\log d}\right)^{1/4}. \tag{2}$$

- $R = \|\theta^*\|_1$ .
- The regularization parameter  $\lambda_n$  can be chosen without knowledge of the true eigenvector  $\theta^*$ .

#### Error bounds

$$\sup_{\substack{\Delta = \theta - \theta^* \\ \|\theta\|_2 = 1}} |\Psi(\Delta; \mathbf{P})| \le c_0 v \|\Delta\|_2^2 + \varphi_v(n, d) \|\Delta\|_1 + \psi_v^2(n, d) \|\Delta\|_1^2$$
 (3)

#### Theorem 8.10

Given a matrix  $\Sigma$  with a unique, unit-norm, s-sparse maximal eigenvector  $\theta^*$  with eigengap v, let  $\hat{\Sigma}$  be any symmetric matrix satisfying the uniform deviation condition (3) with constant  $c_0 < \frac{1}{6}$ , and  $16s\psi_v^2(n,d) \le c_0v$ .

- (a) For any optimal solution  $\widehat{\theta}$  to the constrained program (1) with
- $R = \|\theta^*\|_1$ ,  $\min\left\{\left\|\widehat{\theta} \theta^*\right\|_2, \left\|\widehat{\theta} + \theta^*\right\|_2\right\} \leq \frac{8}{\sqrt{1-4c_0}}\sqrt{s}\varphi_{\nu}(n, d)$ .
- (b) Consider the penalized program (2) with the regularization parameter lower bounded as  $\lambda_n \geq 4 \left(\frac{n}{\log d}\right)^{1/4} \psi_{\nu}^2(n,d) + 2\varphi_{\nu}(n,d)$ . Then any

optimal solution  $\widehat{\theta}$  satisfies the bound

$$\min\left\{\left\|\widehat{\theta}-\theta^*\right\|_2, \left\|\widehat{\theta}+\theta^*\right\|_2\right\} \leq \frac{2\left(\frac{\lambda_n}{\varphi_{\mathcal{V}}(n,d)}+4\right)}{\nu(1-4c_0)}\sqrt{s}\varphi_{\mathcal{V}}(n,d).$$

#### Lemma 8.11

Under the conditions of Theorem 8.10, the error vector  $\widehat{\Delta} = \widehat{\theta} - \theta^*$  satisfies the cone inequality

$$\left\|\widehat{\Delta}_{S^c}\right\|_1 \leq 3 \left\|\widehat{\Delta}_S\right\|_1 \quad \text{ and hence } \|\widehat{\Delta}\|_1 \leq 4\sqrt{s}\|\widehat{\Delta}\|_2.$$

# Proof: Argument for constrained estimator

Note that  $\|\widehat{\theta}\|_1 \leq R = \|\theta^*\|_1$  by construction of the estimator, and moreover  $\theta^*_{S^c} = 0$  by assumption. By Lemma 8.11, we have

$$|\Psi(\hat{\Delta}; \mathbf{P})| \leq c_0 v \|\hat{\Delta}\|_2^2 + 4\sqrt{s}\varphi_v(n, d) \|\hat{\Delta}\|_2 + 16s\psi_v^2(n, d) \|\hat{\Delta}\|_2^2.$$

Substituting back into the basic inequality and performing some algebra yields

$$v\left\{\frac{1}{2}-c_{0}-16\frac{s}{v}\psi_{v}^{2}(n,d)\right\}\|\hat{\Delta}\|_{2}^{2}\leq 4\sqrt{s}\varphi_{v}(n,d)\|\hat{\Delta}\|_{2}.$$

Note that our assumptions imply that  $\kappa > \frac{1}{2} (1 - 4c_0) > 0$ , so that the bound follows.

# Proof: Argument for regularized estimator

With the addition of the regularizer, the basic inequality now takes the slightly modified form

$$\frac{\textit{v}}{2}\|\hat{\boldsymbol{\Delta}}\|_2^2 - |\boldsymbol{\Psi}(\hat{\boldsymbol{\Delta}};\boldsymbol{P})| \leq \lambda_\textit{n}\left\{\|\boldsymbol{\theta}^*\|_1 - \|\widehat{\boldsymbol{\theta}}\|_1\right\} \leq \lambda_\textit{n}\left\{\left\|\hat{\boldsymbol{\Delta}}_\textit{S}\right\|_1 - \left\|\hat{\boldsymbol{\Delta}}_\textit{S^c}\right\|_1\right\},$$

We find that

$$v\underbrace{\left\{\frac{1}{2}-c_0-\frac{16}{v}s\psi_v^2(n,d)\right\}}_{\kappa}\|\hat{\Delta}\|_2^2\leq \sqrt{s}(\lambda_n+4\varphi_v(n,d))\|\hat{\Delta}\|_2.$$

Our assumptions imply that  $\kappa \geq \frac{1}{2} (1 - 4c_0) > 0$ , from which claim (b) follows.

#### Proof of Lemma 8.11

Combining the uniform bound with the basic inequality

$$0 \leq \nu \underbrace{(\frac{1}{2} - c_0)}_{>0} \|\Delta\|_2^2 \leq \varphi_{\nu}(n, d) \|\Delta\|_1 + \psi_{\nu}^2(n, d) \|\Delta\|_1^2 + \lambda_n \left\{ \left\| \widehat{\Delta}_{\mathcal{S}} \right\|_1 - \left\| \widehat{\Delta}_{\mathcal{S}^c} \right\|_1 \right\}$$

Introducing the shorthand  $R = \left(\frac{n}{\log d}\right)^{1/4}$ , the feasibility of  $\widehat{\theta}$  and  $\theta^*$  implies that  $\|\widehat{\Delta}\|_1 \leq 2R$ , and hence

$$0 \leq \underbrace{\left\{\varphi_{v}(n,d) + 2R\psi_{v}^{2}(n,d)\right\}}_{\leq \frac{\lambda n}{2}} \|\hat{\Delta}\|_{1} + \lambda_{n} \left\{ \left\|\hat{\Delta}_{S}\right\|_{1} - \left\|\hat{\Delta}_{Sc}\right\|_{1} \right\}$$
$$\leq \lambda_{n} \left\{ \frac{3}{2} \left\|\hat{\Delta}_{S}\right\|_{1} - \frac{1}{2} \left\|\hat{\Delta}_{Sc}\right\|_{1} \right\},$$

and rearranging yields the claim.



# Spiked model with sparsity

We consider a random vector  $x_i \in \mathbb{R}^d$  generated from the usual spiked ensemble, namely,

$$x_i \stackrel{\mathrm{d}}{=} \sqrt{v} \xi_i \theta^* + w_i,$$

where  $\theta^* \in \mathbb{S}^{d-1}$  is an *s*-sparse vector, corresponding to the maximal eigenvector of  $\mathbf{\Sigma} = \operatorname{cov}(x_i)$ . As before, we assume that both the random variable  $\xi_i$  and the random vector  $w_i \in \mathbb{R}^d$  are independent, each sub-Gaussian with parameter 1, the random vector  $x_i \in \mathbb{R}^d$  has sub-Gaussian tails.

#### Error bounds

#### Corollary 8.12

Consider n i.i.d. samples  $\{x_i\}_{i=1}^n$  from an s-sparse spiked covariance matrix with eigengap v>0 and suppose that  $\frac{s\log d}{n} \leq c \min\left\{1, \frac{v^2}{v+1}\right\}$  for a sufficiently small constant c>0. Then for any  $\delta \in (0,1)$ , any optimal solution  $\widehat{\theta}$  to the constrained program (1) with  $R=\|\theta^*\|_1$ , or to the penalized program (2) with  $\lambda_n=c_3\sqrt{v+1}\left\{\sqrt{\frac{\log d}{n}}+\delta\right\}$ , satisfies the bound

$$\min\left\{\|\widehat{\theta} - \theta^*\|_2, \|\widehat{\theta} + \theta^*\|_2\right\} \leq c_4 \sqrt{\frac{v+1}{v^2}} \left\{\sqrt{\frac{s\log d}{n}} + \delta\right\},$$

for all  $\delta \in (0,1)$  with probability at least  $1-c_1e^{-c_2(n/s)\min\left\{\delta^2, \mathcal{V}, v\right\}}$  .

We claim that

$$|\Psi(\Delta;\mathbf{P})| \leq \underbrace{\frac{1}{8}}_{c_0} v \|\Delta\|_2^2 + \underbrace{16\sqrt{v+1}\left\{\sqrt{\frac{\log d}{n}} + \delta\right\}}_{\varphi_{\nu}(n,d)} \|\Delta\|_1 + \underbrace{\frac{c_3'}{v}\frac{\log d}{n}}_{\psi_{\nu}^2(n,d)} \|\Delta\|_1^2,$$

with probability at least  $1-c_1e^{-c_2n\min\{\delta^2,v^2\}}$ . Here  $(c_1,c_2,c_3')$  are universal constants.

#### Check the condition of Theorem 8.10:

$$\frac{9s\psi_v^2(n,d)}{c_0} = \frac{72c_3'}{v}\frac{s\log d}{n} \le v\left\{72c_3'\frac{v+1}{v^2}\frac{s\log d}{n}\right\} \le v.$$

 $\lambda_n$  satisfies the lower bound requirement in Theorem 8.10. We have

$$4R\psi_{v}^{2}(n,d) + 2\varphi_{v}(n,d) \leq 4v\sqrt{\frac{n}{\log d}} \frac{c_{3}'}{v} \frac{\log d}{n} + 24\sqrt{v+1} \left\{ \sqrt{\frac{\log d}{n}} + \delta \right\}$$

$$\leq \underbrace{c_{3}\sqrt{v+1} \left\{ \sqrt{\frac{\log d}{n}} + \delta \right\}}_{\lambda_{n}}.$$

Recall

$$\mathbf{P} = \underbrace{v(\frac{1}{n}\sum_{i=1}^{n}\xi_{i}^{2}-1)\theta^{*}(\theta^{*})^{\mathrm{T}}}_{\mathbf{P}_{1}} + \underbrace{\sqrt{v}\left(\bar{w}(\theta^{*})^{\mathrm{T}}+\theta^{*}\bar{w}^{\mathrm{T}}\right)}_{\mathbf{P}_{2}} + \underbrace{\left(\frac{1}{n}\sum_{i=1}^{n}w_{i}w_{i}^{\mathrm{T}}-\mathbf{I}_{d}\right)}_{\mathbf{P}_{3}}.$$

#### Control of first component:

Lemma 8.8 guarantees that  $\left|\frac{1}{n}\sum_{i=1}^n \xi_i^2 - 1\right| \leq \frac{1}{16}$  with probability at least  $1 - 2e^{-cn}$ . For any vector  $\Delta = \theta - \theta^*$  with  $\theta \in \mathbb{S}^{d-1}$ , we have

$$|\Psi\left(\Delta; \mathbf{P}_1\right)| \leq \frac{v}{16} \left\langle \Delta, \theta^* \right\rangle^2 = \frac{v}{16} \left(1 - \left\langle \theta^*, \theta \right\rangle \right)^2 \leq \frac{v}{32} \|\Delta\|_2^2.$$

#### Control of second component:

We have

$$\begin{split} |\Psi\left(\Delta; \mathbf{P}_2\right)| &\leq 2\sqrt{\nu} \left\{ \left\langle \Delta, \bar{w} \right\rangle \left\langle \Delta, \theta^* \right\rangle + \left\langle \bar{w}, \Delta \right\rangle + \left\langle \theta^*, \bar{w} \right\rangle \left\langle \Delta, \theta^* \right\rangle \right\} \\ &\leq 4\sqrt{\nu} \|\Delta\|_1 \|\bar{w}\|_{\infty} + 2\sqrt{\nu} |\langle \theta^*, \bar{w} \rangle| \, \frac{\|\Delta\|_2^2}{2}. \end{split}$$

#### Lemma 8.13

Under the conditions of Corollary 8.12, we have

$$\mathbb{P}\left[\|\bar{w}\|_{\infty} \geq 2\sqrt{\frac{\log d}{n}} + \delta\right] \leq c_1 e^{-c_2 n \delta^2} \quad \text{ for all } \delta \in (0,1), \text{ and }$$
 
$$\mathbb{P}\left[|\langle \theta^*, \bar{w} \rangle| \geq \frac{\sqrt{\nu}}{32}\right] \leq c_1 e^{-c_2 n \nu}.$$

Then

$$|\Psi\left(\Delta; \mathbf{P}_2\right)| \leq \frac{v}{32} \|\Delta\|_2^2 + 8\sqrt{v+1} \left\{ \sqrt{\frac{\log d}{n}} + \delta \right\} \|\Delta\|_1.$$

Control of third term: Recalling that  $\mathbf{P}_3 = \frac{1}{n} \mathbf{W}^{\mathrm{T}} \mathbf{W} - \mathbf{I}_d$ , we have

$$\left|\Psi\left(\Delta; \mathbf{P}_{3}\right)\right| \leq \left|\left\langle \Delta, \mathbf{P}_{3} \Delta \right\rangle\right| + 2 \mid \left\|\mathbf{P}_{3} \theta^{*}\right\|_{\infty} \left\|\Delta\right\|_{1}.$$

Our final lemma controls the two terms in this bound:

#### Lemma 8.14

Under the conditions of Corollary 8.12, for all  $\delta \in (0,1)$ , we have

$$\|\mathbf{P}_3\theta^*\|_{\infty} \le 2\sqrt{\frac{\log d}{n}} + \delta$$

and

$$\sup_{\Delta \in \mathbb{R}^d} |\langle \Delta, \mathbf{P}_3 \Delta \rangle| \leq \frac{v}{16} \|\Delta\|_2^2 + \frac{c_3'}{v} \frac{\log d}{n} \|\Delta\|_1^2,$$

where both inequalities hold with probability greater than  $1-c_1e^{-c_2n\min\left(y,v^2,\delta^2\right)}$ .

Combining this lemma, yields the bound

$$|\Psi(\Delta; \mathbf{P}_3)| \le \frac{v}{16} ||\Delta||_2^2 + 8 \left\{ \sqrt{\frac{\log d}{n}} + \delta \right\} ||\Delta||_1 + \frac{c_3'}{v} \frac{\log d}{n} ||\Delta||_1^2.$$

# Thank you!