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

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Motivations

We consider $\Sigma \in S^{d \times d}_+$ 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 Σ 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 $\Pi_{\mathbb{V}^*}(\mathbf{X}) = V_r V_r^{\top} \mathbf{X}$.

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

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 Σ , and \mathbb{V}^* is spanned by those vectors.

Approximation and Perturbation

In practice, we do not know the covariance matrix Σ 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 Σ 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 θ^* .

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,

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

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

$$tr\left[\Sigma^{\top}\left(\theta^{*}(\theta^{*})^{\top}-\hat{\theta}(\hat{\theta})^{\top}\right)\right] = tr\left[\left(\Sigma-\hat{\Sigma}\right)\left(\theta^{*}(\theta^{*})^{\top}-\hat{\theta}(\hat{\theta})^{\top}\right)\right] + tr\left[\hat{\Sigma}\left(\theta^{*}(\theta^{*})^{\top}-\hat{\theta}(\hat{\theta})^{\top}\right)\right] \le -tr\left[P\left(\theta^{*}(\theta^{*})^{\top}-\hat{\theta}(\hat{\theta})^{\top}\right)\right] \\ = -\left(\hat{\theta}^{\top}P\hat{\theta}-(\theta^{*})^{\top}P\theta^{*}\right) = -\psi(\hat{\Delta};P).$$
(*)

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

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

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

$$\mathbf{x}_i \stackrel{d}{=} \sqrt{\nu} \xi_i \theta^* + \mathbf{w}_i,$$

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 ξ_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)

$$P\left(\left\|\frac{1}{n}\sum_{i=1}^{n}w_{i}w_{i}^{\top}-I\right\|_{2} \geq c_{3}\sqrt{\frac{d}{n}}+\delta_{3}\right) \leq 2exp(-c_{2}n\min\{\delta_{3},\delta_{3}^{2}\}).$$
(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.
- ♦ Failure of classical PCA:
- 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

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

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 λ_n can be chosen without knowledge of the true eigenvector θ^* .

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

- (a) For any optimal solution $\widehat{\theta}$ to the constrained program (1) with
- $R = \|\theta^*\|_1, \min\left\{\left\|\widehat{\theta} \theta^*\right\|_2, \left\|\widehat{\theta} + \theta^*\right\|_2\right\} \leq \frac{8}{\nu(1 4c_0)} \sqrt{s} \varphi_{\nu}(n, d).$
- (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

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

We find that

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

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 θ^* 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 ξ_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

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

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:

$$\frac{9s\psi_{v}^{2}(n,d)}{c_{0}} = \frac{72c_{3}'}{v}\frac{s\log d}{n} \leq v\left\{72c_{3}'\frac{v+1}{v^{2}}\frac{s\log d}{n}\right\} \leq v.$$

For the penalized estimator, we need to check $\|\theta^*\|_1 \leq \nu \sqrt{\frac{n}{\log d}}$. θ^* is s-sparse with $\|\theta^*\|_2 = 1$, then $\|\theta^*\|_1 \leq \sqrt{s}$, it suffices to have $\sqrt{s} \leq \nu \sqrt{\frac{n}{\log d}}$, or equivalently $\frac{1}{\nu^2} \frac{s \log d}{n} \leq 1$.

 λ_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

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

Control of second component:

We have

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

Lemma 8.13

Under the conditions of Corollary 8.12, we have

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

$$\mathbb{P}\left[|\langle \theta^*, \bar{w} \rangle| \geq \frac{\sqrt{\nu}}{32}\right] \leq c_1 \mathrm{e}^{-c_2 n \nu}.$$

Then

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

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

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

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

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

Proof of Lemma 8.14

For a constant $\xi>0$ to be chosen, consider the positive integer $k:=\left\lceil \xi v^2\frac{n}{\log d}\right\rceil$, and the collection of submatrices $\left\{ (\mathbf{P}_3)_{SS}, |S|=k \right\}$. Given a parameter $\alpha\in(0,1)$ to be chosen, a combination of the union bound and Theorem 6.5 imply that there are universal constants c_1 and c_2 such that

$$\mathbb{P}\left[\max_{|S|=k} \left\| (\mathbf{P}_3)_{SS} \right\|_2 \ge c_1 \sqrt{\frac{k}{n}} + \alpha v \right] \le 2e^{-c_2 n\alpha^2 v^2 + \log\left(\frac{d}{k}\right)}.$$

Since $\log \binom{d}{k} \le 2k \log(d) \le 4\xi v^2 n$, this probability is at most $e^{-c_2 n v^2 (\alpha^2 - 4\xi)} = e^{-c_2 n v^2 \alpha^2 / 2}$, as long as we set $\xi = \alpha^2 / 8$. The result of Exercise 7.10 then implies that

$$|\langle \Delta, \mathbf{P}_3 \Delta \rangle| \leq 27 c_1' \alpha v \left\{ \|\Delta\|_2^2 + \frac{8}{\alpha^2 v^2} \frac{\log d}{n} \|\Delta\|_1^2 \right\} \quad \text{ for all } \Delta \in \mathbb{R}^d,$$

with the previously stated probability.

Thank you!