Principal Components Analysis in high dimensions

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Overview

1. Motivation and PCA
   - Dimension reduction
   - Perturbations
2. Bounds for generic eigenvectors
   - General result
   - Spiked ensemble
3. 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

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

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

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

By variational representation :

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

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

Uses of PCA

1 Low-rank Approximation:

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

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 $Z^* = P\tilde{Z}P^\top = \sum_{j=1}^{r} \gamma_j(\Sigma) v_j v_j^\top$. And our approximated arror is

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

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

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

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

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

so we should maximize $tr(V_r^\top \Sigma V_r)$. By variational representation we know that $V_r = (v_1, \cdots, v_r)$, 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

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

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

Weyl's Inequality

We claim that

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

To prove this, we only need to prove

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

where $\mathcal{V}_{j-1}$ 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 $x = \sum_{i=1}^k \alpha_i u_i \in S_{k-1}^\perp$, $\|x\| = 1$, satisfying $x^\top Qx \geq \gamma_k$, so that $\max_{u\in\mathbb{V}^\perp\cap\mathcal{S}_{d-1}} u^\top Qu \geq \gamma_k$. 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 $S_{k-1} = span\{u_1, \cdots, u_{k-1}\}$ 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

$$\tilde{P} := U^\top P U = \begin{pmatrix} \tilde{p}_{11} & \tilde{p}^\top \\ \tilde{p} & \tilde{P}_{22} \end{pmatrix}$$

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

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

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^*.

Proof

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 $\tilde{P} = U^\top P U$, then we have

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

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

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

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 $2\rho^2 \leq 1+\rho, \forall \rho \in [0,1]$.

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

$$\begin{aligned}
&tr\left[\Sigma^\top \left(\theta^*(\theta^*)^\top - \hat{\theta}(\hat{\theta})^\top\right)\right] = tr\left[\left(\Sigma - \hat{\Sigma}\right)\left(\theta^*(\theta^*)^\top - \hat{\theta}(\hat{\theta})^\top\right)\right] \\
&+ tr\left[\hat{\Sigma}\left(\theta^*(\theta^*)^\top - \hat{\theta}(\hat{\theta})^\top\right)\right] \leq -tr\left[P\left(\theta^*(\theta^*)^\top - \hat{\theta}(\hat{\theta})^\top\right)\right] \\
&= -\left(\hat{\theta}^\top P\hat{\theta} - (\theta^*)^\top P\theta^*\right) = -\psi(\hat{\Delta}; P). \qquad (*)
\end{aligned}$$

Proof

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

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

Combining *, we have

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

which finishes the proof of Lemma.

Spiked ensemble

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

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

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

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

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 $\boldsymbol{x}_i \in \mathbb{R}^d$ 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 $\{\boldsymbol{x}_i\}_{i=1}^n$ 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 $\hat{\Sigma} = \frac{1}{n}\boldsymbol{x}_i\boldsymbol{x}_i^\top$ such that

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

Proof

In order to apply 9, we let $P = \hat{\Sigma} - \Sigma$, $\tilde{P} = U^\top P U$ 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

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

Proof

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

$$\left\| \frac{1}{n} \sum_{i=1}^n U_2^\top w_i \langle w_i, \theta^* \rangle \right\|_2 \overset{CS}{=} \sup_{v \in \mathcal{S}_{d-1}} \left| (U_2 v)^\top \left(\frac{1}{n} \sum_{i=1}^n w_i w_i^\top - I \right) \theta^* \right|$$

$$\leq \sup_{v \in \mathcal{S}_{d-1}} \| U_2^\top v \|_2 \left\| \frac{1}{n} \sum_{i=1}^n w_i w_i^\top - I \right\|_2 \leq \left\| \frac{1}{n} \sum_{i=1}^n w_i w_i^\top - I \right\|_2$$

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

$$\| \tilde{p} \|_2 \leq \sqrt{\nu} \| \bar{w} \|_2 + \left\| \frac{1}{n} \sum_{i=1}^n w_i w_i^\top - I \right\|_2 . \tag{8.22b}$$

Concentration Lemma

Lemma 8.8

Under the conditions of Corollary 8.7, we have

$$P\left(\left|\frac{1}{n}\sum_{i=1}^{n}\xi_i^2-1\right|\geq\delta_1\right)\leq 2exp(-c_2 n\min\{\delta_1,\delta_1^2\}), \tag{8.23a}$$

$$P\left(\|\bar{w}\|_2\geq 2\sqrt{\frac{d}{n}}+\delta_2\right)\leq 2exp(-c_2 n\min\{\delta_2,\delta_2^2\}), \tag{8.23b}$$

$$P\left(\left\|\frac{1}{n}\sum_{i=1}^{n}w_iw_i^\top-I\right\|_2\geq c_3\sqrt{\frac{d}{n}}+\delta_3\right)\leq 2exp(-c_2 n\min\{\delta_3,\delta_3^2\}). \tag{8.23c}$$

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

Proof

We define
$\phi(\delta_1, \delta_2, \delta_3) = 2e^{-c_2 n \min\{\delta_1, \delta_1^2\}} + 2e^{-c_2 n \min\{\delta_2, \delta_2^2\}} + 2e^{-c_2 n \min\{\delta_3, \delta_3^2\}}$. We apply Lemma 8.8 with $\delta_1 = \frac{1}{16}, \delta_2 = \frac{\delta}{4\sqrt{\nu}}, \delta_3 = \delta/16 \in (0, 1)$, we have

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

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

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

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

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

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

Error bounds

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

Theorem 8.10

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

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

(b) Consider the penalized program (2) with the regularization parameter lower bounded as $\lambda_n \ge 4\left(\frac{n}{\log d}\right)^{1/4}\psi_v^2(n,d) + 2\varphi_v(n,d)$. Then any optimal solution $\widehat{\theta}$ satisfies the bound

$$\min\left\{\left\|\widehat{\theta}-\theta^*\right\|_2, \left\|\widehat{\theta}+\theta^*\right\|_2\right\} \le \frac{2\left(\frac{\lambda_n}{\varphi_v(n,d)}+4\right)}{v(1-4c_0)}\sqrt{s}\varphi_v(n,d).$$

Proof

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

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

Substituting back into the basic inequality and performing some algebra yields

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

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

$$\frac{v}{2}\|\hat{\Delta}\|_2^2 - |\Psi(\hat{\Delta};\mathbf{P})| \le \lambda_n \left\{ \|\theta^*\|_1 - \|\widehat{\theta}\|_1 \right\} \le \lambda_n \left\{ \left\|\hat{\Delta}_S\right\|_1 - \left\|\hat{\Delta}_{S^c}\right\|_1 \right\},$$

We find that

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

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

Proof of Lemma 8.11

Combining the uniform bound with the basic inequality

$$0 \leq \underbrace{v(\frac{1}{2} - c_0)}_{>0} \|\Delta\|_2^2 \leq \varphi_v(n,d)\|\Delta\|_1 + \psi_v^2(n,d)\|\Delta\|_1^2 + \lambda_n \left\{ \left\|\widehat{\Delta}_S\right\|_1 - \left\|\widehat{\Delta}_{S^c}\right\|_1 \right\}$$

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

$$\begin{aligned} 0 &\leq \underbrace{\left\{\varphi_v(n,d) + 2R\psi_v^2(n,d)\right\}}_{\leq \frac{\lambda_n}{2}} \|\hat{\Delta}\|_1 + \lambda_n \left\{ \left\|\hat{\Delta}_S\right\|_1 - \left\|\hat{\Delta}_{Sc}\right\|_1 \right\} \\ &\leq \lambda_n \left\{ \frac{3}{2} \left\|\hat{\Delta}_S\right\|_1 - \frac{1}{2} \left\|\hat{\Delta}_{S^c}\right\|_1 \right\}, \end{aligned}$$

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

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

for all $\delta \in (0,1)$ with probability at least $1 - c_1 e^{-c_2(n/s)\min\{\delta^2, v^2, v\}}$.

Proof

We claim that

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

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

Proof

Check the condition of Theorem 8.10:

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

λ_n satisfies the lower bound requirement in Theorem 8.10.
For the penalized estimator, we need to check $\|\theta^*\|_1 \leq \nu\frac{n}{\log d}$. 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 $\frac{1}{\nu^2}\frac{s\log d}{n} \leq 1$. We have

$$\begin{aligned}4R\psi_v^2(n,d) + 2\varphi_v(n,d) &\leq 4v\sqrt{\frac{n}{\log d}}\frac{c_3'}{v}\frac{\log d}{n} + 24\sqrt{v+1}\left\{\sqrt{\frac{\log d}{n}} + \delta\right\} \\ &\leq \underbrace{c_3\sqrt{v+1}\left\{\sqrt{\frac{\log d}{n}} + \delta\right\}}_{\lambda_n}.\end{aligned}$$

Proof

Recall

$$\mathbf{P} = \underbrace{v(\frac{1}{n}\sum_{i=1}^{n}\xi_i^2 - 1)\theta^*(\theta^*)^{\mathrm{T}}}_{\mathbf{P}_1} + \underbrace{\sqrt{v}\left(\bar{w}(\theta^*)^{\mathrm{T}} + \theta^*\bar{w}^{\mathrm{T}}\right)}_{\mathbf{P}_2} + \underbrace{(\frac{1}{n}\sum_{i=1}^{n} w_i w_i^{\mathrm{T}} - \mathbf{I}_d)}_{\mathbf{P}_3}.$$

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

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

Proof:

Control of second component:

We have

$$|\Psi(\Delta; \mathbf{P}_2)| \leq 2\sqrt{v}\{\langle \Delta, \bar{w}\rangle \langle \Delta, \theta^*\rangle + \langle \bar{w}, \Delta\rangle + \langle \theta^*, \bar{w}\rangle \langle \Delta, \theta^*\rangle\}$$
$$\leq 4\sqrt{v}\|\Delta\|_1\|\bar{w}\|_\infty + 2\sqrt{v}|\langle \theta^*, \bar{w}\rangle| \frac{\|\Delta\|_2^2}{2}.$$

Lemma 8.13

Under the conditions of Corollary 8.12, we have

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

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

Then

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

Proof

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

$$|\Psi(\Delta; \mathbf{P}_3)| \leq |\langle \Delta, \mathbf{P}_3 \Delta \rangle| + 2 \mid \|\mathbf{P}_3 \theta^*\|_\infty \|\Delta\|_1.$$

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

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

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 $1 - c_1 e^{-c_2 n \min\left(y, v^2, \delta^2\right\}}$.

Proof

Combining this lemma, yields the bound

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

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

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

Since $\log \begin{pmatrix} d \\ k \end{pmatrix} \leq 2k \log(d) \leq 4 \xi v^2 n$, this probability is at most $e^{-c_2 n v^2 \left(\alpha^2 - 4\xi\right)} = e^{-c_2 n v^2 \alpha^2 / 2}$, 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 !