How to Round Subspaces: A New Spectral Clustering Algorithm

Ali Kemal Sinop

July 21, 2015

Abstract

A basic problem in spectral clustering is the following. If a solution obtained from the spectral relaxation is close to an integral solution, is it possible to find this integral solution even though they might be in completely different basis? In this paper, we propose a new spectral clustering algorithm. It can recover a $k$-partition such that the subspace corresponding to the span of its indicator vectors is $O(\sqrt{\text{OPT}})$ close to the original subspace in spectral norm with $\text{OPT}$ being the minimum possible ($\text{OPT} \leq 1$ always). Moreover our algorithm does not impose any restriction on the cluster sizes. Previously, no algorithm was known which could find a $k$-partition closer than $o(k \cdot \text{OPT})$.

We present two applications for our algorithm. First one finds a disjoint union of bounded degree expanders which approximate a given graph in spectral norm. The second one is for approximating the sparsest $k$-partition in a graph where each cluster has expansion at most $\phi_k$ provided $\phi_k \leq O(\lambda_{k+1})$ where $\lambda_{k+1}$ is the $(k+1)^{th}$ eigenvalue of Laplacian matrix. This significantly improves upon the previous algorithms, which required $\phi_k \leq O(\lambda_{k+1}/k)$.

1 Introduction

In this paper, we study the following problem. If the solution of spectral relaxation for some $k$-way partitioning problem is close to an integral solution, can we still find this integral solution? The main difficulty is due to the rotational invariance of the spectral relaxation. The basis of an integral solution might be completely different than the basis of solutions for the spectral relaxation. Arguably, this is a fundamental problem in spectral clustering, which is a widely used approach for many data clustering and graph partitioning problems arising in practice.

Formally, we study the problem of approximating a $k$-dimensional linear subspace of $\mathbb{R}^n$ by another subspace which is $k$-piecewise constant: Every vector of this subspace has its coordinates comprised of at most $k$ distinct values. In 2-dimensions, where $k = 2$, optimal solution corresponds to one of the threshold cuts. From this perspective, our problem can be seen as a generalization of thresholding to higher dimensions.

In spectral methods, one uses the top (or bottom) $k$-eigenvectors of some matrix derived from the input to find a $k$-partition, which is usually the Laplacian or adjacency matrix of some graph derived from the distances or nearest neighbors. Usually, there is a close connection between spectral
methods and the basic SDP (semi-definite programming) relaxations of associated clustering and partitioning problems: Top (or bottom) $k$ eigenvectors correspond to an optimal solution of these SDP formulations. If the relaxation is good enough, in the sense that it has a small integrality gap; then one might naturally expect these $k$-eigenvectors to be close to an integral solution in the form of a $k$-partition up to an arbitrary rotation. Hence it is possible to argue that the goal of spectral clustering algorithms is to round these $k$-eigenvectors to a close $k$-partition.

The formal definition of our problem is as follows. Given a $k$-dimensional subspace of $\mathbb{R}^n$ as an orthonormal matrix $Y \in \mathbb{R}^{n \times k}$, $Y^T Y = I_k$, find a $k$-partition of its rows such that, for $C \in \mathbb{R}^{n \times k}$ being the matrix of cluster centers (each row of $C$ is one of the cluster centers), $\|Y - C\|_2$ is as small as possible. Geometrically, this corresponds to a $k$-piecewise constant subspace that makes the minimum angle with $Y$. This problem of finding a $k$-partition so as to minimize the spectral norm was first formalized in [KK10]. Since the spectral norm of difference is bounded, all original spectral properties of $Y$ also apply for our $k$-partition up to a small error. Especially for basic SDP relaxations, this means that such $k$-partitions will be provably good solutions.

Our main contribution is a new spectral clustering algorithm that can recover a $k$-partition whose center matrix $C'$ satisfies $\|Y - C'\|_2 \leq O(\sqrt{\text{OPT}})$, where OPT is the minimum possible. Observe that OPT is always at most one, OPT $\leq 1$. Furthermore, the recovered $k$-partition will be $O(\sqrt{\text{OPT}})$-close to the optimum partition in a very strong sense: Each cluster we found will be close to a unique cluster among the optimum $k$-partition. Previously, no algorithm was known to find a $k$-partition closer than $o(k \cdot \text{OPT})$.

We also study two closely related problems. In the first one, the goal is to approximate a matrix in spectral norm by a block diagonal matrix, with every block being the normalized adjacency matrix of a clique. Our second application is for finding non-expanding sets in a graph whose spectrum exhibits certain gaps.

The choice of spectral norm to measure the closeness of associated subspaces is quite natural from the perspective of our second application. We show how to construct graphs in polynomial time, where finding $k$ non-expanding cuts implies a solution for the clustering problem with spectral norm on any given subspace. From this perspective, we can see that the subspace rounding problem is a prerequisite toward obtaining a $o(k)$-factor approximation algorithm for the problem of $k$-EXPANSION, where the best known is $O(k^4)$ due to [LGT14].

1.1 Related Work

Spectral methods have been successfully used for clustering tasks [Bol13] arising in many different areas such as VLSI [AKY99], machine learning, data analysis [NJW01] and computer vision [SM00, YS03]. They are usually obtained by formulating the clustering task as a combinatorial optimization problem (such as sparsest/normalized cuts [SM00]), then solving the corresponding basic SDP relaxation, whose solution is often given by $k$ extremal eigenvectors of an associated matrix.

One of the first spectral clustering algorithms with worst case guarantees was given in [KVV04] for the graph partitioning problem assuming certain conditions on the internal versus external conductance. The problem of finding a $k$-partition so as to minimize the spectral norm was first introduced by [KK10] in the context of learning mixtures of Gaussians. The best known approximation factor is $O(k)$ due to [AS12].

A problem closely related to spectral clustering is $k$-EXPANSION. Here the goal is to partition the nodes of a graph into $k$-parts so as to minimize the maximum expansion (ratio of the total weight of
edges cut and the total number of pairs cut) of any individual part. When all cluster sizes are con-
strained to be nearly equal, this problem admits a $O(\sqrt{\log n \log k})$-factor approximation [BFK+11].

On the other hand, if a bi-criteria approximation is sought, then one can find $(1 - \Omega(1))k$ clusters
each of which has expansion at most $O(\sqrt{\log n \log k})$ times the optimum [LM14].

If we look at the basic SDP relaxation of $k$-EXPANSION, then the optimal fractional solution is
given by the $k$ smallest eigenvectors of the corresponding graph Laplacian matrix. In fact, this is
the main motivation behind the usage of $k$-eigenvectors for clustering tasks in practice. A natural
question is whether one can “round” these eigenvectors to a $k$-partition (the so called Cheeger inequal-
ities). When $k = 2$, it was shown in [AM85] that simple thresholding yields a 2-partition
with $O(\sqrt{\phi_2})$ expansion, where $\phi_k$ is the optimal value for $k$-EXPANSION. Later a better bound
was given in [KLL+13], assuming there is some gap between eigenvalues. When $k > 2$, bi-criteria
versions of Cheeger’s inequality are known [ABS10, LRTV12, LGT14]. Here the guarantees on the
expansion are of the form $\tilde{O}(\sqrt{\phi_k})$, where $\tilde{O}$ hides the dependencies on logarithmic factors; but the
algorithms can only find $(1 - \Omega(1))k$ parts.

The problem becomes significantly harder when exactly $k$ clusters are desired. In this case, it
was shown in [LGT14] that a method similar to the one proposed in [NJW01] will yield a $k$-
partition with maximum expansion $O(k^{4}\sqrt{\phi_k})$. This is the best known approximation algorithm
for $k$-EXPANSION problem and, as of yet, there is no algorithm known which achieves a poly-
logarithmic approximation.

Perhaps the simplest case of $k$-EXPANSION is when there is a gap between the $(k + 1)^{st}$ smallest
eigenvalue of Laplacian matrix, $\lambda_{k+1}$, and $\phi_k$ of the form $\frac{\lambda_{k+1}}{\phi_k} \geq \frac{1}{\varepsilon}$. One might think of this as a
stability criteria: It implies that all $k$-partitions with maximum expansion $\leq O(\phi_k)$ are $O(\varepsilon)$-close
to each other. To put it in another way, approximating the optimum $k$-partition is at least as easy as
finding a $k$-partition with minimum possible expansion among all its clusters. For the case of $k = 2$,
it is trivial to show that thresholding the second smallest eigenvector of Laplacian yields $\varepsilon$-close
partition to the optimal one. On the other hand, when $k > 2$, the best prior result is due to [AS12];
and it can only find a $k$-partition that is $O(k\varepsilon)$-close to the optimal solution. In other words, when
$\varepsilon \gg \frac{1}{k}$, there is no known algorithm which can find a non-trivial approximation for the optimum
$k$-partition.

1.2 Organization

We first introduce some useful notation and background in Section 2. After this, we state our
main contributions in Section 3. Then we propose a new spectral clustering algorithm in Section 4.
In Section 5, we will prove that our algorithm always finds a $k$-partition that is $\sqrt{\varepsilon}$-close to any given
subspace, where $\varepsilon$ is the optimum. In Section 6, we discuss some applications of our algorithm.
Our main applications will be:

• (Section 6.1) Approximating a graph using disjoint union of expanders and,

• (Section 6.2) $k$-EXPANSION when $\phi_k \leq O(\lambda_{k+1})$.

Finally, in Section 7, we present a simple reduction from $k$-EXPANSION to our problem: This means
any algorithm for $k$-EXPANSION has to solve our subspace rounding problem as well.
2 Notation and Background

Let \([m] \dfn \{1, 2, \ldots, m\}\). We will associate \(V = [n]\) with the set of nodes. For any vector \(q \in \mathbb{R}^\top\), \(\overline{q} \dfn \frac{1}{\|q\|_2} q\) and \(\overline{\overline{q}} \dfn \frac{1}{\|q\|_2} q\). Given a subset \(S \subseteq V\), we use \(e_S \in \mathbb{R}^n\) to denote the indicator vector for \(S\), \(e_S(i) = \begin{cases} 1 & \text{if } i \in S, \\ 0 & \text{else}. \end{cases}\).

Matrices. We use \(\mathbb{R}^{r \times c}\) to denote the set of \(r\)-by-\(c\) real matrices. Likewise, we use \(\mathbb{S}^c\) and \(\mathbb{S}^c_+ \subseteq \mathbb{S}^c\) to denote the set of \(c\)-by-\(c\) symmetric and positive semidefinite matrices, respectively. Finally let \(\mathbb{S}_k(\mathbb{R}^n)\) be the set of all \(n\)-by-\(k\) orthonormal matrices (Stiefel manifold) for \(k \leq n\):

\[
\mathbb{S}_k(\mathbb{R}^n) \dfn \left\{ A \in \mathbb{R}^{n \times k} \mid A^T A = I_k \right\}.
\]

Given an \(r\)-by-\(c\) matrix \(A \in \mathbb{R}^{r \times c}\), we use \(\sigma_i(A), i \in \{1, 2, \ldots, \min(r, c)\}\) to refer to the \(i\)th largest singular value of \(A\). We define \(\sigma_{\min}(A)\) as the minimum singular value of \(A\), and \(\|A\|_2\) as the 2-norm of \(A\), which is \(\|A\|_2 = \sigma_1(A)\). Likewise \(\|A\|_F\) denotes the Frobenius norm of \(A\), \(\|A\|_F = \sqrt{A^T A} = \sqrt{\sum_j \sigma_j^2(A)}\). Given matrix \(R \subseteq [r]\), \(C \subseteq [c]\), we will use \(A_{R,C}\) to refer to the minor corresponding to rows \(R\) and columns \(C\).

Finally, we will use \(A^\Pi, A^\perp \in \mathbb{S}_+^n\) to denote the \(r\)-by-\(r\) projection matrices onto the column space and co-kernel of \(A\), respectively. Observe that for any \(A \in \mathbb{S}_k(\mathbb{R}^n)\), \(A^\Pi = AA^T\) and \(A^\perp = I_n - AA^T\).

One way of measuring how close two subspaces are, is to look at how much (in degrees) we need to rotate a vector in one subspace to the closest vector in the other subspace. It is well known that this quantity is related to the spectral norm. For completeness, we provide a formal version of this statement along with its proof:

**Proposition 2.1 ([SS90]).** Given two linear \(k\)-dimensional subspaces of \(\mathbb{R}^n\) with orthonormal basis \(A, B \in \mathbb{S}_k(\mathbb{R}^n)\) respectively; the cosine of the largest angle between these two subspaces is given by the following:

\[
\cos(\angle AB) \dfn \min_{x \in \text{span}(A)} \max_{y \in \text{span}(B)} \frac{|\langle x, y \rangle|}{\|x\|_2 \|y\|_2}.
\]

We have \(\sin(\angle AB) = \|A^\perp B\|_2 = \|B^\perp A\|_2\).

**Proof.** From the definition of \(\angle AB\), it is easy to see how it measures the maximum degrees necessary to rotate a point in \(A\) to any point in \(B\) and vice versa. We will now prove the second statement. Any point \(x\) in \(\text{span}(A)\) can be written as \(Ap\) for some \(p \in \mathbb{R}^k\). Moreover \(A\) is orthonormal, thus \(\|x\| = \|Ap\| = \|p\|\). This allows us to rewrite \(\cos(\angle AB)\) as follows:

\[
\min_{x \in \text{span}(A)} \max_{y \in \text{span}(B)} \frac{|\langle x, y \rangle|}{\|x\|_2 \|y\|_2} = \min_p \max_{y \in \text{span}(B)} \frac{|\langle Ap, y \rangle|}{\|p\|_2 \|y\|_2}.
\]

For any \(p\), best \(y\) is given by \(B^\Pi Ap\). Moreover \(\|B^\Pi Ap\|_2^2 + \|B^\perp Ap\|_2^2 = \|p\|_2^2\), thus:

\[
\min_p \|B^\Pi Ap\|_2 = \sqrt{1 - \max_p \frac{\|B^\perp Ap\|_2^2}{\|p\|_2^2}}.
\]

Consequently, \(\sin(\angle AB) = \max_p \frac{\|B^\perp Ap\|_2^2}{\|p\|_2^2} = \|B^\perp A\|_2^2\). \(\square\)
Definition 2.2. Let $\text{Set}_V(k)$ be the family of sets of $k$ non-empty subsets of $V$. We will use $\text{Disj}_V(k) \subseteq \text{Set}_V(k)$ to denote the set of $k$ disjoint subsets of $V$: $\Gamma \in \text{Disj}_V(k)$ if and only if $\Gamma \in \text{Set}_V(k)$ and $S \cap T = \emptyset$ for all $S \neq T \in \Gamma$.

In order to compare subspaces with $k$-partitions, we need to identify a canonical representation for the subspaces associated with $k$-partitions. We use the most natural representation, where each basis vector is the normalized indicator of one of the clusters.

Notation 2.3 (Basis Matrices of $k$-Partitions). Given $k$-subsets $\Gamma = \{A_1, \ldots, A_k\}$ of $V$, let $\Gamma \in \mathbb{R}^{n \times k}$ be the corresponding normalized incidence matrix $\Gamma \overset{\text{def}}{=} \begin{bmatrix} \overline{e_{A_1}} & \cdots & \overline{e_{A_k}} \end{bmatrix}$. We will use $\Gamma^\perp \in \mathbb{S}^n_k$ and $\Gamma^\perp \in \mathbb{S}^n_k$ to denote the associated projection matrices so that $\Gamma^\perp \Gamma = \Gamma$ and $\Gamma^\perp \Gamma = 0$.

Multiplication with either of the projection matrices $\Gamma^\perp$ and $\Gamma^\perp$ has a natural correspondence with centers and the differences to centers:

Proposition 2.4. If $\Gamma \in \text{Disj}_V$, then $\Gamma$ is an orthonormal matrix, $\Gamma \in \mathbb{S}_k(\mathbb{R}^n)$, and $\Gamma^\perp$ is a Laplacian matrix. For any $Y \in \mathbb{R}^{k \times n}$, $i^{th}$ column of:

- $Y \Gamma^\perp$ is the mean of points in the same cluster with $i$ provided $i$ is in any cluster of $\Gamma$, and 0 otherwise.
- $Y \Gamma^\perp$ is the difference between $y_i$ and its associated center as defined above.

For example, $\|Y \Gamma^\perp\|^2_F$ measures the sum of squared distances of each point to the center of its cluster or origin if it is not in any cluster.

We will measure the distance between sets in a way very similar to cosine distance.

Notation 2.5. Given $p, q \in \mathbb{R}^n$, we define $\Delta(p, q)$ as $\Delta(p, q) \overset{\text{def}}{=} 1 - \langle p, q \rangle^2$. Note that $\Delta(p, q) = \frac{1}{2} \|p \otimes q - q \otimes p\|^2$. For convenience, we will use $\Delta(S, q)$ as $\Delta(e_S, q)$. In particular, $\Delta(A, B) = 1 - \frac{|A \cap B|^2}{|A||B|}$.

Our measure of set similarity is closely related to the Jaccard index.

Proposition 2.6. For any pair of subsets $A, B \subseteq V$:

$$\frac{1}{4} \frac{|A \Delta B|}{|A \cup B|} \leq \Delta(A, B) \leq \frac{|A \Delta B|}{|A \cup B|}.$$  

Proof. Since $|A \cup B|^2 \geq |A||B|$, we immediately see that $1 - \Delta(A, B) \geq \frac{|A \cap B|}{|A||B|}$. For the other direction, suppose $\Delta(A, B) \leq \epsilon$ and $|A| \geq |B|$. Then:

$$(1 - \epsilon) \sqrt{|A||B|} \leq |A \cap B| \quad \Rightarrow \quad \frac{|A \cap B|}{|A|} \geq (1 - \epsilon) \sqrt{\frac{|B|}{|A|}} \geq (1 - \epsilon) \sqrt{\frac{|A \cap B|}{|A|}}.$$  

Therefore $|A \cap B| \geq (1 - \epsilon)^2 |A|$ and $|A \Delta B| = |A| + |B| - 2|A \cap B| \leq |B| - (1 - 4\epsilon + 2\epsilon^2)|A| \leq 4\epsilon|B|:

$$\frac{|A \Delta B|}{|A \cup B|} \geq 4\Delta(A, B).$$

We will now generalize our set similarity measure to $k$-partitions.
Notation 2.7. Given $\Gamma, \hat{\Gamma} \in \text{Set}_{V}(k)$; we define $\Delta(\Gamma, \hat{\Gamma})$ as:

$$\Delta(\Gamma, \hat{\Gamma}) \overset{\text{def}}{=} \min_{\pi: \Gamma \rightarrow \hat{\Gamma}} \max_{S \subseteq \Gamma} \Delta(S, \pi(S)).$$

We say $A$ (resp. $\Gamma$) is $\varepsilon$-close to $B$ (resp. $\hat{\Gamma}$) whenever $\Delta(A, B) \leq \varepsilon$ (resp. $\Delta(\Gamma, \hat{\Gamma}) \leq \varepsilon$).

Observe that our notion of proximity is a very strong bound. For example if $\Gamma$ is $\varepsilon$-close to $\Gamma_*$, then any subset $S \subseteq \Gamma_*$ of size $|S| < \frac{1}{2}$ has to be preserved exactly in $\Gamma$.

The next theorem says that the similarity measure we use for $k$-partitions in Notation 2.7 is tightly related to the spectral norm distance between the corresponding basis.

Theorem 2.8. Given $\Gamma, \hat{\Gamma} \in \text{Disj}_{V}(k)$; $\Delta(\Gamma, \hat{\Gamma}) \leq \|\Gamma^{-1}\hat{\Gamma}\|_2^2 \leq 2\Delta(\Gamma, \hat{\Gamma})$. Moreover, after appropriately ordering the columns of $\hat{\Gamma}$, $\|\Gamma - \hat{\Gamma}\|_2^2 \leq 4\Delta(\Gamma, \hat{\Gamma})$.

Proof is given in Section 8.1.

Proposition 2.9. Given two symmetric matrices $A, B \in \mathbb{S}^m$; if $A \preceq B$ then $\sigma_r(A) \leq \sigma_r(B)$ for any $r$.

Proof. Recall that $\sigma_r(M) = \max_{P, P^T P = I_r} \sigma_{\min}(P^T M P)$ for any symmetric matrix $M$. Therefore:

$$\sigma_r(A) = \max_{P, P^T P = I_r} \sigma_{\min}(P^T A P) \leq \max_{P, P^T P = I_r} \sigma_{\min}(P^T B P) = \sigma_r(B).$$

\[\blacksquare\]

Proposition 2.10. Given $A, B \in \mathcal{S}_k(\mathbb{R}^n)$, $\sigma_{\min}(A^T B) = \sqrt{1 - \|A^+ B\|_2^2}$.

Proof. $B^T A^+ B = B^T B - B^T A A^T B = I_k - B^T A A^T B$. Since $\|A^T B\|_2 \leq 1$, $\|A^+ B\|_2^2 = 1 - \sigma_{\min}(A^T B)^2$.

\[\blacksquare\]

Consider two subspaces with basis $A$ and $B$. If the angle between these two subspaces is small, then one might intuitively expect that $A A^T$ and $B B^T$ are very close also. In the next lemma, we make this intuition formal.

Lemma 2.11. Given $A, B \in \mathcal{S}_k(\mathbb{R}^n)$; $\|A A^T - B B^T\|_2 \leq 2\sqrt{2}\|A^+ B\|_2$.

Proof. Consider an SVD of the matrix $A^T B = C \Sigma^{1/2} D^T$. Here $C, \Sigma, D \in \mathbb{R}^{k \times k}$. For $R \overset{\text{def}}{=} C D^T$, $R^T R = R R^T = I_k$. Note $\|R - A T B\|_2 = \|I - \Sigma^{1/2}\|_2 = 1 - \sigma_{\min}(A^T B) = \rho$ and $\|A^+ B\|_2^2 = \|B^T A\|_2^2 = 1 - (1 - \rho)^2$ by Proposition 2.10. Using the fact that $A^+ A = 0$:

$$\|AR - B\|_2^2 = \|A(R - A^T B) - A^+ B\|_2^2$$

$$= \|A(R - A^T B)\|_2^2 + \|A^+ B\|_2^2 = \rho^2 + 1 - (1 - \rho)^2 = 2\rho.$$

Thus for any $q$:

$$\|A^T q\|_2^2 - \|B^T q\|_2^2 = \|(AR)^T q\|_2^2 - \|B^T q\|_2^2$$

$$\leq \|B^T q\|_2^2 - \|B^T q\|_2^2 + \|(AR - B)^T q\|_2^2$$

$$= \|(AR - B)^T q\|_2^2 \leq \sqrt{2\rho}\|q\|_2.$$

Consequently:

$$\|q^T (A A^T - B B^T) q\| = \|A^T q\|_2^2 - \|B^T q\|_2^2 (\|A^T q\|_2^2 + \|B^T q\|_2^2) \leq 2\sqrt{2\rho}\|q\|_2^2.$$

We finish the proof by noticing that $\rho = 1 - \sigma_{\min} = 1 - \sqrt{1 - \|A^+ B\|_2^2} \leq \|A^+ B\|_2^2$. \[\blacksquare\]
2.1 Graph Partitioning

Given an undirected graph \( G = (V, C) \) with nodes \( V \) and non-negative edge weights \( C \), we use \( A_G \in \mathbb{S}^V \) and \( L_G \in \mathbb{S}^V \) to denote the adjacency and Laplacian matrices of \( G \). Consider the following \( k \)-way graph partitioning problem where the goal is to minimize the maximum ratio of the total weight of edges cut and the number of nodes inside among all clusters.

**Definition 2.12 (\( k \)-expansion).** Given an undirected graph \( G = (V, C) \) with nodes \( V \) and non-negative edge weights \( C \), we define the \( k \)-way expansion of \( G \) as the following:

\[
\phi_k(G) \overset{\text{def}}{=} \min_{\Gamma \in \text{Disj}_V(k)} \max_{T \in \Gamma} \frac{C(T, T)}{|T|}.
\]

Here \( C(A, B) \) denotes the total weight of unordered edges between \( A \) and \( B \). For fixed \( G \), we will use \( \Gamma_* \in \text{Disj}_V(k) \) to refer to the \( k \)-partition which achieves \( \phi_k(G) \).

At the first glance, our notion of expansion might seem different than the usual definition, which involves dividing by \( \min(|T|, |T'|) \) instead of \( |T| \). However they are indeed the same:

**Proposition 2.13.** For any \( G = (V, C) \) and a \( k \)-partition of \( V \), \( \Gamma \), \( \max_{T \in \Gamma} \frac{C(T, T)}{|T|} = \max_{S \in \Gamma} \frac{C(S, S)}{\min(|S|, |S'|)} \).

*Proof.* For any \( S \), \( \min(|S|, |S'|) \leq |S| \), therefore \( \frac{C(S, S)}{|S|} \leq \frac{C(S, S)}{\min(|S|, |S'|)} \). Now we will prove the other direction. Suppose \( \max_{T \in \Gamma} \frac{C(T, T)}{|T|} \leq \phi \). For any \( T' \in \Gamma \):

\[
C(T', T') \leq \sum_{T \in \Gamma \setminus T'} C(T, T) \leq \phi \sum_{T \in \Gamma \setminus T'} |T| = \phi |V \setminus T'|.
\]

Consequently, \( \frac{C(T', T')}{|V \setminus T'|} \leq \phi \). Combining this with the fact that \( \frac{C(T', T')}{|T'|} \leq \phi \) we see that:

\[
\forall T \in \Gamma : \phi \geq \max \left( \frac{C(T, T)}{|T|}, \frac{C(T, T)}{|T|} \right) = \frac{C(T, T)}{\min(|T|, |T'|)}.
\]

**Lemma 2.14.** Given \( \Gamma \in \text{Disj}_V(k) \), \( \frac{1}{2} \| \Gamma^T LL \|_2 \leq \max_{T \in \Gamma} \frac{C(T, T)}{|T|} \leq \| \Gamma^T LL \|_2 \).

*Proof.* Let \( \phi \overset{\text{def}}{=} \max_{T \in \Gamma} \frac{C(T, T)}{|T|} \). We need to prove \( \phi \leq \sigma_{\text{max}}(\Gamma^T LL) \leq 2\phi \). The lower bound is trivial, so we only give the proof of upper bound. Note \( \Gamma = JD^{-1/2} \) where \( D \) is a matrix whose diagonals are \( |T| \) for \( T \in \Gamma \) and the columns of \( J \) are indicator vectors for every \( T \in \Gamma \). Then \( \Gamma^T LL = D^{-1/2}JTLD^{-1/2}. \) Define \( W \) as the matrix which is equal to \( J^T LJ \) along its diagonals and 0 everywhere else. Since \( J^T LJ \) is a Laplacian matrix \( J^T LJ \leq 2W \). Therefore:

\[
\Gamma^T LL \leq 2D^{-1/2}WD^{-1/2}.
\]

\( D^{-1/2}WD^{-1/2} \) is diagonal whose entries are \( \frac{C(T, T)}{|T|} \leq \phi \) over all \( T \in \Gamma \). Consequently,

\[
\sigma_{\text{max}}(\Gamma^T LL) \leq 2\sigma_{\text{max}}(D^{-1/2}ZD^{-1/2}) \leq 2\phi.
\]
Given Lemma 2.14, a simple relaxation for $\phi_k(G)$ (the basic SDP relaxation) is the following:

$$\min \|Q^T L Q\|_2 \text{ st } Q^T Q = I_k. \tag{1}$$

Note that for any $\Gamma \in \text{Disj}_V(k)$, $\Gamma$ is feasible and eq. (1) is indeed a relaxation. Moreover the Courant-Fischer-Weyl principle implies that the optimum value of eq. (1) is $\lambda_k$ with the corresponding optimal solution being the smallest $k$-eigenvectors of $L$. Therefore:

$$\lambda_k \leq \phi_k(G). \tag{2}$$

3 Our Contributions

We study the following problem. Given a $k$-by-$n$ matrix $Y : Y^T \in S_k(\mathbb{R}^n)$ of the form $Y = [y_1, \ldots, y_n]$ (think of $Y$ as an embedding of $n$ points in $\mathbb{R}^k$), find a $k$-partition $\Gamma \in \text{Disj}_V(k)$ so as to minimize the total variance under any direction:

$$\min_{\Gamma} \max_{z \in \mathbb{R}^k : \|z\|_2 = 1} \sum_{u \in S} (z, y_u - c_u)^2. \tag{3}$$

Here $c_u$ is the mean of points in the same cluster with $u$ if one exists, and $c_u = 0$ otherwise. This is the problem of clustering with spectral norm [KK10].

Remark 3.1 (Covering all points). For simplicity, we allow some points to be left uncovered by any set in $\Gamma$, which corresponds to their “center” being at the origin. However the same guarantees still hold even if we require $\Gamma$ to cover all points.

We can express eq. (3) more succinctly as the following:

$$\min_{\Gamma} \|YT^\perp\|_2^2 \overset{\text{Proposition 2.4}}{=} \text{eq. (3)} \tag{4}$$

There are two closely related problems, whose optimum is within square root of eq. (3) (Lemma 2.11):

- Finding a $k$-by-$k$ rotation matrix $R : R^T R = RR^T = I_k$ and a $k$-partition $\Gamma \in \text{Disj}_V(k)$ so as to minimize the following:

$$\min_{R, \Gamma} \|RY - \Gamma\|_2. \tag{5}$$

- Approximate the Gram matrix of $Y$, $Y^T Y$, using block diagonal matrices with each block being constant. This is equivalent to:

$$\min_{\Gamma} \|Y^T Y - \Gamma \Gamma^T\|_2. \tag{6}$$

Our main contribution is a new spectral clustering algorithm whose pseudo-code is given through Algorithms 1 to 5. We prove the following guarantee on its outputs.

Theorem 3.2 (Restatement of Theorem 5.12). Let $\Gamma^* \in \text{Disj}_V(k)$ with $\|YT^\perp\|^2_2 \leq O(\varepsilon)$. Then $\hat{\Gamma} \leftarrow \text{SPECTRALCLUSTERING}(Y)$ is a $k$-partition so that $\hat{\Gamma} \in \text{Disj}_V(k)$, and it is $O(\sqrt{\varepsilon})$ close to both $\Gamma^*$ and $Y$:

$$\Delta(\Gamma^*, \hat{\Gamma}) \leq O(\sqrt{\varepsilon}) \quad \text{and} \quad \|YT^\perp\|^2_2 \leq O(\sqrt{\varepsilon}).$$
Remark 3.3 (Small Clusters). Our main guarantee as stated in Theorem 5.12 works for any cluster size. For example, consider the case of some optimal cluster $T \in \Gamma_*$ having size $|T| \leq O(1/\sqrt{\varepsilon})$. For such cluster, any $S$ with $\Delta(S, T) \leq O(\sqrt{\varepsilon})$ has to be exactly equal to $T$.

In other words, our algorithm will recover any $T \in \Gamma_*$ with $|T| \leq O(1/\sqrt{\varepsilon})$ exactly.

As an easy consequence, we show how to approximate a graph as a disjoint union of expanders (provided one exists) in polynomial time.

**Corollary 3.4 (Restatement of Corollary 6.4).** Given a graph $G$, if there exists $\Gamma_* \in \Disj_V(k)$ such that Laplacian of $G$ is $\varepsilon$-close (in spectral norm) to the Laplacian corresponding to the disjoint union of normalized cliques on each $T \in \Gamma_*:

$$\|L - \Gamma_*\|_2 \leq \varepsilon,$$

then in polynomial time, we can find $\Gamma \in \Disj_V(k)$ which is $O(\sqrt{\varepsilon})$-close to $\Gamma_*$ and $G$:

$$\|L - \Gamma\|_2 \leq O(\varepsilon^{1/4}).$$

Next we significantly improve the known bounds for recovering a $k$-partition when all clusters have small expansion as in Definition 2.12. Previous spectral clustering algorithms only guarantee recovering each $T \in \Gamma_*$ when the $(k+1)^{st}$ smallest eigenvalue, $\lambda_{k+1}$, of the associated Laplacian matrix for $G$ satisfies

$$\lambda_{k+1} > \Omega(k \cdot \phi_k).$$

Our new algorithm significantly relaxes this requirement to $\lambda_{k+1} > \Omega(\phi_k)$.

**Theorem 3.5 (Restatement of Theorem 6.1).** Given a graph $G$ with Laplacian matrix $L$, let $\Gamma$ be the $k$-partition obtained by running Algorithm 3 on the smallest $k$ eigenvectors of $L$. Then:

$$\Delta(\Gamma, \Gamma_*) \leq O\left(\sqrt{\frac{\phi_k}{\lambda_{k+1}}}\right).$$

Finally, we show that any approximation algorithm for $k$-EXPANSION implies the same approximation bound for the spectral clustering problem restricted to orthonormal matrices. In other words, the spectral clustering problem is a prerequisite for approximating $k$-EXPANSION even on graphs whose normalized Laplacian matrix has its $(k+1)^{st}$ smallest eigenvalue $\lambda_{k+1}$ larger than a constant.

**Theorem 3.6 (Restatement of Theorem 7.1).** Given $Y : Y^T \in S_k(\mathbb{R}^n)$, let $\Gamma_* \defeq \arg\min_{T} \|Y\Gamma_+^{-1}\|_2^2$ with $\varepsilon = \|Y\Gamma_+^{-1}\|_2^2$. Then there exists a weighted, undirected, regular graph $X$, whose normalized Laplacian matrix has its $(k+1)^{st}$ smallest eigenvalue at least $\lambda_{k+1} \geq 1 - O(\sqrt{\varepsilon})$ such that:

- Each $T \in \Gamma_*$ has small expansion, $\phi_X(T) \leq O(\varepsilon)$;
- If $\Gamma \in \Disj_V(k)$ is a $k$-partition with $\max_{S \in \Gamma} \phi_X(S) \leq \delta$, then $\Delta(\Gamma, \Gamma_*) \leq O(\delta + \sqrt{\varepsilon})$.

Moreover such $X$ can be constructed in polynomial time.
4 Our Algorithm

The pseudo-code of our clustering algorithm and its sub-procedures are listed in Algorithms 1 to 5. The main procedure is invoked by \( \hat{\Gamma} = \text{SPECTRALCLUSTERING}(Y) \) (Algorithm 3), where \( Y \) is a \( k \)-by-\( n \) matrix \( Y \) such as the smallest \( k \)-eigenvectors of some Laplacian matrix. The output \( \hat{\Gamma} \) is a \( k \)-partition close to \( Y \). We use \( \Gamma_s = (T_1, \ldots, T_k) \) to denote the closest \( k \)-partition to \( Y \). We will refer to \( T \)'s as true clusters.

4.1 Intuition

First we start with the discussion of some of the main challenges involved in spectral clustering and the intuition behind the major components of our algorithm.

Finding a Cluster. Since there are \( k \) directions and \( k \) clusters, we can think of each direction being associated with one of the clusters. Moreover, for one of the true clusters \( T \), the total correlation of its center with remaining directions will be very small. By utilizing this intuition, we can easily find such a subset, say \( S \) (Algorithm 4). However this property need not be true for all \( T \)'s: Even though each \( T \) will be at most \( \varepsilon \)-close to every non-associated direction, the total correlation might be \((k - 1)\varepsilon \gg 1\), thus overwhelming the correlation it had with its associated direction. In fact, this is the reason why \( k \)-means type procedures will fail to find every cluster when \( \varepsilon > 1/k \). To remedy this, each time we find \( S \), we can try to “peel” it off. A natural approach is to project the columns of \( Y \) onto the orthogonal complement of the center of \( S \). Similar ideas were used before in the context of learning mixtures of anisotropic Gaussians [BV08] and column based matrix reconstruction [DR10, GS12]. After projection, we obtain a new \((k - 1)\)-by-\( n \) orthonormal matrix, \( Z \), corresponding to remaining \( k - 1 \) clusters.

Boosting. Unfortunately we can not iterate the above approach: No matter how accurate we are in \( S \), there will be some error: If \( Y \) were \( \varepsilon \)-close to \((T_1, \ldots, T_k)\), then we can at best guarantee that \( Z \) is \( 2\varepsilon \)-close to \((T_2, \ldots, T_k)\). After \( k \) iterations, our error will be \( 2^O(k)\varepsilon \), which is much worse than \( k \)-means! In our algorithm, we keep the error from accumulating via a boosting step (Algorithm 1).

Unraveling. Even with boosting, there remains one issue: The clusters we found may overlap with each other. Unlike other distance based clustering problems such as \( k \)-means, the assignment problem (“which cluster does this node belong to?”) is quite non-trivial in spectral clustering even if we are given all \( k \)-centers. There is no simple local procedure which can figure out the assignment of node \( u \) by only looking at \( y_u \) and the cluster centers. We deal with this issue by reducing the ownership problem to finding a matching in a bipartite graph (Algorithm 5). Our approach is very similar to the one used in [BS06] for a special case of Santa Claus problem.

Final Algorithm. The final difficulty we face is that, the boosted cluster might cannibalize other much smaller clusters. We overcome this issue by maintaining both estimates for every true cluster: the core found we originally found and the one obtained after boosting. Due to the cascading effect of unraveling whenever we add a new cluster, we have to re-compute the centers and project onto their orthogonal complement at every round.

4.2 Overview

Our algorithm proceeds iteratively. At \( r \)-th iteration, it finds a core \( S_r \) for one of the yet-unseen true clusters, say \( T_r \). The main invariant we need from the core set is the following (Lemma 5.7):
(i) \( S_r \) is noticeably close to \( T_r \), say \( \Delta(S_r, T_r) \leq \frac{1}{100} \).

(ii) All the remaining \( k - r \) true clusters, \( \{T_{r+1}, \ldots, T_k\} \), have small overlap with \( S_r \) in the sense that \( |T_j \cap S_r| \leq \frac{1}{100} |T_j| \) over all \( j > r \).

After having found \( S_r \), our algorithm needs to boost \( S_r \) to \( \hat{S}_r \). For boosting to work however (Theorem 5.8), we need the invariant (ii) to be true for all \( j \neq i \). We do this by \( (U_1, \ldots, U_r) \leftarrow \text{UNRAVEL}(S_1, \ldots, S_r) \). Since \( U_i \)'s are close to \( S_i \)'s, each \( T_j \) with \( j < r \) will still be mostly overlapping with \( S_j \) (Lemma 5.6); hence \( T_j \)'s with \( j < r \) can not overlap with \( U_r \) as \( U_j \)'s are disjoint. Consequently we can use \( U_r \) instead of \( S_r \) for boosting so as to obtain \( \hat{S}_r \). The only invariant we require from \( \hat{S}_r \) is that it is much closer to \( T_r \) than \( S_r \):

\[
\Delta(\hat{S}_r, T_r) \leq O(\sqrt{\varepsilon}).
\]

By using the centers of boosted sets instead of core sets, we can make sure that the error does not accumulate after the projection step \( Z \leftarrow (Y\hat{\Gamma}' \perp Y \) (Lemma 5.5).

After \( k \) iterations, we apply \( \text{UNRAVEL} \) to all boosted sets \( (\hat{S}_1, \ldots, \hat{S}_k) \) one last time and output the result.

**Remark 4.1 (Computing Top Singular Vectors by Power Method [GKB13]).** In Algorithms 1 and 4, the last step involves computing the top singular vector. In both cases, we have:

- A good initial guess (the indicator vector),
- Large separation between \( \sigma_1 \) and \( \sigma_2 \).

Thus, we can simply use power method for \( O(\log 1/\varepsilon) \) many iterations to compute a sufficiently accurate approximation of the top right singular vector, from which we can obtain an approximation of the top left singular vector easily. It was initially shown in [GKB13] that power method is sufficient in the context of spectral clustering.

## 5 Analysis of the Algorithm

In this section, we prove the correctness of our algorithm. Our main result is the following. Its proof is given at the end of Section 5.5.

**Theorem 5.1 (Restatement of Theorem 5.12).** Let \( \Gamma_* \in \text{Disj}_V(k) \) with \( \|Y\Gamma_* \perp \|^2 \leq O(\varepsilon) \). Then \( \hat{\Gamma} \leftarrow \text{SpectralClustering}(Y) \) is a \( k \)-partition so that \( \hat{\Gamma} \in \text{Disj}_V(k) \), and it is \( O(\sqrt{\varepsilon}) \) close to both \( \Gamma_* \) and \( Y \):

\[
\Delta(\Gamma_*, \hat{\Gamma}) \leq O(\sqrt{\varepsilon}) \quad \text{and} \quad \|Y\hat{\Gamma} \perp \|^2 \leq O(\sqrt{\varepsilon}).
\]

In order to keep the analysis simple, we make no effort toward optimizing the constants.
using Wedin’s theorem [SS90], but we chose to give a simple and self-contained proof. The largest eigenvectors of both matrices will be very close to each other. This can also be obtained in spectral norm, if there is a gap between the largest and second largest eigenvalues; then the following proposition, we show that for any pair of symmetric matrices that are close to each other in spectral norm, if there is a gap between the largest and second largest eigenvalues; then in the following proposition, we show that for any pair of symmetric matrices that are close to each other in spectral norm, if there is a gap between the largest and second largest eigenvalues; then

\[ \|Y_{x(i)} - Y_x\| \leq \|Y_{x(i+1)} - Y_x\| \leq \|Y_{x(i+2)} - Y_x\|. \]

In the following proposition, we show that for any pair of symmetric matrices that are close to each other in spectral norm, if there is a gap between the largest and second largest eigenvalues; then the largest eigenvectors of both matrices will be very close to each other. This can also be obtained in spectral norm, if there is a gap between the largest and second largest eigenvalues; then in the following proposition, we show that for any pair of symmetric matrices that are close to each other in spectral norm, if there is a gap between the largest and second largest eigenvalues; then

\[ \|Y_{x(i)} - Y_x\| \leq \|Y_{x(i+1)} - Y_x\| \leq \|Y_{x(i+2)} - Y_x\|. \]

5.1 Preliminaries

In the following proposition, we show that for any pair of symmetric matrices that are close to each other in spectral norm, if there is a gap between the largest and second largest eigenvalues; then the largest eigenvectors of both matrices will be very close to each other. This can also be obtained in spectral norm, if there is a gap between the largest and second largest eigenvalues; then in the following proposition, we show that for any pair of symmetric matrices that are close to each other in spectral norm, if there is a gap between the largest and second largest eigenvalues; then

\[ \|Y_{x(i)} - Y_x\| \leq \|Y_{x(i+1)} - Y_x\| \leq \|Y_{x(i+2)} - Y_x\|. \]

Figure 1 The graph constructed by UNRAVEL on input $S_1 = \{a, b, c, e\}$, $S_2 = \{d, e, f, g\}$, $S_3 = \{g, h, i, j, k\}$, $S_4 = \{k\}$ for $\delta = \frac{1}{4}$.

5.1 Preliminaries

In the following proposition, we show that for any pair of symmetric matrices that are close to each other in spectral norm, if there is a gap between the largest and second largest eigenvalues; then the largest eigenvectors of both matrices will be very close to each other. This can also be obtained in spectral norm, if there is a gap between the largest and second largest eigenvalues; then in the following proposition, we show that for any pair of symmetric matrices that are close to each other in spectral norm, if there is a gap between the largest and second largest eigenvalues; then

\[ \|Y_{x(i)} - Y_x\| \leq \|Y_{x(i+1)} - Y_x\| \leq \|Y_{x(i+2)} - Y_x\|. \]
Proposition 5.2. Given \( A, B \in \mathbb{S}^n \) with maximum eigenvectors \( p, q \in \mathbb{R}^n \):

\[
\langle p, q \rangle^2 \geq 1 - \frac{2\| A - B \|_2}{\sigma_1(A) - \sigma_2(A)}.
\]

Proof. Suppose \( \| p \| = \| q \| = 1 \). Let \( \delta \overset{\text{def}}{=} \| A - B \|_2 \) and \( \theta \overset{\text{def}}{=} \langle p, q \rangle^2 \). We have

\[
\sigma_1(A) = p^T A p \leq \delta + \sigma_2(B) \| p \|_2^2 + \| p \|_2 \| q \|_2^2
\]

\[
\leq \delta + (\sigma_1(A) + \delta) \theta + (\sigma_2(A) + \delta)(1 - \theta)
\]

\[
= \delta + \theta(\sigma_1 - \sigma_2) + (\sigma_2 + 2\delta).
\]

Hence \( \theta \geq \frac{\sigma_1 - \sigma_2 - 2\delta}{\sigma_1 - \sigma_2} \).

The main tool we use to identify the clusters will be the eigenvalues of principal minors of the Gram matrix, \( Y^T Y \). Basically, eigenvalues measure how much true clusters, \( T \), overlap with given principal minor. We make this connection formal in the following claim:

Claim 5.3. Given \( Y \in \mathbb{R}^{m \times n}, \Gamma \in \text{Disj}_V(r) \) and subset \( S \subseteq V \), let \( \rho = (|S \cap T|/|T| \mid T \in \Gamma) \). Then:

\[
|\sigma_1^2(Y_S) - \langle \rho \rangle_{\text{i}}| \leq \| Y^T Y - \Gamma \|_2.
\]

Here \( \langle \rho \rangle_{\text{i}} \) is the \( i \)-th largest element of \( \rho \).

Proof. We have \( \| Y^T Y - \Gamma \|_2^2 \geq \| Y_S^T Y_S - (\Gamma_{\text{s}}^\text{\Pi})_{S,S} \|_2 \). Observe that the eigenvectors of \( (\Gamma_{\text{s}}^\text{\Pi})_{S,S} \) are \( \sigma_{T \cap S} \) with corresponding eigenvalue \( \frac{|T \cap S|}{|T|} \) over all \( T' \in \Gamma_{\text{s}} \). Thus \( \rho \)'s are the eigenvalues of \( (\Gamma_{\text{s}}^\text{\Pi})_{S,S} \).

Consider a principal minor corresponding to some \( S \) whose largest eigenvalue is large, and second largest eigenvalue is small. The previous claim implies that there is a unique optimal cluster \( T \) which is almost contained by \( S \). However this is still not sufficient: \( S \) might be much larger than \( T \). In the next lemma, we show that, one can take the top right singular vector of \( Y_S \) and round (threshold) it to obtain another subset \( \hat{S} \subseteq S \) which is now very close to \( T \).

Lemma 5.4 (Initial Guess). Given \( Y \in \mathbb{R}^{m \times n}, \Gamma_{\text{s}} \in \text{Disj}_V(r) \) with \( \| Y^T Y - \Gamma_{\text{s}}^\text{\Pi} \|_2 \leq \delta \), and subset \( S \subseteq V \), let \( q \in \mathbb{R}^S \) be the top right singular vector of \( Y_S \). If we define \( \sigma_1 \overset{\text{def}}{=} \sigma_1^2(Y_S) \) and \( \sigma_2 \overset{\text{def}}{=} \sigma_2^2(Y_S) \), then the subset \( \hat{S} \subseteq S \) obtained by:

\[
\hat{S} \leftarrow \text{ROUND}(q)
\]

satisfies the following. For \( T \) being \( \text{argmax}_{T \in \Gamma_{\text{s}}} \frac{|S \cap T|}{|T|} ; \)

\[
\frac{|T \cap \hat{S}|}{\sqrt{|T||\hat{S}|}} \geq \frac{\sqrt{\sigma_1 - \delta (1 - \frac{4\delta}{\sigma_1 - \sigma_2})}}{\sqrt{|T||\hat{S}|}} \quad \text{and} \quad \forall T' \neq T \in \Gamma_{\text{s}} : |T' \cap \hat{S}| \leq (\sigma_2 + \delta)|T'|.
\]

Proof. We will use \( \sigma_1 \overset{\text{def}}{=} \sigma_1^2(Y_S), \sigma_2 = \sigma_2^2(Y_S) \) and \( \Delta \overset{\text{def}}{=} \sigma_1 - \sigma_2 \). Since \( q \) is the top right singular vector of \( Y_S \), \( \| Y_S q \|_2^2 = \sigma_1 \) and \( \| q \| = 1 \).
By Claim 5.3, \(|\frac{\|T \cap S\|}{|T|} - \sigma_1| \leq \delta\), which implies \(\frac{|S \cap T|}{|T|} \geq \sigma_1 - \delta\). For any \(T' \neq T\), \(\frac{|S \cap T'|}{|T'|} \leq \sigma_2 + \delta\). Via Proposition 5.2, we see that:
\[
\langle q, e_{T \cap S} \rangle \geq 1 - \frac{2\delta}{\sigma_1 - \sigma_2} \geq 1 - \frac{2\delta}{\Delta} \implies \langle q, e_{S} \rangle \geq 1 - \frac{2\delta}{\Delta}.
\]
Provided that \(\delta \leq \frac{1}{4}\Delta\), both \(\langle q, e_{T \cap S} \rangle\) and \(\langle q, e_{S} \rangle\) have the same sign. Therefore:
\[
\langle e_{T \cap S}, e_{S} \rangle \geq \langle q, e_{T \cap S} \rangle \langle q, e_{S} \rangle - \|q^\perp e_{T \cap S}\|\|q^\perp e_{S}\| \geq 1 - \frac{4\delta}{\Delta}.
\]
Consequently, using the fact \(\hat{S} \subseteq S\), we see that any \(T' \neq T\) has \(|T' \cap \hat{S}| \leq (\alpha + \delta)|T'|\) and \(T \cap S \cap \hat{S} = T \cap \hat{S}\):
\[
1 - \frac{4\delta}{\Delta} \leq \frac{|T \cap S|}{|T \cap S||\hat{S}|} \leq \frac{1}{\sqrt{|T||\hat{S}|}} \frac{|T \cap \hat{S}|}{\sqrt{|\sigma_1 - \delta|}}.
\]

After we found new clusters, we iterate by projecting \(Y\) onto the orthogonal complement of their center. In the following lemma, we prove that, as long as the clusters were close to optimal ones, the projection preserves remaining clusters.

**Lemma 5.5.** Given \(Y : Y^T \in S_k(\mathbb{R}^n)\) and \(\Gamma \in \text{Disj}_V(r)\) with the cluster centers in \(\Gamma\) being linearly independent, suppose there exists \(\Gamma_\ast \in \text{Disj}_V(k)\) of the form \(\Gamma_\ast = \Gamma_\ast' \cup \Gamma_\ast''\): \(\Gamma_\ast' \in \text{Disj}_V(r), \Gamma_\ast'' \in \text{Disj}_V(k-r)\) such that:
- \(\|\Gamma - \Gamma_\ast\|_2^2 \leq \alpha\).
- \(\|YT_\ast^\perp\|_2^2 \leq \varepsilon\).

Then \(\Gamma_\ast''\) is a good spectral clustering for \(Z \defeq (YT)^\perp Y\), in the sense that \(\|Z(\Gamma_\ast'')^\perp\|_2^2 \leq \varepsilon + \alpha\). In addition, \(\sigma_1(Z) = \ldots = \sigma_{k-r}(Z) = 1, \sigma_{k-r+1}(Z) = 0\).

**Proof.** Note that \(Z\) has all singular values either 0 or 1:
\[
ZZ^T = (YT)^\perp YY^T (YT)^\perp = (YT)^\perp.
\]
Moreover \((YT)^\perp\) has rank \(\text{rank}(Y) - \text{rank}(YT) = k - r\). Since spectral clustering is invariant under change of basis, we can assume \(Z \in \mathbb{R}^{(k-r)\times n}\) so that all singular values of \(Z\) are 1. This means \(Z\) is orthonormal. It is obtained from \(Y\) by a linear transformation, therefore \(\Gamma_\ast\) is a good spectral clustering for \(Z\) also:
\[
\varepsilon \geq \|YT_\ast^\perp Y^T\|_2 \geq \|ZT_\ast^\perp Z^T\|_2 = \|ZZ^T - (Z\Gamma_\ast)(Z\Gamma_\ast)^T\|_2 = \|I_{k-r} - (Z\Gamma_\ast)(Z\Gamma_\ast)^T\|_2.
\]
In other words,
\[
(1 - \varepsilon)I_{k-r} \preceq Z\Gamma_\ast^\perp Z^T = Z[(\Gamma_\ast')^\perp + (\Gamma_\ast'')^\perp]Z^T,
\]
\[
\varepsilon I_{k-r} \preceq Z(\Gamma_\ast'')^\perp Z^T - Z^T\Gamma_\ast^\perp Z^T.
\]
Now we will upper bound \(\|Z(\Gamma_\ast')^\perp Z^T\|_2 = \|ZT_\ast'\|_2 = \|(YT)^\perp(YT_\ast')\|_2\):
\[
\|(YT)^\perp(YT_\ast')\|_2^2 = \|(YT)^\perp(YT_\ast') - (YT)^\perp(YT)\|_2^2 = \|(YT)^\perp(Y(\Gamma_\ast' - \Gamma))\|_2^2 \leq \|\|(YT)^\perp\|_2^2\|\Gamma_\ast' - \Gamma\|_2^2 \leq \|\Gamma_\ast' - \Gamma\|_2^2 \leq \alpha.
\]
As a consequence, \(\|Z(\Gamma_\ast'')^\perp\|_2^2 \leq \varepsilon + \|ZT_\ast'\|_2^2 \leq \varepsilon + \alpha\).
Now we will start with the proof of correctness for our unraveling procedure.

5.2 Correctness of UNRAVEL (Algorithm 5)

We will now prove that if the input of UNRAVEL($\Gamma$) (Algorithm 5) is a list of (possibly overlapping) sets which are close to some $k$-partition (ground truth), then the output will be a list of $k$ disjoint sets which are also close to the ground truth. Our algorithm is based on formulating this as a simple maximum bipartite matching problem.

**Lemma 5.6.** Given $\Gamma \in \text{Set}_V(k)$, if there exists $\Gamma^* \in \text{Disj}_V(k)$ which is $\delta$-close to $\Gamma$, then UNRAVEL($\Gamma$) (Algorithm 5) will output $\hat{\Gamma} \in \text{Disj}_V(k)$ such that:

- For each $S \in \Gamma$, there exists $U \in \hat{\Gamma}$ with $U \subseteq S$ and $|U| \geq (1 - \delta)|S|$.
- $\hat{\Gamma}$ is $4\delta$-close to $\Gamma^*$.

**Proof.** It is easy to see that, if all blocks are matched, the resulting assignment is a collection of $k$-disjoint subsets and it has the first property. For the second property, consider any $S \in \Gamma$ with corresponding subsets $U \in \hat{\Gamma}$ and $T \in \Gamma^*$.

$$
\Delta(U, S) = 1 - \frac{|S \cap U|^2}{|S||U|} = 1 - \frac{|U|}{|S|} = \frac{|S \setminus U|}{|S|} \leq \delta.
$$

Hence $\sqrt{\Delta(U, T)} \leq \sqrt{\Delta(U, S)} + \sqrt{\Delta(S, T)} \leq 2\sqrt{\delta}$. This implies $\hat{\Gamma}$ is $4\delta$-close to $\Gamma^*$.

Now we will prove that if $\delta$-close $\Gamma^* \in \text{Disj}_V(k)$ exists, then there is always a matching of all blocks. Suppose $\pi : \Gamma \leftrightarrow \Gamma^*$ is a matching which minimizes $\max_S \Delta(S, \pi(S))$. Then:

$$
|S \cap \pi(S)|^2 \geq (1 - \delta)|S||\pi(S)| \implies |S \cap \pi(S)| \geq (1 - \delta)|S|.
$$

By Hall’s theorem, we have to show that for any set of right nodes, $B \subseteq R$, $B$’s neighbors on the left, $N(B)$, are more than $B$: $|N(B)| \geq |B|$. Observe that if $B$ contains some nodes of block $B_S$, then adding the whole block $B_S$ to $B$ does not increase $|N(B)|$, because all nodes in $B_S$ have the same set of neighbors. Hence the only subsets we need to consider are of the form $B = \cup_{S \in A} B_S$ over all $A \subseteq \Gamma$:

$$
|N(B)| = \left| \cup_{S \in A} S \right| \geq \left| \cup_{S \in A} (S \cap \pi(S)) \right| = \sum_{S \in A} |S \cap \pi(S)| \geq (1 - \delta) \sum_{S} |S| = |B|. \quad \Box
$$

5.3 Correctness of FINDCLUSTER (Algorithm 4)

Here we prove that, given an orthonormal basis $Y$, if it is close to a $k$-partition up to rotation, then FINDCLUSTER($Y$) (Algorithm 4) will output a set which is close to one of the clusters in this $k$-partition.

**Lemma 5.7.** Given $Y \in \mathbb{R}^{m \times n}$, whose singular values are 0 or 1, if there exists $\Gamma^* \in \text{Disj}_V(k)$ with $\|Y^TY - \Gamma^*\|_2^2 \leq \delta$ for some small enough constant $\delta$, then FINDCLUSTER($Y$) (Algorithm 4) will output $S' \subseteq V$ such that:

- There exists $T \in \Gamma^*$ with $\Delta(S', T) \leq O(\sqrt{\delta})$. 

15
• Any $T' \neq T : T' \in \Gamma_s$ has $|T' \cap S'| \leq O(\sqrt{\delta})|T'|$.

Proof. $\|Y^TY - \Gamma_s^2\|_2^2 \leq \delta$ implies $\sigma_k(Y) = 1$ and $\sigma_{k+1}(Y) = 0$. Therefore $\|Y\Gamma_s^{-1}\|_F^2 \leq \delta k$. In other words,

$$\sum_{T \in \Gamma_s} (\|Y_T\|_F^2 - \|Y\|_F^2) = \sum_{T \in \Gamma_s} (1 - \|Y\|_F^2) \leq \delta k.$$  

So:

$$\sum_{T \in \Gamma_s} \left[ \max(1, \|Y_T\|_F^2) - \|Y\|_F^2 \right] \leq 2\delta k.$$  

As a consequence, there exists $T \in \Gamma_s$ and some $c \in T$ such that:

$$\|Y_T\|_F^2 \geq \|Y\|_F^2 \geq 1 - 2\delta.$$  

$$4\delta \geq \frac{1}{|T|} \sum_{u \in T, v \in T} \|Y_u - Y_v\|_F^2 \geq \sum_{u \in T} \|Y_u - Y_c\|_F^2.$$  

$$\frac{4\delta}{1 - 2\delta} \geq \mathbb{E}_{u \sim \|Y_u\|_F^2} \left[ \frac{\|Y_u - Y_c\|_F^2}{\|Y_u\|_F^2} \right].$$  

Let’s define $\rho_u \overset{\text{def}}{=} \frac{\|Y_u - Y_c\|_F^2}{\|Y_u\|_F^2}$ and sort the nodes in ascending order so that $\rho_1 \leq \rho_2 \leq \ldots \leq \rho_n$:

$$\mathbb{E}_{u \sim \|Y_u\|_F^2} [\rho_u] \leq \frac{4\delta}{1 - 2\delta} \leq 9\delta. \quad \text{(provided $\delta \leq \frac{1}{2}$)}$$  

By a simple Markov inequality, sum of all $\|Y_u\|_F^2$ over $u \in T$ with $\rho_u \leq 3\sqrt{\delta}$ is at least $1 - 3\sqrt{\delta}$. Consequently, the smallest integer $m$ for which $\sum_{1 \leq u \leq m} \|Y_u\|_F^2 \geq 1 - 3\sqrt{\delta}$ satisfies $\sum_{1 \leq u \leq m} \|Y_u - Y_c\|_F^2 \leq 3\sqrt{\delta}$.

From now on, we assume $S$ is a subset and $\delta' : \delta' \leq 3\sqrt{\delta}$ with:

$$\|Y_S\|_F^2 = \sum_j \sigma^2_j(Y_S) \geq 1 - \delta' \quad \text{and} \quad \delta' \geq \sum_{u \in S} \|Y_u - Y_c\|_F^2.$$  

Recall that variance is lower bounded by sum of the squares of all but largest singular values:

$$\sum_{u \in S} \|Y_u - Y_c\|_F^2 \geq \|Y_S\|_F^2 - \sigma^2_1(Y_S) = \sum_{j \geq 2} \sigma^2_j(Y_S).$$  

Hence $\sigma^2_1(Y_S) \geq 1 - 2\delta'$ and $\sigma^2_2(Y_S) \leq \delta'$. Provided that $\delta \leq \frac{1}{100}$, which implies $\delta' \leq \frac{3}{10}$:

$$(\sigma_1 - \delta) \left( 1 - \frac{4\delta}{\sigma_1 - \sigma_2} \right) \geq 1 - 8\sqrt{\delta}.$$  

For such $S$, Lemma 5.4 tells us that the new subset $\hat{S} \subseteq S$ obtained by rounding the top right singular vector of $Y_S$ satisfies, for $T \overset{\text{def}}{=} \arg\max_{T \in \Gamma_s} \frac{|S \cap T|}{|T|}$:

• $\Delta(\hat{S}, T) \leq 1 - (\sigma_1 - \delta) \left( 1 - \frac{4\delta}{\sigma_1 - \sigma_2} \right) \leq 8\sqrt{\delta}.$  

• For any $T' \neq T \in \Gamma_s$, $|T' \cap \hat{S}| \leq 4\sqrt{\delta}|T'|$.  

\[\square\]
5.4 Correctness of BOOST (Algorithm 1)

As we mentioned earlier, if we keep finding clusters and removing them iteratively, the error will quickly accumulate and degrade the quality of remaining clusters. To prevent this, we apply a boosting procedure as described in $\hat{S} \leftarrow$ BOOST($Y, S$) (Algorithm 1) every time we find a new cluster. The main idea is that, if $S$ is close to some cluster in ground truth, say $T$, and far from others; then the top left singular vector, say $p$, of the vectors associated with $S$ will be close to the ones $S \cap T$. Unfortunately, we can not use simple perturbation bounds such as Wedin’s theorem. We have to make full use of eq. (3) instead: Under projection by $\Gamma_*$, vectors in $T \setminus S$ will be very close to the vectors in $S \cap T$. Hence indeed $p$ will be close most of $T \setminus S$ in addition to $S \cap T$.

**Theorem 5.8 (Boosting).** Given $Y \in S_k(\mathbb{R}^n)$ and $\Gamma_* \in \text{Disj}_k(k)$ with $\|Y \Gamma_*\|_2^2 \leq \varepsilon$, consider any subset $S \subseteq V$. Suppose there exists $T \in \Gamma_*$ with $|S \cap T| \geq (1 - \alpha)|T|$ such that for any $T' \neq T \in \Gamma_*$, $|S \cap T'| \leq \alpha|T'|$ for some $\alpha \leq \frac{1}{2}$. Then for $\hat{S} \leftarrow$ BOOST($Y, S$) (Algorithm 1), $\hat{S}$ satisfies:

$$\Delta(\hat{S}, T) \leq c_0\sqrt{\varepsilon}$$

for some constant $c_0 \leq 200$.

**Remark 5.9.** Note that Theorem 5.8 allows us to convert a subset with non-negligible overlap into a subset which is very close. Unfortunately, the new subset we obtain is no longer guaranteed to have small intersection with other $T' \neq T$.

**Proof of Theorem 5.8.** By Lemma 2.11, for $\delta \overset{\text{def}}{=} \sqrt{8\varepsilon}$:

$$\|Y^T Y - \Gamma_*\|_2 \leq \delta.$$

We will use $\sigma_1 \overset{\text{def}}{=} \sigma_1^2(Y_S)$ and $\sigma_2 \overset{\text{def}}{=} \sigma_2^2(Y_S)$. By Claim 5.3, $|\sigma_1 - |S \cap T||/|T|| \leq \delta$ and $\sigma_2 \leq \beta + \delta$.

Since $p$ is the left top singular vector of $Y_S$, $\|Y_S^T p\|^2 = \sigma_1$. We define $q \overset{\text{def}}{=} Y^T p$ so that $\|q_S\|^2 = \sigma_1$:

$$\frac{\|q_S\|^2}{|S \cap T|/|T|} \geq 1 - \frac{\delta}{|S \cap T|/|T|} \geq 1 - \delta \geq 1 - \frac{4\delta}{3}. \quad (7)$$

Since $\sigma_1((\Gamma_*^H)_{S,S}) - \sigma_2((\Gamma_*^H)_{S,S}) \geq 1 - 2\alpha$, Proposition 5.2 implies:

$$\langle \mathbf{e}_{T \cap S}, q \rangle^2 \geq \|q_S\|^2 \left(1 - \frac{2\delta}{1 - 2\alpha}\right) \geq \|q_S\|^2 \left(1 - 4\delta\right).$$

Let’s use $\mu_A$ to denote the mean of $p$ on subset $A$, $\mu_A \overset{\text{def}}{=} \langle \mathbf{e}_A, q \rangle$. We will assume, without loss of generality, $\mu_{S \cap T} \geq 0$. Hence $\mu_{S \cap T} \geq \frac{\|q_S\|}{\sqrt{|S \cap T|}} \sqrt{1 - 4\delta}$. On the other hand,

$$\varepsilon \geq p^T Y \Gamma_* \perp Y^T p = q^T \Gamma_* \perp q \geq q^T K_T q \geq |S \cap T| (\mu_{S \cap T} - \mu_T)^2.$$

$$\mu_T \geq \mu_{S \cap T} - \frac{\varepsilon}{|S \cap T|},$$

$$\langle \mathbf{e}_T, q \rangle \geq \sqrt{|T| \mu_{S \cap T}} - \sqrt{\frac{\varepsilon |T|}{|S \cap T|}} \geq \sqrt{|T|} \left(\|q_S\| \sqrt{1 - 4\delta} - \sqrt{\varepsilon}\right).$$
Using eq. (7), we can lower bound this quantity as:

\[
\geq \sqrt{(1 - \frac{4\delta}{3})(1 - 4\delta)} - \sqrt{\frac{\varepsilon}{1 - \alpha}} \geq 1 - 4\delta - \sqrt{\frac{4\varepsilon}{3}} \geq 1 - 5\delta.
\]

Since \(\|q\| = \|Y^T p\| \leq 1\), we have \(\Delta(p, T) \leq 1 - \langle e_T, q \rangle^2 \leq 10\delta\). Using Proposition 5.10, we see that \(\hat{S} \leftarrow \text{ROUND}(q)\) satisfies:

\[
\Delta(\hat{S}, T) \leq 4\Delta(q, T) \leq 40\delta.
\]

\[\square\]

5.5 Correctness of ROUND (Algorithm 2)

Possibly the simplest case for our problem is when \(Y\) is 1-dimensional, i.e. it is a vector. As we argued in the introduction, our algorithm boils down to simple thresholding in this case.

**Proposition 5.10.** Given \(q \neq 0 \in \mathbb{R}^n\), for any \(T \neq \emptyset\), \(S \leftarrow \text{ROUND}(q)\) (Algorithm 2) satisfies \(\Delta(S, T) \leq 4\Delta(q, T)\).

**Proof.** Let \(\varepsilon \coloneqq \Delta(q, T)\). Without loss of generality, we may assume \(q_1 \geq \ldots \geq q_m > 0 \geq \ldots \geq q_n\), \(\|q\| = 1\) and \(\langle q, e_T \rangle \geq 0\). We have:

\[
\sqrt{1 - \varepsilon} \leq \frac{\langle q, e_T \rangle}{\|T\|} \leq \frac{\sum_{j \leq |T|} q_j}{\|T\|} \leq \max_{S'} \frac{\sum_{j \leq |S'|} q_j}{\sqrt{|S'|}} \leq \frac{\sum_{j \leq |S|} q_j}{\sqrt{|S|}} \leq |\langle q, e_S \rangle|.
\]

So \(\Delta(S, q) \leq \varepsilon\) and \(\sqrt{\Delta(S, T)} \leq \sqrt{\Delta(S, q)} + \sqrt{\Delta(q, T)} \leq 2\sqrt{\varepsilon}\).

\[\square\]

5.6 Correctness of SPECTRALCLUSTERING (Algorithm 3)

Finally, we put everything together and prove the correctness of SPECTRALCLUSTERING(\(Y\)) (Algorithm 3). In the following lemma, we will show that the algorithm will iteratively find sets \(S_1, S_2, \ldots\) (think of them as coarse approximations of \(T_i\)’s) and \(\hat{S}_1, \hat{S}_2, \ldots\) (think of them as fine approximations of \(T_i\)’s) such that at each iteration, each \(S_i\) and \(\hat{S}_i\) will correspond to a unique \(T_i\). Moreover, each \(S_i\) will have very small overlap with remaining \(T_j\)’s coming after themselves. Even though \(S_i\)’s might still have large overlap with previous \(T_j\)’s for \(j < i\), we can easily use UNRAVEL(\(\Gamma\)) (Algorithm 5) to rectify this issue.

**Lemma 5.11.** Let \(\Gamma_* \in \text{Disj}_r(k)\) with \(\|Y^T \Gamma_*^{-1}\|^2 \leq \varepsilon\) for some \(\varepsilon \leq \varepsilon_0\), where \(\varepsilon_0 \in (0, 1)\) is a constant. For any \(r \in [k]\), consider the sequences \(\Gamma = (S_1, \ldots, S_r)\) and \(\hat{\Gamma} = (\hat{S}_1, \ldots, \hat{S}_r)\) as found by SPECTRALCLUSTERING(\(Y\)) at the start of \(r\)th iteration. Then there exists an ordering of \(\Gamma_*\):

\[
\Gamma_* = (T_1, T_2, \ldots, T_r, T_{r+1}, \ldots, T_k),
\]

with the following properties for some \(\alpha \leq \frac{1}{16}\) and \(\beta \leq 100\):

(a) For every \(i \leq r\):

- \(\Delta(S_i, T_i) \leq \alpha\).

(b) For every \(i > r\):

- \(\Delta(S_i, T_i) \leq \beta\).

(c) For every \(i > r\):

- \(\Delta(S_i, \hat{S}_i) \leq \beta\).

\[\square\]
• For all \( j > i \), \(|T_j \cap S_i| \leq \alpha|T_j|\).

(b) For every \( i \leq r \), \( \Delta(S_i, T_i) \leq \beta \epsilon \).

Proof. By induction on \( r \). For \( r = 0 \), (a) and (b) are trivially true.

Given \( r \), suppose (a) and (b) are true with \((T_1, \ldots, T_k), \Gamma^r\) and \(\Gamma''^r\) being as described.

At the beginning of \((r+1)\)th iteration, we have \(\Gamma = (S_1, \ldots, S_r)\) and \(\tilde{\Gamma} = (\hat{S}_1, \ldots, \hat{S}_r)\). (b) means \(\tilde{\Gamma}\) is \(\beta \epsilon\)-close to \(\Gamma^r\).

After \(\tilde{\Gamma}' \leftarrow \text{UNRAVEL}(\Gamma)\), by Lemma 5.6, \(\tilde{\Gamma}'\) is \(4\beta \epsilon\)-close to \(\Gamma^r\) and \(\tilde{\Gamma}' \in \text{Disj}_v(r)\). Using Theorem 2.8, we see that \(\|\tilde{\Gamma}' - \Gamma'^r\|_2^2 \leq 8\beta \epsilon\). Now we can invoke Lemma 5.5, which implies:

\[
\|Z(\Gamma^r)\|^2_2 \leq \epsilon + 8\beta \epsilon \leq 9\beta \epsilon.
\]

Provided \(9\beta \epsilon \leq \delta_0\) for some small enough constant \(\delta_0\), we can use Lemma 5.7 to see that the subset \(S_{r+1} \leftarrow \text{FINDCLUSTER}(Z)\) satisfies

\[
\Delta(S_{r+1}, T) \leq \alpha,
\]

and

\[
\forall T' \in \Gamma^r : T' \neq T \implies |T' \cap S_{r+1}| \leq \alpha|T'|.
\]

We reorder \((T_{r+1}, \ldots, T_k)\) so that \(T_{r+1} = T\). Then (a) holds true when \(i = r + 1\). Since \(T_1, \ldots, T_r\) remain the same, (a) is true for all \(i \leq r + 1\).

Consider \((U_1, \ldots, U_{r+1}) \leftarrow \text{UNRAVEL}(\Gamma)\). By Lemma 5.6, we know that \(\Delta(U_i, T_i) \leq 4\alpha\) and \(U_i \subseteq S_i, |U_i| \geq (1 - \alpha)|S_i|\) for each \(i \in [r+1]\). In particular, for all \(i \leq r + 1\):

\[
|U_i \cap T_i| \geq (1 - 4\alpha)|T_i|.
\]

\(U_{r+1}\) being a subset of \(S_{r+1}\) means \(|U_{r+1} \cap T_j| \leq \alpha|T_j|\) whenever \(j > r + 1\). Now we will prove the case of \(j \leq r\). Using the fact that \(U\)'s are disjoint, for any \(j \leq r\):

\[
|U_{r+1} \cap T_j| \leq |T_j| - |T_j \cap U_j| \leq |T_j| - (1 - 4\alpha)|T_j| = 4\alpha|T_j|.
\]

Consequently, for any \(j \neq r + 1\):

\[
|U_{r+1} \cap T_j| \leq 4\alpha|T_j|.
\]

After executing \(\hat{S}_{r+1} \leftarrow \text{BOOST}(Y, U_{r+1})\), noting \(\alpha \leq \frac{1}{16}\), we see via Theorem 5.8:

\[
\Delta(\hat{S}_{r+1}, T_{r+1}) \leq c_0\sqrt{\epsilon} = \beta \epsilon.
\]

Combined with the fact that \(\hat{S}_i\) and \(T_i\) remain the same for \(i \leq r\), (b) also remains true for all \(i \leq r + 1\).

By induction, we now see that both (a) and (b) are true for all \(r \leq k\). \(\square\)

**Theorem 5.12.** Let \(\Gamma_* \in \text{Disj}_v(k)\) with \(\|YT_*\|^2_2 \leq O(\epsilon)\). Then \(\hat{\Gamma} \leftarrow \text{SPECTRALCLUSTERING}(Y)\) is a \(k\)-partition so that \(\hat{\Gamma} \in \text{Disj}_v(k)\), and it is \(O(\sqrt{\epsilon})\) close to both \(\Gamma_*\) and \(Y\):

\[
\Delta(\Gamma_*, \hat{\Gamma}) \leq O(\sqrt{\epsilon}) \quad \text{and} \quad \|YT\|^2_2 \leq O(\sqrt{\epsilon}).
\]
Proof. By Lemma 5.11, \( \hat{\Gamma} = (\hat{S}_1, \ldots, \hat{S}_k) \) is \( \beta \sqrt{\varepsilon} \)-close to \( \Gamma_* \). Lemma 5.6 implies that UNRAVEL(\( \hat{\Gamma} \)) outputs a disjoint collection of \( k \)-subsets which is \( 4\beta \sqrt{\varepsilon} \)-close to \( \Gamma_* \). For the second bound:

\[
\frac{1}{2} \|Y \hat{\Gamma} \|^2 \leq \|YT_* \hat{\Gamma} \|^2 + \|YT_* \hat{\Gamma} \|^2 \\
\leq \|YT_* \|^2 \cdot \|\hat{\Gamma} \|^2 + \|YT_* \|^2 \cdot \|\hat{\Gamma} \|^2 \\
\leq \varepsilon + \|\hat{T}_* \|^2 \leq \varepsilon + 2\Delta(\Gamma, \hat{\Gamma}) \leq O(\sqrt{\varepsilon}).
\]

In the second to last inequality, we used Theorem 2.8.

\( \square \)

6 Applications

In this section, we will show some applications of our spectral clustering algorithm.

6.1 \( k \)-EXPANSION

Our first application is approximating non-expanding \( k \)-partitions in graphs. One may also interpret this as applying our subspace rounding algorithm on the basic SDP relaxation for \( k \)-EXPANSION problem.

Theorem 6.1. Given a graph \( G \) with Laplacian matrix \( L \), let \( \Gamma \) be the \( k \)-partition obtained by running Algorithm 3 on the smallest \( k \) eigenvectors of \( L \). Then:

\[
\Delta(\Gamma, \Gamma_*) \leq O\left(\sqrt{\phi_k \lambda_{k+1}}\right).
\]

Remark 6.2 (Faster Algorithm). By slightly modifying our algorithm to take advantage of the underlying graph structure, one can obtain a faster randomized algorithm having the same guarantees with Theorem 6.1 with expected running time \( O(k^2(n + m)) \).

Proof. From Lemma 2.14, we know that \( \phi_k \leq \sigma_{\max}(\Gamma_*^T L \Gamma_*) \leq 2\phi_k \). Now consider the matrix \( Z = Y^T \), whose columns are the smallest \( k \) eigenvectors of \( L \). We have \( L \succeq \lambda_{k+1} Z^T \) which means:

\[
\lambda_{k+1} \cdot \Gamma_*^T Z \Gamma_* \leq \Gamma_*^T L \Gamma_* \leq 2\phi_k I_k \implies O(\varepsilon) \geq \|\Gamma_*^T Z \Gamma_*\|_2 = \|I_k - \Gamma_*^T ZZ^T \Gamma_*\|_2.
\]

Thus \( \sigma_k(Z^T \Gamma_*) = \sigma_{\min}(Z^T \Gamma_*) \geq \sqrt{1 - O(\varepsilon)} \) and:

\[
\|Y \Gamma_* \|^2 = \|Z^T \Gamma_* \|^2 = \|I_k - \Gamma_*^T ZZ^T \Gamma_*\|_2 = 1 - \sigma_{\min}(\Gamma_*^T Z) \leq O(\varepsilon).
\]

The claim follows from Theorem 5.12. \( \square \)

6.2 Matrix and Graph Approximations

Our next application is for approximating a matrix in terms of \( k \)-block diagonal matrices corresponding to the adjacency matrices of normalized cliques, under spectral norm.
Theorem 6.3. Given a matrix $X \in \mathbb{S}^n$, let $\varepsilon \eqdef \min_{\Gamma \in \text{Disj}_V(k)} \|X - \Gamma \|_2$. In polynomial time, we can find $\Gamma \in \text{Disj}_V(k)$ such that $\Delta(\Gamma, \Gamma) \leq O(\sqrt{\varepsilon})$ and:

$$\|X - \Gamma\|_2 \leq O(\varepsilon^{1/4}).$$

Proof. Let $Y$ be the matrix whose rows are the top $k$ eigenvectors of $X$. Consider $\Gamma \leftarrow \text{SPECTRALCLUSTERING}(Y)$:

$$\|Y^TY - X\|_2 \leq \|X - \Gamma, \Gamma^T\|_2 \leq \varepsilon \implies \|Y^TY - \Gamma, \Gamma^T\|_2 \leq 2\varepsilon \implies \|Y\Gamma \|_2 \leq 2\varepsilon.$$

By Theorem 5.12, $\Delta(\Gamma, \Gamma) \leq O(\sqrt{\varepsilon})$ and $\|Y\Gamma \|_2 \leq O(\sqrt{\varepsilon})$:

$$\|\Gamma\Gamma^T - X\|_2 \leq \varepsilon + \|\Gamma, \Gamma^T\|_2 \leq O(\varepsilon^{1/4}).$$

Our final application is for approximating a graph Laplacian via another Laplacian corresponding to the disjoint union of $k$ normalized cliques (expanders), again under spectral norm. Since we are working with Laplacian matrices, this means the new graph approximates cuts of the original graph also.

Corollary 6.4. Given a graph $G$, if there exists $\Gamma \in \text{Disj}_V(k)$ such that Laplacian of $G$ is $\varepsilon$-close (in spectral norm) to the Laplacian corresponding to the disjoint union of normalized cliques on each $T \in \Gamma$:

$$\|L - \Gamma\|_2 \leq \varepsilon,$$

then we can find $\Gamma \in \text{Disj}_V(k)$ which is $O(\sqrt{\varepsilon})$-close to $\Gamma$ and $G$ in polynomial time:

$$\|L - \Gamma\|_2 \leq O(\varepsilon^{1/4}).$$

Proof. Since $\|L - \Gamma\|_2 = \|(I - L) - \Gamma\|_2$, we can apply Theorem 6.3 on the matrix $I - L$. The rest follows easily.

7. $k$-EXPANSION Implies Spectral Clustering

In this section, we will show that approximation algorithms for various graph partitioning problems imply similar approximation guarantees for our clustering problem.

Theorem 7.1. Given $Y : Y^T \in S_k(\mathbb{R}^n)$, let $\Gamma \coloneqq \arg\min_{\Gamma} \|Y\Gamma\|_2^2$ with $\varepsilon = \|Y\Gamma\|_2^2$. Then there exists a weighted, undirected, regular graph $X$, whose normalized Laplacian matrix has its $(k+1)^{st}$ smallest eigenvalue $\lambda_{k+1}$ is at least $\lambda_{k+1} \geq 1 - O(\sqrt{\varepsilon})$ such that:

- Each $T \in \Gamma$ has small expansion, $\phi_X(T) \leq O(\varepsilon)$,

- If $\Gamma \in \text{Disj}_V(k)$ is a $k$-partition with $\max_{S \in \Gamma} \phi_X(S) \leq \delta$, then $\Delta(\Gamma, \Gamma) \leq O(\delta + \sqrt{\varepsilon})$.

Moreover such $X$ can be constructed in polynomial time.

Proof. Consider the following SDP. Here we chose $\varepsilon \in [0, 1]$ to be the minimum value where this SDP remains feasible:

(i) $X \succeq Y^2 + 2\sqrt{2\varepsilon}Y^\perp$. 

21
We finish our proof with Claims 8.2 to 8.4.

Therefore

\[ \text{Claim 8.2.} \]

Moreover, after appropriately ordering the columns of \( \hat{\Gamma} \),

\[ \text{By Claim 8.2, } \Gamma \text{ and } \Gamma^* \] are within factor-

\[ \text{Consider } M \text{ as the following:} \]

\[ \forall S \in \Gamma: \pi_1(S) = \arg\max_{T \in \hat{\Gamma}} \frac{|S \cap T|}{|T|} \quad \text{and} \quad \forall T \in \hat{\Gamma}: \pi_2(T) = \arg\max_{S \in \Gamma} \frac{|S \cap T|}{|S|}. \]

Consider \( M = \{(S, \pi_1(S)) \mid S \in \Gamma\} \): By Claims 8.3 and 8.4, \( M \) is indeed a perfect matching between \( \Gamma \) and \( \hat{\Gamma} \). Now consider any matched pair \( (S, T) \in M \). Without loss of generality, say \( |S| \geq |T| \).

\[ \text{By Claim 8.2, } |S \cap T| \geq (1 - \varepsilon)|S|. \]

Since \( |S \Delta T| = |S| + |T| - 2|S \cap T| \):

\[ |S \Delta T| \leq |S| + |T| - 2(1 - \varepsilon)|S| = 2\varepsilon|S| + (|T| - |S|) \leq 2\varepsilon|S|. \]

We finish our proof with Claims 8.2 to 8.4.

**Claim 8.2.** If \( \pi_1(S) = T \), then \( |S \cap T| \geq (1 - \varepsilon)|T| \). Similarly, if \( \pi_2(T) = S \), then \( |S \cap T| \geq (1 - \varepsilon)|S| \).
Proof. Consider the matrix $P = \Gamma^T \hat{\Gamma}^T \Gamma \in S^k_+$ so that $\lambda_{\text{min}}(P) = \sigma_{\text{min}}^2(\Gamma^T \hat{\Gamma})$. Thus $\lambda_{\text{min}}(P) = \sigma_{\text{min}}(\Gamma^T \hat{\Gamma})^2 \geq 1 - \varepsilon$. In particular, all diagonals of $P$ are at least $1 - \varepsilon$. Consider any diagonal corresponding to $S \in \Gamma$:

$$1 - \varepsilon \leq \frac{e_S^T \hat{\Gamma}^T \Gamma e_S}{|S|} = \sum_{T \in \Gamma} \frac{|S \cap T|^2}{|S||T|} \leq \left( \max_{T' \in \Gamma} \frac{|S \cap T'|}{|T'|} \right) \sum_{T \in \Gamma} \frac{|S \cap T|}{|S|} = \max_{T' \in \Gamma} \frac{|S \cap T'|}{|T'|},$$

which, by construction, is equal to $\frac{|S \cap \pi_1(S)|}{|\pi_1(S)|}$. This proves the first part of the claim. The second part follows immediately by applying the same argument on $\hat{\Gamma}$ and $\Gamma$.

Claim 8.3. Both $\pi_1$ and $\pi_2$ are bijections.

Proof. Suppose $\pi_1(S) = \pi_1(S') = T$ for some $S \neq S'$. Since $S, S'$ are disjoint and $\varepsilon < \frac{1}{2}$:

$$|T| \geq |S \cap T| + |S' \cap T| \geq 2(1 - \varepsilon)|T| > |T|,$$

a contradiction. A similar argument shows that $\pi_2$ is a bijection as well.

Claim 8.4. $\pi_1 = \pi_2^{-1}$.

Proof. Suppose not. Since both $\Gamma$ and $\hat{\Gamma}$ are bijections by Claim 8.3, there exists a cycle of the form

$$(S_0, T_0, \ldots, S_{m-1}, T_{m-1}, S_m = S_0)$$

where $\pi_1(S_i) = T_i$ and $\pi_2(T_i) = S_{i+1}$ for some $m \geq 2$. By construction, $|S_i \cap T_i| \geq (1 - \varepsilon)|T_i|$ which means $\varepsilon|T_i| \geq |T_i \setminus S_i|$. Since $S_i$ and $S_{i+1}$ are disjoint, $|T_i \setminus S_i| \geq |T_i \cap S_{i+1}|$. Again, by construction, $|T_i \cap S_{i+1}| \geq (1 - \varepsilon)|S_{i+1}|$. Therefore $\varepsilon|T_i| \geq (1 - \varepsilon)|S_{i+1}|$ which implies $|T_i| \geq \frac{1-\varepsilon}{\varepsilon}|S_{i+1}| > |S_{i+1}|$ since $\varepsilon < 1/2$. By a similar argument, we can also show that $|S_i| > |T_i|$. Consequently, $|S_0| > |S_1| > \ldots > |S_m| = |S_0|$ which is a contradiction. So all cycles have length 2, which implies $\pi_1 = \pi_2^{-1}$.

\[\square\]

Acknowledgments

We thank Moses Charikar and Ravishankar Krishnaswamy for stimulating discussions about the problem.

References

[ABS10] Sanjeev Arora, Boaz Barak, and David Steurer. Subexponential algorithms for Unique Games and related problems. In 51th Annual IEEE Symposium on Foundations of Computer Science, FOCS 2010, October 23-26, 2010, Las Vegas, Nevada, USA, pages 563–572, 2010.

[AKY99] Charles J. Alpert, Andrew B. Kahng, and So-Zen Yao. Spectral partitioning with multiple eigenvectors. Discrete Applied Mathematics, 90(1-3):3–26, 1999.
Noga Alon and V. D. Milman. $\lambda_1$, Isoperimetric inequalities for graphs, and superconcentrators. J. Comb. Theory, Ser. B, 38(1):73–88, 1985.

Pranjal Awasthi and Or Sheffet. Improved spectral-norm bounds for clustering. In Approximation, Randomization, and Combinatorial Optimization. Algorithms and Techniques - 15th International Workshop, APPROX 2012, and 16th International Workshop, RANDOM 2012, Cambridge, MA, USA, August 15-17, 2012. Proceedings, pages 37–49, 2012.

Nikhil Bansal, Uriel Feige, Robert Krauthgamer, Konstantin Makarychev, Viswanath Nagarajan, Joseph Naor, and Roy Schwartz. Min-max graph partitioning and small set expansion. In IEEE 52nd Annual Symposium on Foundations of Computer Science, FOCS 2011, Palm Springs, CA, USA, October 22-25, 2011, pages 17–26, 2011.

Marianna Bolla. Spectral Clustering and Biclustering: Learning Large Graphs and Contingency Tables. Wiley, 2013.

Nikhil Bansal and Maxim Sviridenko. The Santa Claus problem. In Proceedings of the 38th Annual ACM Symposium on Theory of Computing, Seattle, WA, USA, May 21-23, 2006, pages 31–40, 2006.

S. Charles Brubaker and Santosh Vempala. Isotropic PCA and affine-invariant clustering. In 49th Annual IEEE Symposium on Foundations of Computer Science, FOCS 2008, October 25-28, 2008, Philadelphia, PA, USA, pages 551–560, 2008.

Amit Deshpande and Luis Rademacher. Efficient volume sampling for row/column subset selection. In 51th Annual IEEE Symposium on Foundations of Computer Science, FOCS 2010, October 23-26, 2010, Las Vegas, Nevada, USA, pages 329–338, 2010.

Alex Gittens, Prabhanjan Kambadur, and Christos Boutsidis. Spectral clustering via the power method – provably. CoRR, abs/1311.2854, 2013.

Venkatesan Guruswami and Ali Kemal Sinop. Optimal column-based low-rank matrix reconstruction. In Proceedings of the Twenty-Third Annual ACM-SIAM Symposium on Discrete Algorithms, SODA 2012, Kyoto, Japan, January 17-19, 2012, pages 1207–1214, 2012.

Amit Kumar and Ravindran Kannan. Clustering with spectral norm and the k-Means algorithm. In 51th Annual IEEE Symposium on Foundations of Computer Science, FOCS 2010, October 23-26, 2010, Las Vegas, Nevada, USA, pages 299–308, 2010.

Tsz Chiu Kwok, Lap Chi Lau, Yin Tat Lee, Shayan Oveis Gharan, and Luca Trevisan. Improved Cheeger’s inequality: analysis of spectral partitioning algorithms through higher order spectral gap. In Symposium on Theory of Computing Conference, STOC’13, Palo Alto, CA, USA, June 1-4, 2013, pages 11–20, 2013.

Ravi Kannan, Santosh Vempala, and Adrian Vetta. On clusterings: Good, bad and spectral. Journal of the ACM, 51(3):497–515, 2004.

James R. Lee, Shayan Oveis Gharan, and Luca Trevisan. Multiway spectral partitioning and higher-order Cheeger inequalities. Journal of the ACM, 61(6):37, 2014.
[LM14] Anand Louis and Konstantin Makarychev. Approximation algorithm for sparsest $k$-partitioning. In *Proceedings of the Twenty-Fifth Annual ACM-SIAM Symposium on Discrete Algorithms, SODA 2014, Portland, Oregon, USA, January 5-7, 2014*, pages 1244–1255, 2014.

[LRTV12] Anand Louis, Prasad Raghavendra, Prasad Tetali, and Santosh Vempala. Many sparse cuts via higher eigenvalues. In *Proceedings of the 44th Symposium on Theory of Computing Conference, STOC 2012, New York, NY, USA, May 19 - 22, 2012*, pages 1131–1140, 2012.

[NJW01] Andrew Y. Ng, Michael I. Jordan, and Yair Weiss. On spectral clustering: Analysis and an algorithm. In *Advances in Neural Information Processing Systems 14 [Neural Information Processing Systems: Natural and Synthetic, NIPS 2001, December 3-8, 2001, Vancouver, British Columbia, Canada]*, pages 849–856, 2001.

[SM00] Jianbo Shi and Jitendra Malik. Normalized cuts and image segmentation. *IEEE Trans. Pattern Anal. Mach. Intell.*, 22(8):888–905, 2000.

[SS90] G. W. Stewart and Ji-guang Sun. *Matrix Perturbation Theory*. Academic Press, 1990.

[YS03] Stella X. Yu and Jianbo Shi. Multiclass spectral clustering. In *9th IEEE International Conference on Computer Vision (ICCV 2003), 14-17 October 2003, Nice, France*, pages 313–319, 2003.