CS 798 - Algorithmic Spectral Graph Theory, Fall 2015, Waterloo

Lecture 5: Higher-order Cheeger's inequality

We show a generalization of Cheeger's inequality relating lk to multiway partitioning.

The proofs use the spectral embedding of a graph, and provide some new ideas to analyzing it.

Higher eigenvalues and graph multipartitioning

We assume the graph is d-regular.

Let $L = \frac{1}{\alpha}L$ be the normalized Laplacian matrix, with eigenvalues $0 = \lambda_1 \le \lambda_2 \le ... \le \lambda_n \le 2$.

It is not difficult to show that $\lambda_{k=0}$ if and only if the graph has at least k connected components.

In other words, $\lambda_{k}=0$ if and only if there are disjoint subsets $S_{1},S_{2},...,S_{k}\subseteq V$ with $\phi(S_{1})=0$, where $\phi(S_{1})$ denotes the conductance of S_{1} .

Similar to the pattern that we have seen in previous lectures, we will show that this spectral characterization allows us to prove a quantitative generalization, that λ_K is small if and only if there are disjoint subsets $S_1, S_2, ..., S_K \leq V$ all with small conductance.

Let $\phi_{\kappa}(G) := \min_{S_1, S_2, ..., S_K \leq V} \max_{i} \phi(S_i^*)$ be the k-way conductance of the graph G. $S_i \cap S_j = \emptyset \ \forall i, j$

The following result is called the higher-order Cheeger's inequality.

Theorem [LOT12] $\frac{\lambda_k}{2} \leq \phi_k(q) \leq O(k^2) \sqrt{\lambda_k}$

Another research group also proved a similar result using different techniques, which shows that the dependency on k can be improved considerably if we construct slightly fewer disjoint sparse cuts. Theorem [LOTIZ, LRTV 12] $\phi_k(G) \leq O(\text{polylog}(k)) \int_{\lambda_{2k}}^{\infty}$

Both results were inspired by the result in [ABS10] that if λ_k is small for a large k, then there exists a set S with $\phi(S) \approx O(J\lambda_k)$ and $|S| \approx |V|/k$.

We will study the result in [ABS10] later when we talk about random walks in graphs.

The direction $\frac{1}{2}\lambda_k \leq \Phi_k(G)$ is called the easy direction, and the other direction is the hard direction. Again, the easy direction can be seen as showing that λ_k is a relaxation of the k-way partitioning problem, while the hard direction can be seen as a rounding algorithm for the relaxation.

Spectral embedding

We have proved the following result when we proved Cheeger's inequality.

Lemma (Cheeper's rounding) Given $x \in \mathbb{R}^n$, there is an efficient algorithm (the "sweep" algorithm) that finds $S \subseteq \text{supp}(x)$ such that $\Phi(S) \subseteq \int 2R(x)$, where $\text{supp}(x) := \{i \mid xi \neq 0\}$ is the support of vector x and $R(x) := \frac{x^T \mathcal{L}x}{x^T x}$ is the Rayleigh quotient of x.

If λ_k is small, then we know that there are k orthogonal eigenvectors each with small Rayleigh quotient. We can apply Cheeger's rounding on each eigenvector to find a sparse cut.

(Note that to apply the above lemma, we don't need X to be an eigenvector, just that R(X) is small.)

Since the K vectors are orthogonal, intuitively, we expect that the sparse cuts produced by

Cheeger's rounding on them are quite different (e.g. imagine the k vectors are all \$0,1]-vectors).

So, this suggests that there are K different sparse cuts in the graph, and it should be

possible to combine them to find k disjoint sparse cuts in the graph.

It is not clear how to proceed with this idea, by dealing with each vector independently.

Instead, we take a more global view that considers all the k vectors at the same time.

Let U be an nxk matrix where the i-th column is the i-th eigenvector, i.e. $U = \begin{bmatrix} v_1 v_2 & \dots & v_k \\ v_1 v_2 & \dots & v_k \\ \vdots & \ddots & \ddots & \vdots \end{bmatrix}$ For each vertex $j \in V$, we map j to the j-th row of U, denoted by U_j .

We think of this maps vertex j to a point in the k-dimensional space.

This is what we mean by the <u>Spectral embedding</u> of the graph.

The spectral embedding is actually used in pratical heuristics for graph k-way partitioning for some time. One popular heuristic is to apply some well-known geometric clustering algorithms, in particular the k-means algorithm, to partition the point set in the spectral embedding into k groups, and use this partitioning to cut the graph into k sets.

It is reported that this heuristic works very well in applications, like image segmentation and data clustering, but no theoretical guarantees were known about these heuristics.

The proofs of the higher-order Cheeper's inequality can be seen as proving rigorously the performance

Isotropy condition

For the Spectral partitioning to provide useful information for us to find k disjoint sparse cuts, a necessary condition is that the points should be reasonably well spread out (e.g. if all the vertices are only mapped into only two distinct points in \mathbb{R}^k , then we have no clue how to find k disjoint sparse cuts for k > 2).

Of course, this kind of bad cases would not happen because the k vectors are orthogonal. The question is how to use the orthogonality to give us useful conditions for clustering.

Recall that U is the nxk matrix where the i-th column is the i-th eigenvector, and U_j denotes the j-th row of U, the k-dimensional point associated to vertex j in the spectral embedding.

Then $U^TU=I$, because the columns of U are orthonormal.

Note that $U^TU=I$ can also be written as $\sum_{i=1}^n U_i^T U_i^T=I$.

We say the vectors U,..., Un ERk are in isotropy condition for the following reason.

Claim (isotropy condition) For any $X \in \mathbb{R}^k$ with ||X|| = 1, we have $\sum_{i=1}^n \langle X_i U_i \rangle^2 = 1$.

$$\frac{\text{proof}}{\text{U}} \quad \text{U}^{\text{T}} \cup \text{I} \quad \Rightarrow \quad \text{X}^{\text{T}} \cup \text{U}^{\text{T}} \cup \text{X} = \text{X}^{\text{T}} \times \text{I} \quad \Rightarrow \quad \text{I} = \text{X}^{\text{T}} \left(\sum_{i=1}^{n} \cup_{i} \cup_{i}^{i} \right) \times = \sum_{i=1}^{n} \text{X}^{\text{T}} \cup_{i}^{i} \cup_{i}^{i} \times \text{X} = \sum_{i=1}^{n} \left\langle \times_{i} \cup_{i}^{i} \right\rangle^{2}. \quad \square$$

This claim says that for any direction $x \in \mathbb{R}^k$, the sum of the square of the projection of x_i on u is equal to one.

To get an idea, suppose $U_1=U_2=...=U_Q=y\in\mathbb{R}^k$ (that the first l vertices all mapped to the same pointy), then the claim implies that $1=\sum\limits_{i=1}^{\infty}<\frac{y}{\|y\|}$, $|y|>^2>\sum\limits_{i=1}^{2}<\frac{|y|}{\|y|}$, $|y|>^2=\sum\limits_{i=1}^{2}\||y||^2$.

On the other hand, $\sum_{i=1}^{n} ||V_i||^2 = \sum_{i=1}^{K} ||V_i||^2 = K$, where V_i is the i-th eigenvector (of unit length).

Therefore, if we think of the <u>mass</u> of a point i is $\|V_i\|^2$, then the above discussion says that the total mass mapped to the same point y is one, while the total mass is k.

That is, only & fraction of the total mass is mapped to the same point.

This, for example, shows that the vertices cannot be mapped to less than K distinct points, and that's why the bad cases that we mentioned won't happen in the spectral embedding.

Generalizing this idea, suppose U, U2,...,Ue are all pointing to similar direction, such that costij>1-E.

By setting $X = U_1$. the isotropy condition tells us that $1 = \sum_{i=1}^{n} \left\langle \frac{U_1}{||U_1||}, U_i \right\rangle^2 \geqslant \sum_{i=1}^{k} \frac{1}{||U_1||^2} \left\langle U_1, U_i \right\rangle^2 = \sum_{i=1}^{k} \frac{1}{||U_2||^2} ||U_1||^2 ||U_2||^2 ||U_1||^2 ||U_2||^2 ||U_1||^2 (1-\epsilon)^2 \geqslant (1-2\epsilon) \sum_{i=1}^{k} ||U_i||^2.$

This implies that $\sum_{i=1}^{k} ||U_i||^2 \leq \frac{1}{1-2\epsilon}$. When ϵ is small, the RHS is very close to one.

This is saying that points in very similar direction can carry at most & k fraction of total mass. So, by using the direction of the points to guide us to cluster the points, we see that the points will be reasonably well spread out.

Clustering using directions

We formalize the above discussions into a lemma.

For a vertex i, the mass of i is defined as IVIII.

Recall that the total mass is $\frac{n}{n} \|V_i\|^2 = k$.

For two vertices i,j, we define the <u>distance</u> d(i,j) as $\|\frac{Ui}{\|V_i\|} - \frac{Uj}{\|V_j\|}\|$.

Note that d(i,j) & Oij, where Oij is the angle between Ui and Uj.

Lemma Let $S \leq V$ be such that $d(i,j) \leq \Delta$ for all $i,j \in S$. Then $\sum_{i \in S} ||U_i||^2 \leq \left(\frac{1}{1-\Delta^2}\right)$.

<u>proof</u> For two unit vectors u,v, ||u-v||^= ||u||^+ ||v||^- 2(u,v) = 2-2(u,v), and so (u,v) = 1- d(u,v).

Pick an arbitrary vertex jes and consider the unit vector Uj/110j11.

The isotropy claim says that $1 = \sum_{i=1}^{n} \left\langle \frac{U_i}{\|U_j\|} - U_i \right\rangle^2 \geqslant \sum_{i \in S} \left\| |U_i||^2 \left\langle \frac{U_i}{\|U_j\|} , \frac{U_i}{\|U_i||} \right\rangle^2$

 $= \sum_{i \in S} \|U_i\|^2 \left(1 - \frac{d(i,j)}{2}\right)^2 \quad (by the above)$ $\geq \sum_{i \in S} \|U_i\|^2 \left(1 - \frac{\partial^2}{2}\right)^2 \quad (by the assumption)$ $\geq \sum_{i \in S} \|U_i\|^2 \left(1 - \partial^2\right).$

To apply the lemma, we choose \triangle so that $\frac{1}{1-\Delta^2} \le 1+\frac{1}{2k}$ (say when $\triangle = \frac{1}{2Jk}$). We will only take a subset S with diameter \triangle (i.e. $d(ij) \le \triangle = \forall i,j \in S$). Then, the lemma implies that each such subset has mass at most $1+\frac{1}{2k}$.

So, after taking k-1 subsets, the remaining mass is still at least \pm , a $\Omega(k)$ fraction of the total mass. This will ensure that we can form k groups of $\Omega(k)$ fraction of mass by clustering using directions. This distance function (using directions) is used in a practical heuristic before [NJW01].

Disjoint Clusters

The previous section shows that bad cases won't happen if we do the clustering based on directions.

In this section, we think about the good case when the spectral embedding really gives what we want, k clusters that are far apart from each other.

Suppose there are k disjoint subsets $S_1, S_2, ..., S_K$ such that each has mass 1 and $d(S_i, S_j) \ge \delta$ $\forall i,j$ where $d(S_i, S_j) := \min \left\{ d(a,b) \mid a \in S_i, b \in S_j \right\}$.

Can we conclude that these correspond to k disjoint sparse cuts in the graph?

Rayleigh quotients

Let $U_1, U_2, ..., U_n \in \mathbb{R}^k$ be the spectral embedding of the graph.

We can define the Rayleigh quotient of the spectral embedding as \frac{\sum_{\infty} || \Ui-Ui||^2}{d\xi_{\infty} || \Ui-Ui||^2}.

Note that $\|U_{\hat{i}} - U_{\hat{j}}\|^2 = \sum_{l=1}^k \left(|U_{\hat{i}}(l) - U_{\hat{j}}(l)|^2 \right)^2$ (sum of the k coordinates) $= \sum_{l=1}^k \left(|V_l(\hat{i}) - V_l(\hat{j})|^2 \right)^2 \qquad \text{(the l-th coordinate is the l-th eigenvector)}$

Let $R(v_i) = A_i/B_i = \lambda_i$ for $1 \le i \le k$.

Then, we see that the Rayleigh quotient of the spectral embedding is $\frac{\sum_{k=1}^{k}A_{k}}{\sum_{k=1}^{k}B_{k}} \leq \lambda_{k}$.

On the other hand, if we have a spectral embedding (in \mathbb{R}^k) with Rayleigh quotient $\leq \alpha$, then we can find a one-dimensional embedding with Rayleigh quotient $\leq \alpha$.

The reasoning is similar: we write the Rayleigh quotient of the spectral embedding as $\frac{\sum\limits_{k=1}^{k}A_{k}}{\sum\limits_{k=1}^{k}B_{k}}$, where A_{k} , B_{k} are the sums of the k-th coordinate.

Then, $\min \frac{AR}{B_{e}} \le \frac{\sum_{k=1}^{K}AR}{\sum_{k=1}^{K}B_{e}}$, and so the best coordinate has Rayleigh quotient no larger than that of the K-dimensional embedding.

So, from a k-dimensional embedding. We can find a sparse cut by first restricting to the best coordinate, and then use Cheeper rounding in that coordinate to obtain a sparse cut.

The plan

Now we are ready to analyze the good case.

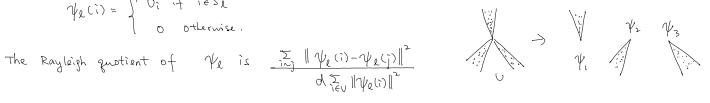
From the above discussion, we know that the Rayleigh quotient of the spectral embedding is $\leq \lambda_K$.

In the good case, there are k disjoint subsets S1, S2,..., SKEV, each has mass 1, and d(S1,S1) > 6 4:1. We would like to construct k spectral embedding $V_1, V_2, ..., V_k$, such that V_ℓ is only supported on So (i.e. in No, every vertex i & So is mapped to the zero vector).

If we can do this such that the Rayleigh quotient of ψ_{ℓ} is small for all $1 \le \ell \le k$, then we can apply the argument in the above discussion to reduce to the best wordinate in the Then, we can apply the Cheeger rounding lemma to obtain a sparse cut, with support on Sx.

The important question is how to construct the and upper bound its Rayleigh quotient.

The most natural way to define be is simply to zero out everything outside Se:



$$= \frac{\sum_{i=1}^{\infty} and (es and jes ||U_i-U_j||^2 + \sum_{i=1}^{\infty} and (es and jes ||U_i||^2)}{d (es and jes ||U_i||^2)}$$

Compare it to the Rayleigh quotient of the spectral embedding of U.

Since is ||Vill=1 (by our assumption of the good case) and is ||uill=k, the denominator of the is * times the denominator of U.

Clearly, each term in the first summation of We is at most that in U.

The interesting case is for those edges with iES and j&S.

For those edges, it contributes 110:11 in We while it contributes 110:-Ujll in U.

By our assumption. Oij \approx d(i,j) \geqslant δ , the smallest $\|U_i - U_j\|^2$ one could get is $\|U_{i}\| \sin^{2}\theta_{ii} \approx \|U_{i}\| e^{i}_{ii} > \|U_{i}\| s^{2}$



Therefore, each term in the numerator of ψ_{ℓ} is at most $\frac{1}{8^2}$ times that of the corresponding term in U, and thus the numerator of the is at most & times the numerator of U.

Combining, the Rayleigh quotient of Ve is at most $\frac{k}{s^2}$ times the Rayleigh quotient of V, and thus $R(\gamma_k) \le \frac{k \lambda_k}{s^2}$. So, by Cheeger's rounding, we get a sparse cut $S_{\ell}' \subseteq S_{\ell}$ with $\phi(S_{\ell}') \le \frac{1}{5} \sqrt{2k \lambda_k}$.

Assuming δ is a constant, then we get k disjoint sparse cuts of conductance $O(\sqrt{2k}\lambda_k)$.

Smooth localization

In the general case, we use a similar strategy.

We would like to find k disjoint subsets S1, S2, ..., SK EV such that

- (2) $d(S_i, S_j) \ge 2\delta$ \forall $1 \le i + j \le k$, where $d(S_i, S_j) = \min_{a \in S_i, b \in S_j} d(a, b)$.

If we can do this, then we would like to define k disjoint supported functions $\psi_1, \psi_2, ..., \psi_k$ with Rayleigh quotient $R(\psi_\ell) \leq \frac{k \lambda_k}{S^2}$ as above.

There is one subtlety here.

There are some points $j \notin S_1 \cup ... \cup S_k$ but are very close to some point $i \in S_k$. In this case, when we define $\forall \ell$ by zeroing out everything outside S_k .

The length of this edge in Ve is $\|V_{\ell}(i) - V_{\ell}(j)\|^2 = \|U_i\|^2$ could be much larger than $\|U_i - U_j\|^2$.

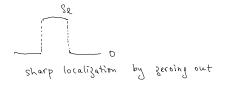
The ratio $\|V_{\ell}(i) - V_{\ell}(j)\|$ could be unbounded and our term-by-term analysis above does not work.

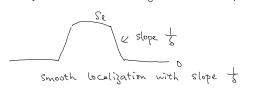
To handle this issue, we use the condition that $d(S_i, S_j) \geqslant \delta$ to give us some room to "Smoothly" decrease the length of the points close to S_A to zero.

Formally, for each $j \notin S_{\ell}$, let $d(j, S_{\ell}) = \min_{i \in S_{\ell}} d(i, j)$.

We define $c_j = \max \{ 1 - \frac{d(j, S_k)}{s}, o \}$ and $\psi_k(j) = c_j U_j$.

So, if d(j,Sl) ≥ 8, then \u03c4(j)=0; if d(j,Sl)≤8, cj decreases linearly with a slope of





By doing smooth localization, the following claim shows that the same term-by-term analysis still works.

<u>proof</u> Note that $|c_i - c_j| \le \frac{1}{8} d(i,j)$, as $d(j,S) - d(i,S) \le d(i,j)$.

Now, 11 /2 (1) - /2 (1) 11 = 11 ci vi - cj vj 11 = 11 ci vi - cj vi + cj vi - cj vj 11

Note that the first term $|e_{i}-e_{j}| \|U_{i}\| \leq \frac{1}{\delta} \|u_{i,j}\| \|u_{i,j}\| = \frac{1}{\delta} \|\frac{U_{i}}{\|U_{j,j}\|} \||u_{i,j}\|| = \frac{1}{\delta} \||u_{i}-\frac{U_{i,j}}{\|U_{j,j}\|} \|u_{i,j}\| = \frac{1}{\delta} \||u_{i}-\frac{U_{i,j}}{\|U_{j,j}\|} \|u_{i,j}\| = \frac{1}{\delta} \||u_{i}-\frac{U_{i,j}}{\|U_{j,j}\|} \|u_{i,j}\| = \frac{1}{\delta} \||u_{i}-\frac{U_{i,j}}{\|U_{i,j}\|} \|u_{i,j}\| = \frac{1}{\delta} \||u_{i,j}-\frac{U_{i,j}}{\|U_{i,j}\|} \|u_{i,j}\| = \frac{1}{\delta} \||u_{i,j}-\frac{U_{i,j}}{\|U_{i,j}-\frac{U_{i,j}}{\|U_{i,j}-\frac{U_{i,j}}{\|U_{i,j}-\frac{U_{i,j}}{\|U_{i,j}-\frac{U_{i,j}}{\|U_{i,j}-\frac{U_{i,j}}{\|U_{i,j}-\frac{U_{i,j}}{\|U_{i,j}-\frac{U_{i,j}}{\|U_{i,j}-\frac{U_{i,j}}{\|U_{i,j}-\frac{U_{i,j}}{\|U_{i,j}-\frac{U_{i,j}}{\|U_{i,j}-\frac{U_{i,j}}{\|U_{i,j}-\frac{U_{i,j}}{\|U_{i,j}-\frac{U_{i,j}}{\|U_{i,j}-\frac{U_{i,j}}{\|U_{i,j}-\frac{U_{i,j}}{\|U_{i,j}-\frac{U_{i,j}}{\|U_{i,j}-\frac{U_{i,j}}{\|U_{i,j}-\frac{U_{i,j}}{\|U_{i,j}-\frac{U_{i,j}}{\|U_{i,j}-\frac{U_{i,j}}{\|U_{i,j}-\frac{U_{i,j}}{\|U_{i,j}-\frac{U_{i,j}}{\|U_{i,j}-\frac{U_{i,j}}{\|U_{i,j}-\frac{U_{i,j}}{\|U_{i,j}-\frac{U_{i,j}}{\|U_{i,j}-\frac{U_{i,j}}{\|U_{i,j}-\frac{U_{i,j}}{\|U_{i,j}-\frac{U_{i,j}}{\|U_{i,j}-\frac{U_{i,j}}{\|U_{i,j}-\frac{U_{i,j}}{\|U_{i,j}-\frac{U_{i,j}}{\|U_{i,j}-\frac{U_{i,j}}{\|U_{i,j}-\frac{U_{i,j}}{\|U_{i,j}-\frac{U_{i,j}}{\|U_{i,j}-\frac{U_{i,j}}{\|U_{i$

With this (technical) claim, we are about to complete the proof.

Partitioning space

The difficult case seems to be when the points distributed evenly in the space, in which it is not clear how to find the disjoint sets $S_1,...,S_k$ with the required properties.

The idea is to partition the directions in S^k (the k-dimensional sphere) into cubes each with side length $L=\frac{1}{2k}$.

(This cube argument is presented in [L13].)

All the points with directions in the same cube are put into a block.

The diameter in each cube is $LJK = \frac{1}{2JK}$.



By the isotropy lemma, the points in each block has mass ≤ 1+ 1/2k.

To construct disjoint $S_1,...,S_k \in V$ where each S_1 has mass $\gg \frac{1}{2}$, we just greedily group the blocks so that their mass is at least $\frac{1}{2}$.

Since no block is too heavy, it is always possible.



Finally, we need to guarantee that the sets are 8-far apart.

To do this, for each cube, we delete all the directions that are of distance at most $\frac{L}{4k^2}$ from some side, and then we delete all the points with those directions in the conserponding block.

By doing so, the fraction of the volume of each cube remained is $(1 - \frac{1}{4k^2})^k \ge (1 - \frac{1}{4k}).$



Therefore, if we choose a uniformly random translation of the partition, the expected total massed removed is only $\frac{1}{4}$, and this is small enough so that it doesn't affect the graping argument. Now, the sets S_7 are at least 8-far apart with $8 = \frac{L}{2k^2} = \frac{1}{4k^3}$

So, following our plan (with smooth localization), we can construct disjoint supported functions, each with Rayleigh quotient $O(\frac{k\lambda k}{5^2}) = O(k^7 \lambda k)$, and hence we get k disjoint subsets with conductance $O(k^3 5 \lambda k)$ by Cheeger rounding.

Discussions

- The tighter bound $O(k^2 J \lambda_k)$ is obtained by some random partitioning technique in metric embedsing.
- The bound $\phi_{\kappa}(G) \leq O(polylog(k) \int \lambda_{2k})$ is proved by using some dimension reduction technique

to reduce the spectral embedding from k-dimensional space to O(logk)-dimensional space.

This bound is tight as shown by the noisy hypercube example (we may talk about later).

- The algorithm in [LRTV12] is very simple. Compute the spectral embedding. Generate k random directions $r_1,...,r_k$. Put point j into cluster l if $\langle U_j,r_k\rangle \geqslant \langle U_j,r_i\rangle \forall i$.

 This is it, but the analysis is less intuitive.
- It is still open whether $\phi_{\mathcal{K}}(G_1) \leq O\left(\frac{1}{2}\log(k)\right) \sqrt{\lambda_{\mathcal{K}}}$.

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