ELE 538B: Mathematics of High-Dimensional Data

Spectral methods



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Outline

- A motivating application: graph clustering
- Distance and angles between two subspaces
- Eigen-space perturbation theory
- Extension: singular subspaces
- Extension: eigen-space for asymmetric transition matrices

A motivating application: graph clustering

Graph clustering / community detection

Community structures are common in many social networks



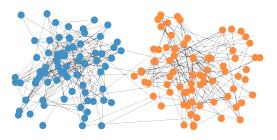
figure credit: The Future Buzz



figure credit: S. Papadopoulos

Goal: partition users into several clusters based on their friendships / similarities

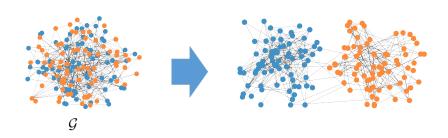
A simple model: stochastic block model (SBM)



- $x_i = 1$: 1st community $x_i = -1$: 2nd community

- n nodes $\{1, \cdots, n\}$
- 2 communities
- n unknown variables: $x_1, \dots, x_n \in \{1, -1\}$
 - encode community memberships

A simple model: stochastic block model (SBM)



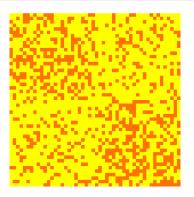
ullet observe a graph ${\mathcal G}$

$$(i,j) \in \mathcal{G}$$
 with prob. $\begin{cases} p, & \text{if } i \text{ and } j \text{ are from same community} \\ q, & \text{else} \end{cases}$

Here, p > q and $p, q \gtrsim \log n/n$

• Goal: recover community memberships of all nodes, i.e. $\{x_i\}$

Adjacency matrix

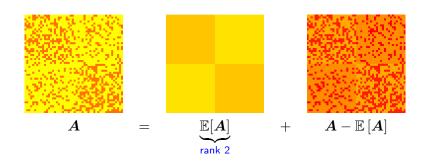


Consider the adjacency matrix $\mathbf{A} \in \{0,1\}^{n \times n}$ of \mathcal{G} :

$$A_{i,j} = \begin{cases} 1, & \text{if } (i,j) \in \mathcal{G} \\ 0, & \text{else} \end{cases}$$

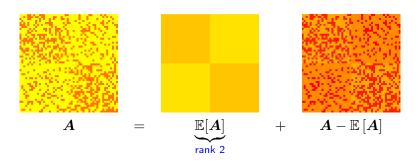
• WLOG, suppose $x_1 = \cdots = x_{n/2} = 1$; $x_{n/2+1} = \cdots = x_n = -1$

Adjacency matrix



$$\mathbb{E}[\boldsymbol{A}] = \begin{bmatrix} p\mathbf{1}\mathbf{1}^\top & q\mathbf{1}\mathbf{1}^\top \\ q\mathbf{1}\mathbf{1}^\top & p\mathbf{1}\mathbf{1}^\top \end{bmatrix} = \underbrace{\frac{p+q}{2}}_{\text{uninformative bias}} + \underbrace{\frac{p-q}{2}}_{=\boldsymbol{x} := [x_i]_{1 \leq i \leq n}} \begin{bmatrix} \mathbf{1} \\ -\mathbf{1} \end{bmatrix} \begin{bmatrix} \mathbf{1}^\top, -\mathbf{1}^\top \end{bmatrix}$$

Spectral clustering



- 1. computing the leading eigenvector $\hat{m{u}} = [\hat{u}_i]_{1 \leq i \leq n}$ of $m{A} \frac{p+q}{2} \mathbf{1} \mathbf{1}^{ op}$
- 2. rounding: output $\hat{x}_i = \begin{cases} 1, & \text{if } \hat{u}_i > 0 \\ -1, & \text{if } \hat{u}_i < 0 \end{cases}$

Spectral clustering

Rationale: recovery is reliable if $\underbrace{A - \mathbb{E}[A]}_{\text{perturbation}}$ is sufficiently small

ullet if $A-\mathbb{E}[A]=0$, then

$$\hat{u} \propto \pm \left| egin{array}{c} 1 \ -1 \end{array}
ight| \quad \Longrightarrow \quad {\sf perfect \; clustering}$$

Question: how to quantify the effect of perturbation $A-\mathbb{E}[A]$ on \hat{u} ?

Distance and angles between two subspaces

Setup and notation

Consider 2 symmetric matrices $m{M}$, $\hat{m{M}} = m{M} + m{H} \in \mathbb{R}^{n \times n}$ with eigen-decompositions

$$m{M} = \sum_{i=1}^n \lambda_i m{u}_i m{u}_i^ op$$
 and $\hat{m{M}} = \sum_{i=1}^n \hat{\lambda}_i \hat{m{u}}_i \hat{m{u}}_i^ op$

where $\lambda_1 \geq \cdots \geq \lambda_n$; $\hat{\lambda}_1 \geq \cdots \geq \hat{\lambda}_n$. For simplicity, write

$$egin{aligned} m{M} &= [m{U}_0, m{U}_1] \left[egin{array}{ccc} m{\Lambda}_0 & & \ & m{\Lambda}_1 \end{array}
ight] \left[egin{array}{ccc} m{U}_0^ op \ m{U}_1^ op \end{array}
ight] \ \hat{m{M}} &= [\hat{m{U}}_0, \hat{m{U}}_1] \left[egin{array}{cccc} \hat{m{\Lambda}}_0 & & \ & \hat{m{\Lambda}}_1 \end{array}
ight] \left[egin{array}{cccc} \hat{m{U}}_0^ op \ \hat{m{U}}_1^ op \end{array}
ight] \end{aligned}$$

Here, $U_0 = [u_1, \cdots, u_r]$, $\Lambda_0 = \operatorname{diag}([\lambda_1, \cdots, \lambda_r])$, \cdots

Setup and notation

$$egin{aligned} egin{aligned} oldsymbol{M} &= egin{bmatrix} oldsymbol{u}_1 & \cdots & oldsymbol{u}_r & oldsymbol{u}_1 \ & \lambda_1 & & & & \ & \ddots & & & \ & \lambda_r & & & \ & & \lambda_r & & & \ & & \lambda_{r+1} & & & \ & & \ddots & & \ & & \lambda_n & & \ & & oldsymbol{u}_1^ op & & \ & oldsymbol{u}_1^ op & & \ & oldsymbol{u}_1^ op & \ & oldsymbol{u}_1^ o$$

Setup and notation

ullet $\|M\|$: spectral norm (largest singular value of M)

• $\| m{M} \|_{\mathrm{F}}$: Frobenius norm $(\| m{M} \|_{\mathrm{F}} = \sqrt{\mathrm{tr}(m{M}^{ op} m{M})} = \sqrt{\sum_{i,j} M_{i,j}^2})$

Eigen-space perturbation theory

Main focus: how does the perturbation H affect the distance between U and \hat{U} ?

Question #0: how to define distance between two subspaces?

ullet $\|m{U} - \hat{m{U}}\|_{ ext{F}}$ and $\|m{U} - \hat{m{U}}\|$ are not appropriate, since they fall short of accounting for global orthonormal transformation.

 \forall orthonormal $m{R} \in \mathbb{R}^{r \times r}, \ m{U}$ and $m{U}m{R}$ represent same subspace

Distance between two eigen-spaces

One metric that takes care of global orthonormal transformation is

$$dist(X_0, Z_0) := \|X_0 X_0^{\top} - Z_0 Z_0^{\top}\|$$
 (2.1)

This metric has several equivalent expressions:

Lemma 2.1

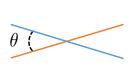
Suppose $X:=[X_0,\underbrace{X_1}]$ and $Z:=[Z_0,\underbrace{Z_1}]$ are orthonormal complement subspace matrices. Then

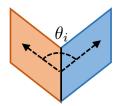
$$\mathsf{dist}(oldsymbol{X}_0, oldsymbol{Z}_0) = \|oldsymbol{X}_0^ op oldsymbol{Z}_1\| = \|oldsymbol{Z}_0^ op oldsymbol{X}_1\|$$

ullet sanity check: if $oldsymbol{X}_0 = oldsymbol{Z}_0$, then $\operatorname{dist}(oldsymbol{X}_0, oldsymbol{Z}_0) = \|oldsymbol{X}_0^ op oldsymbol{Z}_1\| = 0$

Principal angles between two eigen-spaces

In addition to "distance", one might also be interested in "angles"





We can quantify the similarity between two lines (represented resp. by unit vectors x_0 and z_0) by an angle between them

$$\theta = \arccos\langle \boldsymbol{x}_0, \boldsymbol{z}_0 \rangle$$

Principal angles between two eigen-spaces

For r-dimensional subspaces, one needs r angles

Specifically, given $\|\boldsymbol{X}_0^{\top}\boldsymbol{Z}_0\| \leq 1$, we write SVD of $\boldsymbol{X}_0^{\top}\boldsymbol{Z}_0 \in \mathbb{R}^{r \times r}$ as

$$oldsymbol{X}_0^ op oldsymbol{Z}_0 = oldsymbol{U} egin{bmatrix} \cos heta_1 & & & \ & \ddots & \ & & \cos heta_r \end{bmatrix} oldsymbol{V}^ op := oldsymbol{U}\cosoldsymbol{\Theta} oldsymbol{V}^ op := oldsymbol{V}$$

where $\{\theta_1,\cdots,\theta_r\}$ are called the principal angles between $m{X}_0$ and $m{Z}_0$

Relations between principal angles and $dist(\cdot, \cdot)$

As expected, principal angles and distance are closely related

Lemma 2.2

Suppose $m{X}:=[m{X}_0,m{X}_1]$ and $m{Z}:=[m{Z}_0,m{Z}_1]$ are orthonormal matrices. Then

$$\|\boldsymbol{X}_0^{\top}\boldsymbol{Z}_1\| = \|\sin\boldsymbol{\Theta}\| = \max\{|\sin\theta_1|, \cdots, |\sin\theta_r|\}$$

Lemmas 2.1 and 2.2 taken collectively give

$$dist(\mathbf{X}_0, \mathbf{Z}_0) = \max\{|\sin \theta_1|, \cdots, |\sin \theta_r|\}$$
 (2.2)

Proof of Lemma 2.2

$$\|\boldsymbol{X}_{0}^{\top}\boldsymbol{Z}_{1}\| = \|\boldsymbol{X}_{0}^{\top} \boldsymbol{Z}_{1}\boldsymbol{Z}_{1}^{\top} \boldsymbol{X}_{0}\|^{\frac{1}{2}}$$

$$= \|\boldsymbol{X}_{0}^{\top}\boldsymbol{X}_{0} - \boldsymbol{X}_{0}^{\top}\boldsymbol{Z}_{0}\boldsymbol{Z}_{0}^{\top}\boldsymbol{X}_{0}\|^{\frac{1}{2}}$$

$$= \|\boldsymbol{I} - \boldsymbol{U}\cos^{2}\boldsymbol{\Theta}\boldsymbol{U}^{\top}\|^{\frac{1}{2}} \qquad (\text{since } \boldsymbol{X}_{0}^{\top}\boldsymbol{Z}_{0} = \boldsymbol{U}\cos\boldsymbol{\Theta}\boldsymbol{V}^{\top})$$

$$= \|\boldsymbol{I} - \cos^{2}\boldsymbol{\Theta}\|^{\frac{1}{2}}$$

$$= \|\sin\boldsymbol{\Theta}\|$$

Proof of Lemma 2.1

We first claim that SVD of $\boldsymbol{X}_1^{\top} \boldsymbol{Z}_0$ can be written as

$$\boldsymbol{X}_{1}^{\top}\boldsymbol{Z}_{0} = \tilde{\boldsymbol{U}}\sin\boldsymbol{\Theta}\boldsymbol{V}^{\top} \tag{2.3}$$

for some orthonormal $ilde{U}$ (to be proved later). With this claim in place, one has

$$oldsymbol{Z}_0 = \left[oldsymbol{X}_0, oldsymbol{X}_1
ight] \left[egin{array}{c} oldsymbol{X}_0^{ op} \ oldsymbol{X}_1 \end{array}
ight] \left[egin{array}{c} oldsymbol{U}\cosoldsymbol{\Theta}oldsymbol{V}^{ op} \ \hat{oldsymbol{U}}\sinoldsymbol{\Theta}oldsymbol{V}^{ op} \end{array}
ight]$$

$$\implies \boldsymbol{Z}_0 \boldsymbol{Z}_0^\top = [\boldsymbol{X}_0, \boldsymbol{X}_1] \left[\begin{array}{cc} \boldsymbol{U} \cos^2 \boldsymbol{\Theta} \boldsymbol{U}^\top & \boldsymbol{U} \cos \boldsymbol{\Theta} \sin \boldsymbol{\Theta} \tilde{\boldsymbol{U}}^\top \\ \tilde{\boldsymbol{U}} \cos \boldsymbol{\Theta} \sin \boldsymbol{\Theta} \boldsymbol{U}^\top & \tilde{\boldsymbol{U}} \sin^2 \boldsymbol{\Theta} \tilde{\boldsymbol{U}}^\top \end{array} \right] \left[\begin{array}{c} \boldsymbol{X}_0^\top \\ \boldsymbol{X}_1^\top \end{array} \right]$$

As a consequence,

$$\begin{split} \boldsymbol{X}_0 \boldsymbol{X}_0^\top - \boldsymbol{Z}_0 \boldsymbol{Z}_0^\top \\ &= \left[\boldsymbol{X}_0, \boldsymbol{X}_1 \right] \left[\begin{array}{cc} \boldsymbol{I} - \boldsymbol{U} \cos^2 \Theta \, \boldsymbol{U}^\top & - \boldsymbol{U} \cos \Theta \sin \Theta \, \tilde{\boldsymbol{U}}^\top \\ - \tilde{\boldsymbol{U}} \cos \Theta \sin \Theta \, \boldsymbol{U}^\top & - \tilde{\boldsymbol{U}} \sin^2 \Theta \, \tilde{\boldsymbol{U}}^\top \end{array} \right] \left[\begin{array}{c} \boldsymbol{X}_0^\top \\ \boldsymbol{X}_1^\top \end{array} \right] \end{split}$$

Proof of Lemma 2.1 (cont.)

This further gives

$$\begin{split} & \left\| \boldsymbol{X}_{0} \boldsymbol{X}_{0}^{\top} - \boldsymbol{Z}_{0} \boldsymbol{Z}_{0}^{\top} \right\| \\ & = \left\| \begin{bmatrix} \boldsymbol{U} & \sin^{2}\boldsymbol{\Theta} & -\cos\boldsymbol{\Theta}\sin\boldsymbol{\Theta} \\ -\cos\boldsymbol{\Theta}\sin\boldsymbol{\Theta} & -\sin^{2}\boldsymbol{\Theta} \end{bmatrix} \begin{bmatrix} \boldsymbol{U}^{\top} & \\ \tilde{\boldsymbol{U}}^{\top} \end{bmatrix} \right\| \\ & = \left\| \underbrace{\begin{bmatrix} \sin^{2}\boldsymbol{\Theta} & -\cos\boldsymbol{\Theta}\sin\boldsymbol{\Theta} \\ -\cos\boldsymbol{\Theta}\sin\boldsymbol{\Theta} & -\sin^{2}\boldsymbol{\Theta} \end{bmatrix}}_{\text{each block is diagonal matrix}} \right\| \quad (\|\cdot\| \text{ is rotationally invariant}) \\ & = \max_{1 \leq i \leq r} \left\| \begin{bmatrix} \sin^{2}\theta_{i} & -\cos\theta_{i}\sin\theta_{i} \\ -\cos\theta_{i}\sin\theta_{i} & -\sin^{2}\theta_{i} \end{bmatrix} \right\| \\ & = \max_{1 \leq i \leq r} \left\| \sin\theta_{i} \begin{bmatrix} \sin\theta_{i} & -\cos\theta_{i} \\ -\cos\theta_{i} & -\sin\theta_{i} \end{bmatrix} \right\| \\ & = \max_{1 \leq i \leq r} \left\| \sin\theta_{i} \right\| = \left\| \sin\boldsymbol{\Theta} \right\| \end{split}$$

Proof of Lemma 2.1 (cont.)

It remains to justify (2.3). To this end, observe that

$$egin{aligned} oldsymbol{Z}_0^ op oldsymbol{X}_1 oldsymbol{X}_1^ op oldsymbol{Z}_0 &= oldsymbol{Z}_0^ op oldsymbol{Z}_0 - oldsymbol{Z}_0^ op oldsymbol{X}_0^ op oldsymbol{Z}_0 \\ &= oldsymbol{I} - oldsymbol{V} \cos^2 oldsymbol{\Theta} oldsymbol{V}^ op \\ &= oldsymbol{V} \sin^2 oldsymbol{\Theta} oldsymbol{V}^ op \end{aligned}$$

and hence right singular space (resp. singular values) of $m{X}_1^ op m{Z}_0$ is given by $m{V}$ (resp. $\sin m{\Theta}$)

Eigen-space perturbation theory

Davis-Kahan $\sin \Theta$ Theorem: a simple case







William Kahan

Theorem 2.3

Suppose $M \succeq \mathbf{0}$ and has rank r. If $\|\mathbf{H}\| < \lambda_r(\mathbf{M})$, then

$$\mathsf{dist}ig(\hat{oldsymbol{U}}_0, oldsymbol{U}_0ig) \leq rac{ig\|oldsymbol{H}oldsymbol{U}_0ig\|}{\lambda_r(oldsymbol{M}) - ig\|oldsymbol{H}ig\|} \leq rac{ig\|oldsymbol{H}ig\|}{\lambda_r(oldsymbol{M}) - ig\|oldsymbol{H}ig\|}$$

ullet depends on the smallest non-zero eigenvalue of M and perturbation

Proof of Theorem 2.3

We intend to control $\hat{m{U}}_1^{ op} m{U}_0$ by studying their interactions through $m{H}$:

$$\begin{split} \left\| \hat{\boldsymbol{U}}_{1}^{\top} \boldsymbol{H} \boldsymbol{U}_{0} \right\| &= \left\| \hat{\boldsymbol{U}}_{1}^{\top} \left(\underline{\hat{\boldsymbol{U}}} \hat{\boldsymbol{\Lambda}} \underline{\hat{\boldsymbol{U}}}^{\top} - \underline{\boldsymbol{U}} \underline{\boldsymbol{\Lambda}} \underline{\boldsymbol{U}}^{\top} \right) \boldsymbol{U}_{0} \right\| \\ &= \left\| \hat{\boldsymbol{\Lambda}}_{1} \hat{\boldsymbol{U}}_{1}^{\top} \boldsymbol{U}_{0} - \hat{\boldsymbol{U}}_{1}^{\top} \boldsymbol{U}_{0} \boldsymbol{\Lambda}_{0} \right\| \qquad (\text{since } \boldsymbol{U}_{1}^{\top} \boldsymbol{U}_{0} = \hat{\boldsymbol{U}}_{1}^{\top} \hat{\boldsymbol{U}}_{0} = \boldsymbol{0}) \\ &\geq \left\| \hat{\boldsymbol{U}}_{1}^{\top} \boldsymbol{U}_{0} \boldsymbol{\Lambda}_{0} \right\| - \left\| \hat{\boldsymbol{\Lambda}}_{1} \hat{\boldsymbol{U}}_{1}^{\top} \boldsymbol{U}_{0} \right\| \qquad (\text{triangle inequality}) \\ &\geq \left\| \hat{\boldsymbol{U}}_{1}^{\top} \boldsymbol{U}_{0} \right\| \lambda_{r} - \left\| \hat{\boldsymbol{U}}_{1}^{\top} \boldsymbol{U}_{0} \right\| \left\| \hat{\boldsymbol{\Lambda}}_{1} \right\| \end{aligned} \tag{2.4}$$

In view of Weyl's Theorem, $\|\hat{\boldsymbol{\Lambda}}_1\| \leq \|\boldsymbol{H}\|$, which combined with (2.4) gives

$$\left\|\hat{\boldsymbol{U}}_1^{\top}\boldsymbol{U}_0\right\| \leq \frac{\left\|\hat{\boldsymbol{U}}_1^{\top}\boldsymbol{H}\boldsymbol{U}_0\right\|}{\lambda_r - \left\|\boldsymbol{H}\right\|} \leq \frac{\left\|\hat{\boldsymbol{U}}_1\right\| \cdot \left\|\boldsymbol{H}\boldsymbol{U}_0\right\|}{\lambda_r - \left\|\boldsymbol{H}\right\|} = \frac{\left\|\boldsymbol{H}\boldsymbol{U}_0\right\|}{\lambda_r - \left\|\boldsymbol{H}\right\|}$$

This together with Lemma 2.1 completes the proof

Davis-Kahan $\sin \Theta$ Theorem: more general case

Theorem 2.4 (Davis-Kahan $\sin \Theta$ Theorem)

Suppose $\lambda_r(M) \geq a$ and $\lambda_{r+1}(\hat{M}) \leq a - \Delta$ for some $\Delta > 0$. Then

$$\mathsf{dist}(\hat{oldsymbol{U}}_0, oldsymbol{U}_0) \leq rac{\|oldsymbol{H} oldsymbol{U}_0\|}{\Delta} \leq rac{\|oldsymbol{H}\|}{\Delta}$$

ullet immediate consequence: if $\lambda_r(M) > \lambda_{r+1}(M) + \|H\|$, then

$$\operatorname{dist}(\hat{\boldsymbol{U}}_{0}, \boldsymbol{U}_{0}) \leq \underbrace{\frac{\|\boldsymbol{H}\|}{\lambda_{r}(\boldsymbol{M}) - \lambda_{r+1}(\boldsymbol{M})} - \|\boldsymbol{H}\|}_{\text{spectral gap}} \tag{2.5}$$

Back to stochastic block model ...

Let
$$M = \underbrace{\mathbb{E}[A] - \frac{p+q}{2}\mathbf{1}\mathbf{1}^{\top}}_{=\frac{p-q}{2}\left[\begin{array}{c}\mathbf{1}\\-\mathbf{1}\end{array}\right]\left[\mathbf{1}^{\top},-\mathbf{1}^{\top}\right]}_{=\frac{p-q}{2}\left[\begin{array}{c}\mathbf{1}\\-\mathbf{1}\end{array}\right]\left[\mathbf{1}^{\top},-\mathbf{1}^{\top}\right]}$$

Then the Davis-Kahan $\sin \Theta$ Theorem yields

$$dist(\hat{u}, u) \le \frac{\|\hat{M} - M\|}{\lambda_1(M) - \|\hat{M} - M\|} = \frac{\|A - \mathbb{E}[A]\|}{\frac{(p-q)n}{2} - \|A - \mathbb{E}[A]\|}$$
(2.6)

Question: how to bound $||A - \mathbb{E}[A]||$?

A hammer: matrix Bernstein inequality

Consider a sequence of independent random matrices $\{oldsymbol{X}_l \in \mathbb{R}^{d_1 imes d_2}\}$

•
$$\mathbb{E}[X_l] = \mathbf{0}$$

•
$$\|\boldsymbol{X}_l\| \leq B$$
 for each l

variance statistic:

$$v := \max \left\{ \left\| \mathbb{E} \left[\sum_{l} \boldsymbol{X}_{l} \boldsymbol{X}_{l}^{\top} \right] \right\|, \left\| \mathbb{E} \left[\sum_{l} \boldsymbol{X}_{l}^{\top} \boldsymbol{X}_{l} \right] \right\| \right\}$$

Theorem 2.5 (Matrix Bernstein inequality)

For all
$$\tau \geq 0$$
,
$$\mathbb{P}\left\{\left\|\sum_{l} \boldsymbol{X}_{l}\right\| \geq \tau\right\} \leq (d_{1} + d_{2}) \exp\left(\frac{-\tau^{2}/2}{v + B\tau/3}\right)$$

A hammer: matrix Bernstein inequality

$$\mathbb{P}\left\{\left\|\sum_{l} \mathbf{X}_{l}\right\| \geq \tau\right\} \leq (d_{1} + d_{2}) \exp\left(\frac{-\tau^{2}/2}{v + B\tau/3}\right)$$

- moderate-deviation regime (τ is small):
 - sub-Gaussian tail behavior $\exp(-\tau^2/2v)$
- large-deviation regime (τ is large):
 - sub-exponential tail behavior $\exp(-3\tau/2B)$ (slower decay)
- user-friendly form (exercise): with prob. $1 O((d_1 + d_2)^{-10})$

$$\left\| \sum_{l} X_{l} \right\| \lesssim \sqrt{v \log(d_{1} + d_{2})} + B \log(d_{1} + d_{2})$$
 (2.7)

Bounding $\|A - \mathbb{E}[A]\|$

The Matrix Bernstein inequality yields

Lemma 2.6

Consider SBM with $p>q\gtrsim \frac{\log n}{n}.$ Then with high prob.

$$\|\boldsymbol{A} - \mathbb{E}[\boldsymbol{A}]\| \lesssim \sqrt{np\log n} \tag{2.8}$$

Statistical accuracy of spectral clustering

Substitute (2.8) into (2.6) to reach

$$\mathsf{dist}(\hat{\boldsymbol{u}},\boldsymbol{u}) \leq \frac{\|\boldsymbol{A} - \mathbb{E}[\boldsymbol{A}]\|}{\frac{(p-q)n}{2} - \|\boldsymbol{A} - \mathbb{E}[\boldsymbol{A}]\|} \lesssim \frac{\sqrt{np\log n}}{(p-q)n}$$

provided that $(p-q)n \gg \sqrt{np\log n}$

Thus, under condition $\frac{p-q}{\sqrt{p}}\gg\sqrt{\frac{\log n}{n}}$, with high prob. one has

$$\mathsf{dist}(\hat{\boldsymbol{u}},\boldsymbol{u}) \ll 1 \qquad \Longrightarrow \qquad \mathsf{nearly perfect clustering}$$

Statistical accuracy of spectral clustering

$$\frac{p-q}{\sqrt{p}}\gg\sqrt{\frac{\log n}{n}}\quad\Longrightarrow\quad \text{nearly perfect clustering}$$

ullet dense regime: if $p \asymp q \asymp 1$, then this condition reads

$$p - q \gg \sqrt{\frac{\log n}{n}}$$

• "sparse" regime: if $p=\frac{a\log n}{n}$ and $q=\frac{b\log n}{n}$ for $a,b\asymp 1$, then $a-b\gg \sqrt{a}$

This condition is information-theoretically optimal (up to log factor)

— Mossel, Neeman, Sly '15, Abbe '18

Proof of Lemma 2.6

To simplify presentation, assume $A_{i,j}$ and $A_{j,i}$ are independent (check: why this assumption does not change our bounds)

Proof of Lemma 2.6

Write $m{A} - \mathbb{E}[m{A}]$ as $\sum_{i,j} m{X}_{i,j}$, where $m{X}_{i,j} = \left(A_{i,j} - \mathbb{E}[A_{i,j}]\right) m{e}_i m{e}_j^{ op}$

• Since ${\sf Var}(A_{i,j}) \leq p$, one has $\mathbb{E}\left[m{X}_{i,j} m{X}_{i,j}^{ op}
ight] \preceq p m{e}_i m{e}_i^{ op}$, which gives

$$\sum\nolimits_{i,j} \mathbb{E}\left[\boldsymbol{X}_{i,j} \boldsymbol{X}_{i,j}^{\top}\right] \preceq \sum\nolimits_{i,j} p \boldsymbol{e}_{i} \boldsymbol{e}_{i}^{\top} \preceq n p \boldsymbol{I}$$

Similarly, $\sum_{i,j} \mathbb{E}\left[m{X}_{i,j}^{ op} m{X}_{i,j}
ight] \preceq np \, m{I}$. As a result,

$$v = \max\left\{\left\|\sum\nolimits_{i,j} \mathbb{E}\left[\boldsymbol{X}_{i,j}\boldsymbol{X}_{i,j}^{\top}\right]\right\|, \left\|\sum\nolimits_{i,j} \mathbb{E}\left[\boldsymbol{X}_{i,j}^{\top}\boldsymbol{X}_{i,j}\right]\right\|\right\} \leq np$$

- In addition, $\|\boldsymbol{X}_{i,j}\| \leq 1 := B$
- Take the matrix Bernstein inequality to conclude that with high prob.,

$$\|\boldsymbol{A} - \mathbb{E}[\boldsymbol{A}]\| \lesssim \sqrt{v \log n} + B \log n \lesssim \sqrt{np \log n} \quad (\text{since } p \gtrsim \frac{\log n}{n})$$



Singular value decomposition

Consider two matrices $oldsymbol{M}, \hat{oldsymbol{M}} = oldsymbol{M} + oldsymbol{H}$ with SVD

$$egin{aligned} m{M} &= [m{U}_0, m{U}_1] \left[egin{array}{ccc} m{\Sigma}_0 & m{0} \ m{0} & m{\Sigma}_1 \ m{0} & m{0} \end{array}
ight] \left[m{V}_0^ op \ m{V}_1^ op \end{array}
ight] \ \hat{m{M}} &= \left[\hat{m{U}}_0, \hat{m{U}}_1
ight] \left[egin{array}{cccc} \hat{m{\Sigma}}_0 & m{0} \ m{0} & \hat{m{\Sigma}}_1 \ m{0} & m{0} \end{array}
ight] \left[m{\hat{V}}_0^ op \ \hat{m{V}}_1^ op \end{array}
ight] \end{aligned}$$

where U_0 (resp. \hat{U}_0) and V_0 (resp. \hat{V}_0) represent the top-r singular subspaces of M (resp. \hat{M})

Wedin $\sin \Theta$ Theorem

The Davis-Kahan Theorem generalizes to singular subspace perturbation:

Theorem 2.7 (Wedin $\sin \Theta$ Theorem)

Suppose
$$\underbrace{\sigma_r(M)} \geq a$$
 and $\sigma_{r+1}(\hat{M}) \leq a - \Delta$ for some $\Delta > 0$. Then th singular value
$$\max \left\{ \mathsf{dist}(\hat{U}_0, U_0), \mathsf{dist}(\hat{V}_0, V_0) \right\} \leq \underbrace{\frac{\max \left\{ \| HV_0 \|, \| H^\top U_0 \| \right\}}{\Delta}}_{two\text{-sided interactions}} \leq \underbrace{\frac{\| H \|}{\Delta}}_{two}$$



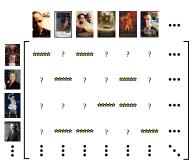
- Netflix challenge: Netflix provides highly incomplete ratings from 0.5 million users for & 17,770 movies
- How to predict unseen user ratings for movies?

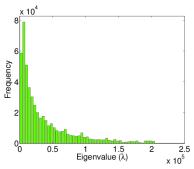
In general, we cannot infer missing ratings

```
      ✓
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      ✓
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— this is an underdetermined system (more unknowns than observations)

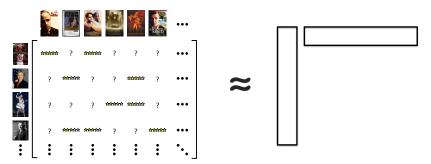
... unless rating matrix has other structure





A few factors explain most of the data

... unless rating matrix has other structure



A few factors explain most of the data \longrightarrow low-rank approximation

How to exploit (approx.) low-rank structure in prediction?

Model for low-rank matrix completion

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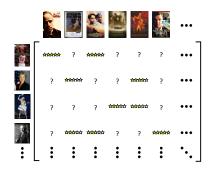


figure credit: Candès

- ullet consider a low-rank matrix M
- ullet each entry $M_{i,j}$ is observed independently with prob. p

• goal: fill in missing entries

Spectral estimate for matrix completion

1. set $\hat{m{M}} \in \mathbb{R}^{n imes n}$ as

$$\hat{M}_{i,j} = \begin{cases} \frac{1}{p} M_{i,j} & \text{if } M_{i,j} \text{ is observed} \\ 0, & \text{else} \end{cases}$$

- \circ rationale for rescaling: $\mathbb{E}[\hat{M}] = M$
- 2. compute the rank-r SVD $\hat{U}\hat{\Sigma}\hat{V}^{\top}$ of \hat{M} , and return $(\hat{U},\hat{\Sigma},\hat{V})$

Statistical accuracy of spectral estimate

Let's analyze a simple case where $oldsymbol{M} = oldsymbol{u} oldsymbol{v}^ op$ with

$$oldsymbol{u} = rac{1}{\| ilde{oldsymbol{u}}\|_2} ilde{oldsymbol{u}}, \quad oldsymbol{v} = rac{1}{\| ilde{oldsymbol{v}}\|_2} ilde{oldsymbol{v}}, \quad ilde{oldsymbol{u}}, ilde{oldsymbol{v}} \sim \mathcal{N}(oldsymbol{0}, oldsymbol{I}_n)$$

From Wedin's Theorem: if $p \gg \log^3 n/n$, then with high prob.

$$\max \left\{ \mathsf{dist}(\hat{\boldsymbol{u}}, \boldsymbol{u}), \mathsf{dist}(\hat{\boldsymbol{v}}, \boldsymbol{v}) \right\} \leq \frac{\|\hat{\boldsymbol{M}} - \boldsymbol{M}\|}{\sigma_1(\boldsymbol{M}) - \|\hat{\boldsymbol{M}} - \boldsymbol{M}\|} \approx \underbrace{\|\hat{\boldsymbol{M}} - \boldsymbol{M}\|}_{\mathsf{controlled by Bernstein}} \\ \ll 1 \quad (\mathsf{nearly accurate estimates}) \quad (2.9)$$

Sample complexity

For rank-1 matrix completion,

$$p \gg \frac{\log^3 n}{n} \implies \text{nearly accurate estimates}$$

Sample complexity needed for obtaining reliable spectral estimates is

$$\underbrace{n^2p \asymp n\log^3 n}_{\text{optimal up to log factor}}$$

Proof of (2.9)

Write
$$\hat{m{M}}-m{M}=\sum_{i,j}m{X}_{i,j}$$
, where $m{X}_{i,j}=(\hat{M}_{i,j}-M_{i,j})m{e}_im{e}_j^{ op}$

First,

$$\|\boldsymbol{X}_{i,j}\| \leq \frac{1}{p} \max_{i,j} |M_{i,j}| \lesssim \frac{\log n}{pn} := B \quad (\mathsf{check})$$

ullet Next, $\mathbb{E}[oldsymbol{X}_{i,j}oldsymbol{X}_{i,j}^{ op}] = \mathsf{Var}(\hat{M}_{i,j})oldsymbol{e}_ioldsymbol{e}_i^{ op}$ and hence

$$\mathbb{E}\big[\sum\nolimits_{i,j} \boldsymbol{X}_{i,j} \boldsymbol{X}_{i,j}^{\top} \big] \preceq \Big\{ \max_{i,j} \mathsf{Var}\big(\hat{M}_{i,j}\big) \Big\} n\boldsymbol{I} \preceq \Big\{ \frac{n}{p} \max_{i,j} M_{i,j}^2 \Big\} \boldsymbol{I}$$

$$\implies \qquad \left\| \mathbb{E} \big[\sum\nolimits_{i,j} \boldsymbol{X}_{i,j} \boldsymbol{X}_{i,j}^\top \big] \right\| \leq \frac{n}{p} \max_{i,j} M_{i,j}^2 \lesssim \frac{\log^2 n}{np} \quad (\mathsf{check})$$

Similar bounds hold for $\|\mathbb{E}\left[\sum_{i,j} X_{i,j}^{\top} X_{i,j}\right]\|$. Therefore,

$$v := \max \left\{ \left\| \mathbb{E} \left[\sum\nolimits_{i,j} \boldsymbol{X}_{i,j} \boldsymbol{X}_{i,j}^\top \right] \right\|, \left\| \mathbb{E} \left[\sum\nolimits_{i,j} \boldsymbol{X}_{i,j}^\top \boldsymbol{X}_{i,j} \right] \right\| \right\} \lesssim \frac{\log^2 n}{np}$$

• Take the matrix Bernstein inequality to yield: if $p \gg \log^3 n/n$, then

$$\|\hat{\boldsymbol{M}} - \boldsymbol{M}\| \lesssim \sqrt{v \log n} + B \log n \ll 1$$

Extension: eigen-space for asymmetric transition matrices

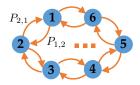
Eigen-decomposition for asymmetric matrices

Eigen-decomposition for asymmetric matrices is much more tricky; for example:

- 1. both eigenvalues and eigenvectors might be complex-valued
- 2. eigenvectors might not be orthogonal to each other

This lecture focuses on a special case: **probability transition matrices**

Probability transition matrices



Consider Markov chain $\{X_t\}_{t\geq 0}$

- n states
- transition probability $\mathbb{P}\{X_{t+1}=j\mid X_t=i\}=P_{i,j}$
- transition matrix $\boldsymbol{P} = [P_{i,j}]_{1 \leq i,j \leq n}$
- ullet stationary distribution $\underline{\pi=[\pi_1,\cdots,\pi_n]}_{\pi_1+\cdots+\pi_n=1}$ is 1st eigenvector of $m{P}$

$$\pi P = \pi$$

• $\{X_t\}_{t\geq 0}$ is said to be reversible if $\pi_i P_{i,j} = \pi_j P_{j,i}$ for all i,j

Eigenvector perturbation for transition matrices

Define
$$\|oldsymbol{a}\|_{oldsymbol{\pi}}:=\sqrt{\pi_1a_1^2+\cdots+\pi_na_n^2}$$

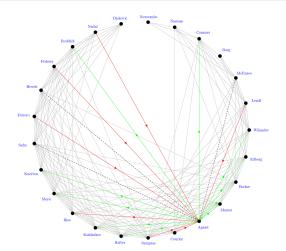
Theorem 2.8 (Chen, Fan, Ma, Wang '17)

Suppose P, \hat{P} are transition matrices with stationary distributions π , $\hat{\pi}$, respectively. Assume P induces reversible Markov chain. If $1 > \max{\{\lambda_2(P), -\lambda_n(P)\}} + \|\hat{P} - P\|_{\pi}$, then

$$\|\hat{\boldsymbol{\pi}} - \boldsymbol{\pi}\|_{\boldsymbol{\pi}} \leq \underbrace{\frac{\|\boldsymbol{\pi}(\hat{\boldsymbol{P}} - \boldsymbol{P})\|_{\boldsymbol{\pi}}}{1 - \max\left\{\lambda_2(\boldsymbol{P}), -\lambda_n(\boldsymbol{P})\right\}} - \underbrace{\|\hat{\boldsymbol{P}} - \boldsymbol{P}\|_{\boldsymbol{\pi}}}_{\text{perturbation}}}_{\text{spectral gap}}$$

ullet \hat{P} does not need to induce reversible Markov chain

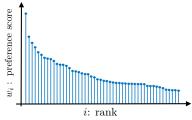
Example: ranking from pairwise comparisons



pairwise comparisons for ranking tennis players

figure credit: Bozóki, Csató, Temesi

Bradley-Terry-Luce (logistic) model



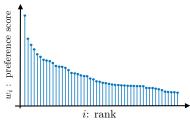
- n items to be ranked
- ullet assign a latent score $\{w_i\}_{1 \le i \le n}$ to each item, so that

item
$$i \succ$$
 item j if $w_i > w_j$

ullet each pair of items (i,j) is compared independently

$$\mathbb{P}\left\{\text{item } j \text{ beats item } i\right\} = \frac{w_j}{w_i + w_j}$$

Bradley-Terry-Luce (logistic) model



- n items to be ranked
- assign a latent score $\{w_i\}_{1 \le i \le n}$ to each item, so that

item
$$i \succ$$
 item j if $w_i > w_j$

ullet each pair of items (i,j) is compared independently

$$y_{i,j} \stackrel{\text{ind.}}{=} \begin{cases} 1, & \text{with prob. } \frac{w_j}{w_i + w_j} \\ 0, & \text{else} \end{cases}$$

Spectral ranking method

ullet construct a probability transition matrix \hat{P} obeying

$$\hat{P}_{i,j} = \begin{cases} \frac{1}{2n} y_{i,j}, & \text{if } i \neq j \\ 1 - \sum_{l:l \neq i} \hat{P}_{i,l}, & \text{if } i = j \end{cases}$$

ullet return the score estimate as the leading left eigenvector $\hat{\pi}$ of \hat{P}

— closely related to PageRank!

Rationale behind spectral method

$$\mathbb{E}[\hat{P}_{i,j}] = \frac{1}{2n} \cdot \frac{w_j}{w_i + w_j}, \qquad i \neq j$$

ullet $oldsymbol{P}:=\mathbb{E}[\hat{oldsymbol{P}}]$ obeys

$$w_i P_{i,j} = w_j P_{j,i}$$
 (detailed balance)

ullet Thus, the stationary distribution π of P obeys

$$\pi = \frac{1}{\sum_{l} w_{l}} \boldsymbol{w}$$
 (reveal true scores)

Statistical guarantees for spectral ranking

— Negahban, Oh, Shah'16, Chen, Fan, Ma, Wang'17

Suppose $\max_{i,j} \frac{w_i}{w_j} \lesssim 1$. Then with high prob.

$$\frac{\|\hat{\boldsymbol{\pi}} - \boldsymbol{\pi}\|_2}{\|\boldsymbol{\pi}\|_2} \asymp \frac{\|\hat{\boldsymbol{\pi}} - \boldsymbol{\pi}\|_{\boldsymbol{\pi}}}{\|\boldsymbol{\pi}\|_2} \lesssim \underbrace{\frac{1}{\sqrt{n}}}_{\text{nearly perfect estimate}} 0$$

• consequence of Theorem 2.8 and the matrix Bernstein (exercise)

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