EE 381V: Large Scale Learning

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Lecture 7 — February 5

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7.1 Topics covereed

• The planted model for spectral clustering

7.2 Perturbation approach

In the previous lecture, we proved the $\sin \theta$ theorem. Applying the theorem, we can find a performance guarantee for the spectral clustering.

Let us first recap the $\sin \theta$ theorem. The distance $d_p(E_0, F_0)$ between two subspaces spanned by the columns of E_0 and F_0 , respectively, is defined as

$$d_p(E_0, F_0) \triangleq ||E_0 E_0^* - F_0 F_0^*||_2 = ||\sin\Theta||_2$$
(7.1)

where Θ is a diagonal matrix with principal angles.

Theorem 7.1 (The $\sin \theta$ theorem). Consider matrices $M, \Delta \in \mathbb{S}_n$ where

$$M = [E_0|E_1] \begin{bmatrix} \operatorname{diag}(M_0) & 0 \\ 0 & \operatorname{diag}(M_1) \end{bmatrix} [E_0|E_1]^*,$$

$$M + \Delta = [F_0|F_1] \begin{bmatrix} \operatorname{diag}(\hat{M}_0) & 0 \\ 0 & \operatorname{diag}(\hat{M}_1) \end{bmatrix} [F_0|F_1]^*$$

are the eigenvalue decompositions of the matrices. If $M_0 \subseteq [a, b]$, $\hat{M}_1 \subseteq (-\infty, a - \delta) \cup (b + \delta, \infty)$, then

$$d_p(E_0, F_0) \le \frac{1}{\delta} ||\Delta||_2.$$
 (7.2)

The $\sin \theta$ theorem bounds the distance between the column spaces of E_0 and F_0 . In spectral clustering, once we take the k eigenvectors with the k smallest eigenvalues, we cluster n rows of the matrix whose columns are the k eigenvectors. Therefore, the performance of the spectral clustering must be measured as the gap between the n rows obtained from the perturbed Laplacian, \hat{L}_n , and the n rows from the unperturbed Laplacian, L_n , up to rotation. In other words, let Y and \hat{Y} denote the matrices with the first k eigenvectors of L and \hat{L} ,

respectively. They are described as

$$Y = \begin{bmatrix} | & & | \\ u_1 & \cdots & u_k \\ | & & | \end{bmatrix} = \begin{bmatrix} - & y_1 & - \\ & \vdots & \\ - & y_n & - \end{bmatrix}, \ \hat{Y} = \begin{bmatrix} | & & | \\ \hat{u}_1 & \cdots & \hat{u}_k \\ | & & | \end{bmatrix} Q = \begin{bmatrix} - & \hat{y}_1 & - \\ & \vdots & \\ - & \hat{y}_n & - \end{bmatrix} Q,$$
(7.3)

where u_1, \ldots, u_k are the first k eigenvectors of L, and $\hat{u}_1, \ldots, \hat{u}_k$ are the first k eigenvectors of \hat{L} . Q is a $k \times k$ unitary matrix. The performance of spectral clustering gets better as $\hat{y}_1, \ldots, \hat{y}_n$ are closer to y_1, \ldots, y_n , respectively. Hence we need to measure $\frac{1}{n} \sum_{i=1}^n ||y_i - \hat{y}_i||_2^2$. Since we have

$$\frac{1}{n} \sum_{i=1}^{n} \|y_i - \hat{y}_i\|_2^2 \le \frac{1}{n} \|Y - \hat{Y}\|_F^2 \le \frac{k}{n} \|Y - \hat{Y}\|_2^2, \tag{7.4}$$

we need to bound $||Y - \hat{Y}||_2^2$. To do so, we define another measure of distance between two subspaces.

Definition 7.2.

$$d_c(E_0, F_0) \triangleq \min_{Q, R \in O(k)} ||E_0 Q - F_0 R||_2$$

= $\min_{R \in O(k)} ||E_0 - F_0 R||_2$ (7.5)

Before we consider the main theorem, we check two useful lemmas.

Lemma 7.3.

$$d_p(E_0, F_0) \le d_c(E_0, F_0) \le \sqrt{2} d_p(E_0, F_0) \tag{7.6}$$

Proof: (Proof)

Lemma 7.4. Let λ_{k+1} and $\hat{\lambda}_{k+1}$ be the (k+1)-th smallest eigenvalue of matrices L and \hat{L} , respectively. Then

$$\hat{\lambda}_{k+1} \ge \lambda_{k+1} - \|\hat{L} - L\|_2. \tag{7.7}$$

Proof: Let u_1, \ldots, u_k be the first k eigenvectors (with the k smallest eigenvalues) of L. Then it follows that

$$\begin{split} \hat{\lambda}_{k+1} &= \max_{V: \dim(V) = k} \min_{x: x \in V^{\perp}, \|x\| = 1} \langle x, \hat{L}x \rangle \\ &\geq \min_{x: x \in \operatorname{span}\{u_1, \dots, u_k\}^{\perp}, \|x\| = 1} \left\{ \langle x, \hat{L}x \rangle - \langle x, (\hat{L} - L)x \rangle \right\} \\ &= \min_{x: x \in \operatorname{span}\{u_1, \dots, u_k\}^{\perp}, \|x\| = 1} \left\{ \langle x, Lx \rangle - \max_{\|x\| = 1} \langle x, (\hat{L} - L)x \rangle \right\} \\ &\geq \min_{x: x \in \operatorname{span}\{u_1, \dots, u_k\}^{\perp}, \|x\| = 1} \langle x, Lx \rangle - \max_{\|x\| = 1} \langle x, (\hat{L} - L)x \rangle \\ &\geq \min_{x: x \in \operatorname{span}\{u_1, \dots, u_k\}^{\perp}, \|x\| = 1} \langle x, Lx \rangle - \max_{\|x\| = \|y\| = 1} \langle y, (\hat{L} - L)x \rangle \\ &= \lambda_{k+1} - \|\hat{L} - L\|_2. \end{split}$$

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An interpretation of Lemma 7.4 is the following: If we add $\hat{L} - L$ to L, λ_{k+1} will change. It is maximally reduced when the kth eigenvector of L is perfectly aligned to the eigenvector with the smallest (negative) eigenvalue of $\hat{L} - L$. Since the value is greater than $-\|\hat{L} - L\|_2$, λ_{k+1} cannot be reduced more than $\|\hat{L} - L\|_2$. There is a chance that another eigenvalue of L smaller than λ_{k+1} will become the (k+1)-th smallest eigenvalue of \hat{L} , but it doesn't matter because the value will be greater than $\lambda_{k+1} - \|\hat{L} - L\|_2$.

Using the above lemmas, we obtain the main theorem.

Theorem 7.5. There exists a unitary matrix $Q \in O(k)$ such that if

$$Y = \begin{bmatrix} | & & | \\ u_1 & \cdots & u_k \\ | & & | \end{bmatrix}, \ \hat{Y} = \begin{bmatrix} | & & | \\ \hat{u}_1 & \cdots & \hat{u}_k \\ | & & | \end{bmatrix} Q, \tag{7.8}$$

then $d_c(E_0, F_0) = ||Y - \hat{Y}||_2$, and

$$\frac{1}{n} \sum_{i=1}^{n} \|y_i - \hat{y}_i\|_2^2 \le \frac{2k}{n(\lambda_{k+1} - \lambda_k - \|\hat{L}_n - L_n\|)^2} \|\hat{L}_n - L_n\|_2^2. \tag{7.9}$$

Proof:

$$\frac{1}{n} \sum_{i=1}^{n} \|y_i - \hat{y}_i\|_2^2 = \frac{1}{n} \|Y - \hat{Y}\|_F^2
\leq \frac{k}{n} \|Y - \hat{Y}\|_2^2
= \frac{k}{n} d_c(Y, \hat{Y})^2
\leq \frac{2k}{n} d_p(Y, \hat{Y})^2
\leq \frac{2k}{n} (\hat{\lambda}_{k+1} - \lambda_k)^2 \|L_n - \hat{L}_n\|_2^2
\leq \frac{2k}{n(\hat{\lambda}_{k+1} - \lambda_k)^2} \|L_n - \hat{L}_n\|_2^2
\leq \frac{2k}{n(\lambda_{k+1} - \lambda_k)^2} \|L_n - \hat{L}_n\|_2^2$$

- The first equality holds by the definition of Frobenius norm.
- The second inequality holds because $||X||_F \leq \sqrt{k}||X||_2$ for any matrix X with rank k.
- The third equality holds by the definition of the distance measure d_c .
- The fourth inequality holds by Lemma 7.3.
- The fifth inequality follows from Theorem 7.1.
- The last inequality follows from Lemma 7.4.

In the next section, we apply this theorem to the planted model.

7.3 The planted model

Consider a graph with k clusters. There is an edge with probability p between a pair of vertices in the same cluster, while vertices in different cluster are connected with probability q. It is natural that we should have p > q to correctly split the vertices into k clusters. The main question is that: How big must the gap p - q be?

Let us build a mathematical model before we consider the problem. The matrices P^{un} and P are defined as

$$P_{ij}^{\mathrm{un}} = \left\{ \begin{array}{l} p & \text{if vertices } i \text{ and } j \text{ are in the same cluster,} \\ 0 & \text{if vertices } i \text{ and } j \text{ are in different clusters,} \end{array} \right.$$

$$P_{ij} = \left\{ \begin{array}{l} p & \text{if vertices } i \text{ and } j \text{ are in the same cluster,} \\ q & \text{if vertices } i \text{ and } j \text{ are in different clusters.} \end{array} \right.$$

Then an adjacency matrix A based on P is generated as

$$A_{ij} = \begin{cases} 1 & \text{with probability } P_{ij} & \text{if } i \leq j, \\ 0 & \text{with probability } 1 - P_{ij} & \text{if } i \leq j, \\ A_{ji} & \text{with probability } P_{ij} & \text{if } i > j. \end{cases}$$

Once we have an adjacency matrix A, we do the spectral clustering.

Note that P and A can be thought of as perturbations of P^{un} and P, respectively. Therefore, we apply Theorem 7.5 for the following two cases.

- A deterministic model : $L_n=I-D^{-\frac{1}{2}}P^{\mathrm{un}}D^{-\frac{1}{2}}, \hat{L}_n=I-D^{-\frac{1}{2}}PD^{-\frac{1}{2}}$
- The planted model : $L_n = I D^{-\frac{1}{2}}PD^{-\frac{1}{2}}, \hat{L}_n = I D^{-\frac{1}{2}}AD^{-\frac{1}{2}}$

In the following sections, we will find a lower bound on p-q for exact partitioning by spectral clustering. The planted model is what we are interested in, but we first consider the deterministic model.

7.3.1 Spectral clustering for the deterministic model

Let $P = U\Lambda U^{-1}$ be the eigenvalue decomposition of P. Since D = (qn + (p-q)n/k)I is a multiple of identity, we have that

$$\hat{L}_n = I - D^{-\frac{1}{2}}PD^{-\frac{1}{2}}$$

$$= UU^{-1} - \frac{1}{\sqrt{\gamma}}I \cdot U\Lambda U^{-1} \cdot \frac{1}{\sqrt{\gamma}}I$$

$$= U\left(I - \frac{1}{\gamma}\Lambda\right)U^{-1}$$

$$(7.10)$$

where $\gamma = qn + (p-q)n/k$. Note that $I - \frac{1}{\gamma}\Lambda$ is diagonal. This means that (7.10) is the eigenvalue decomposition of \hat{L}_n . Therefore, the eigenvectors corresponding to the k smallest eigenvalues of \hat{L}_n are equal to the eigenvectors with the k largest eigenvalues of P. This leads to the following fact.

Proposition 7.6. Clustering according to the bottom k eigenvectors of \hat{L}_n is equivalent to clustering by the top k eigenvectors of P.

Can we also consider the bound in Theorem 7.5 in terms of P and P^{un} ? The following proposition is the key property.

Proposition 7.7. The bound (7.9) is invariant to scaling and translation by addition of a multiple of identity.

Proof:
$$(Proof)$$

As D is a multiple of identity, P is obtained by scaling \hat{L}_n and adding a multiple of identity to it. It follows that the gap between two eigenvalues of \hat{L}_n are scaled by the absolute number of the scaling factor. Therefore, the bound (7.9) is written as

$$\frac{1}{n} \sum_{i=1}^{n} \|y_i - \hat{y}_i\|_2^2 \le \frac{2k}{n(\lambda_{n-k+1}(P) - \lambda_{n-k}(P) - \|P - P^{\mathrm{un}}\|_2)^2} \|P - P^{\mathrm{un}}\|_2^2. \tag{7.11}$$

Since the eigenvalues of P are given by

$$\lambda_n(P) = qn + (p - q)\frac{n}{k},$$

$$\lambda_{n-1}(P) = \dots = \lambda_{n-k+1}(P) = (p - q)\frac{n}{k},$$

$$\lambda_{n-k}(P) = \dots = \lambda_1(P) = 0,$$

the bound is written as

$$\frac{1}{n} \sum_{i=1}^{n} \|\hat{y}_i - e_{\text{cluster}(i)}\|^2 \le \frac{2k}{n(qn + (p-q)n/k - \|P - P^{\text{un}}\|_2)^2} \|P - P^{\text{un}}\|_2^2$$

$$= \frac{2k}{n(qn + (p-q)n/k - qn)^2} (qn)^2$$

$$= \frac{2k^3 q^2}{n(p-q)^2} \tag{7.12}$$

which means that the spectral clustering works while

$$q \le p \left\{ 1 - \frac{ck^{3/2}}{n^{1/2}} \right\}. \tag{7.13}$$

7.3.2 Spectral clustering for the planted model

As mentioned in the previous case, we can consider the k largest eigenvalues and their corresponding eigenvectors of A instead of the k smallest eigenvalues and eigenvectors of L_n , when D for A is a multiple of identity. Here, we also look at A because each diagonal entry

of D is given by the sum of independent random variables, $d_i = \sum_{j=1}^n A_{ij}$, and for sufficiently large n, it is close to a constant $\sum_{j=1}^n P_{ij} = \frac{n}{k}(p-q) + nq$.

The planted model can be rewritten as

$$A = P + X$$
.

where

$$X_{ij} = \begin{cases} 1 - P_{ij} & \text{with probability } P_{ij}, \\ -P_{ij} & \text{otherwise.} \end{cases}$$

Note that E[X] = 0. The bound (7.9) is then given by

$$\frac{1}{n} \sum_{i=1}^{n} \|y_i - \hat{y}_i\|_2^2 \le \frac{2k}{n(\lambda_{n-k+1}(P) - \lambda_{n-k}(P) - \|X\|_2)^2} \|X\|_2^2$$
 (7.14)

Since the eigenvalues of P are given by

$$\lambda_n(P) = qn + (p - q)\frac{n}{k},$$

$$\lambda_{n-1}(P) = \dots = \lambda_{n-k+1}(P) = (p - q)\frac{n}{k},$$

$$\lambda_{n-k}(P) = \dots = \lambda_1(P) = 0,$$

the bound is written as

$$\frac{1}{n} \sum_{i=1}^{n} \|y_i - \hat{y}_i\|_2^2 \le \frac{2k}{n((p-q)(n/k) - \|X\|_2)^2} \|X\|_2^2$$

$$= \frac{2k}{n(n\epsilon/k - \|X\|_2)^2} \|X\|_2^2 \tag{7.15}$$

where $\epsilon = p - q$. Since $||X||_2$ is still a random variable, we need an expression to bound it with high probability.

One reasonable try can be to use Chebyshev's inequality: For any random variable Z with mean μ and variance σ^2 ,

$$P(|Z - \mu| \ge \alpha \sigma) \le \frac{1}{\alpha^2} \tag{7.16}$$

for any number $\alpha > 0$. Since we have that

$$\sigma^2 = E[\|X\|_2^2] \le E[\|X\|_F^2] = \sum_{i,j} E[X_{ij}^2] \le n^2, \tag{7.17}$$

it follows that

$$P(\|X\|_2 \ge 10n) \le P(\|X\|_2 \ge 10\sigma^2) \le \frac{1}{100}.$$
 (7.18)

Putting the bound $||X||_2 \le 10n$ to Theorem 7.5, we get

$$\frac{1}{n} \sum_{i=1}^{n} \|y_i - \hat{y}_i\|_2^2 \le \frac{2k}{n(n\epsilon/k - \|X\|_2)^2} \|X\|_2^2$$

$$\le \frac{2k}{n(n(\epsilon/k - 10))^2} (10n)^2$$

$$\le \frac{200k}{n(\epsilon/k - 10)^2}.$$

This bound doesn't give any useful result for ϵ . In the above derivation, (7.17) and (7.18) hold even if the entries of X are correlated. To obtain a useful bound, we must exploit independence of i and j.

Another try is to use the Matrix Bernstein inequality. [1]

Theorem 7.8 (Matrix Bernstein inequality). Let $Z_1, \ldots, Z_m \in \mathbb{S}^n$ be independent random matrices where $E[Z_i] = 0$, $||Z_i||_2 \leq R$, and $||\sum_{i=1}^m E[Z_i^2]|| \leq \sigma^2$, and let $X = \sum_{i=1}^m Z_i$. Then we have that

$$P(\|X\|_2 > t) \le n \exp\left(-\frac{t^2}{6(Rt + \sigma^2)}\right).$$
 (7.19)

We can apply Theorem 7.8 to X = P - A by defining

$$Z_{(ij)} \triangleq X_{ij}(e_i e_i^* + e_j e_i^*)$$

where the superscript * denotes the transpose. Note that all the entries of $Z_{(ij)}$ are zero except for the entries at (i,j) and (j,i) that are equal to $X_{ij} = X_{ji}$. Then X can be described as the sum of n^2 matrices

$$X = \sum_{i,j} Z_{(ij)}.$$

The random matrices $Z_{(ij)}$ have the following properties.

- $E[Z_{(ij)}] = 0, ||Z_{(ij)}||_2 \le 2.$
- $Z_{(ij)}^2 = X_{ij}(e_i e_j^* + e_j e_i^*)^* \cdot X_{ij}(e_i e_j^* + e_j e_i^*) = X_{ij}^2(e_i e_i^* + e_j e_j^*).$

$$\sum_{i,j:i \le j} E[Z_{(ij)}^2] = \begin{pmatrix} \sum_{j=1}^n X_{1j}^2 & & \\ & \ddots & \\ & & \sum_{i=1}^n X_{nj}^2 \end{pmatrix}, \quad \sigma^2 = \left\| \sum_{i \le j} E[Z_{(ij)}^2] \right\|_2 \le n.$$

Using Theorem 7.8 and the above properties, we obtain that

$$P(\|X\|_2 > t) \le n \exp\left(-\frac{t^2}{6(Rt + \sigma^2)}\right)$$

$$\le n \exp\left(-\frac{t^2}{6(2t + n)}\right). \tag{7.20}$$

Consider $t = 10\sqrt{n \log n}$. Then we have that

$$P\left(\|X\|_{2} > 10\sqrt{n\log n}\right) \le n \exp\left(-\frac{100n\log n}{6(n+20\sqrt{n\log n})}\right)$$

$$\le n \exp\left(-\frac{100n\log n}{10n}\right)$$

$$\le n \exp\left(-10\log n\right) = n^{-9}.$$
(7.21)

This implies that for sufficiently large n, we have that

$$||X||_2 \le 10\sqrt{n\log n} \tag{7.22}$$

with high probability. Let us drop the $\log n$ factor just to make bounds look clean. Then we obtain that

$$\frac{1}{n} \sum_{i=1}^{n} \|y_i - \hat{y}_i\|_2^2 \le \frac{2k}{n(n\epsilon/k - \|X\|_2)^2} \|X\|_2^2
\le \frac{200k}{(n\epsilon/k - 10\sqrt{n})^2}
\le \frac{200k}{\gamma^2 n}$$

where $\epsilon \geq \frac{10k}{\sqrt{n}} + \gamma$. This concludes that we need

$$p - q = \epsilon \ge \frac{10k}{\sqrt{n}} \tag{7.23}$$

for the planted model to be correctly partitioned using spectral clustering for sufficiently large n.

Remark 7.9. If k = O(1) as $n \to \infty$, then we need $\epsilon = O(1/\sqrt{n})$. This implies that if n >> k, the spectral clustering can correctly partition the planted model even with a very small gap $\epsilon = p - q$.

Bibliography

[1] Tropp, J. (2010). User-friendly tail bounds for sums of random matrices. Foundations of Computational Mathematics, 12(4), 389–434.