A Performance Guarantee for Spectral Clustering*

March Boedihardjo † , Shaofeng Deng ‡, and Thomas Strohmer §

4 Abstract. The two-step spectral clustering method, which consists of the Laplacian eigenmap and a rounding step, is a widely used method for graph partitioning. It can be seen as a natural relaxation to 56the NP-hard minimum ratio cut problem. In this paper we study the central question: when is 7 spectral clustering able to find the global solution to the minimum ratio cut problem? First we provide a condition that naturally depends on the intra- and inter-cluster connectivities of a given 8 9 partition under which we may certify that this partition is the solution to the minimum ratio cut 10 problem. Then we develop a deterministic two-to-infinity norm perturbation bound for the the invariant subspace of the graph Laplacian that corresponds to the k smallest eigenvalues. Finally 11 12by combining these two results we give a condition under which spectral clustering is guaranteed 13 to output the global solution to the minimum ratio cut problem, which serves as a performance 14guarantee for spectral clustering.

15 Key words. graph partitioning, ratio cut, spectral clustering, Laplacian eigenmap, matrix perturbation theory

16 AMS subject classifications. 90B10, 62H30, 47A55

17**1.** Introduction. The graph partitioning problem is ubiquitous in data analysis [4]: how to partition a graph into a given number of subgraphs so that the connections among them 18 are weak? One popular measurement for how well the graph is partitioned is the ratio cut of 19this partition. Let G be an undirected graph with vertex set $V = \{v_1, \dots, v_n\}$. We assume 20that the graph G is weighted, that is each edge between two vertices v_i and v_j carries a 21 non-negative weight $w_{ij} \ge 0$ ($w_{ii} = 0$). The weighted adjacency matrix of the graph is the 22 symmetric matrix $W = (w_{ij})$. Given a k-way partition of the vertices $\{V_i\}_{i=1}^k (\sqcup_{i=1}^k V_i = V)$, 2324 the ratio cut of this partition is defined to be

RatioCut
$$\left(\{V_i\}_{i=1}^k \right) = \sum_{i=1}^k \frac{\operatorname{Cut}\left(V_i, V_i^c\right)}{|V_i|},$$

26 where

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$$\operatorname{Cut}\left(V_{i}, V_{i}^{c}\right) = \sum_{v_{j} \in V_{i}, v_{k} \in V_{i}^{c}} w_{jk}$$

is the total weight between V_i and V_i^c . The ratio cut measures the connections among the subgraphs normalized by the size of the subgraphs. The purpose of the normalization is to discourage unbalanced partitions. Hence we are interested in finding a k-way partition that

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[†]Department of Mathematics, University of California Los Angeles (Email: march@math.ucla.edu).

[‡]Department of Mathematics, University of California Davis (Email: sfdeng@math.ucdavis.edu).

[§]Center of Data Science and Artificial Intelligence Research and Department of Mathematics, University of California at Davis (Email: strohmer@math.ucdavis.edu).

has the minimum ratio cut, which is presumed to be a NP-hard problem ([23]). Spectral clustering is a natural relaxation to this NP-hard problem. We begin by defining the graph

- 32 clustering is a natur 33 Laplacian of G. Let
- 34

$$d_i = \deg(v_i) = \sum_{j \neq i} w_{ij}$$

denote the degree of vertex v_i . Let the diagonal matrix D be the degree matrix with the degrees d_1, \dots, d_n on the diagonal. The graph Laplacian of the graph is then defined to be

$$37 L = D - W$$

38 Note that we can rewrite

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40
$$\operatorname{RatioCut}(\{V_i\}_{i=1}^k) = \sum_{i=1}^k \frac{\mathbb{1}_{V_i}^T L \mathbb{1}_{V_i}}{|V_i|} = \operatorname{Tr}\left(U^T L U\right),$$

41 where $U \in \mathbb{R}^{n \times k}$ has its *i*th column U_i being $\frac{1}{\sqrt{|V_i|}} \mathbb{1}_{V_i}$ and $\mathbb{1}_{V_i}$ is the indicator vector that 42 take value 1 on the vertices in V_i and 0 elsewhere. Therefore the minimum ratio cut problem 43 can be formulated as

44 (1.1)
$$\min_{\{V_i\}_{i=1}^k} \operatorname{Tr} \left(U^T L U \right) \quad \text{s.t. } U_i = \frac{1}{\sqrt{|V_i|}} \mathbb{1}_{V_i} \text{ for } i \in [k].$$

45 Spectral clustering relaxes the combinatorial constraint of U and instead seeks a solution 46 among all matrices U with orthonormal columns. So the relaxed problem is

47 (1.2)
$$\min_{U \in \mathbb{R}^{n \times k}} \operatorname{Tr} \left(U^T L U \right) \quad \text{s.t. } U^T U = I_k,$$

whose solution U can be shown to be the eigenvectors w.r.t. the k smallest eigenvalues of L. Since the columns of U are no longer a collection of indicator vectors, a rounding step is necessary to obtain the partition. The rounding step is performed on the rows of U. Namely one should treat the *i*th row U_{i} as the embedding of vertex v_i in \mathbb{R}^k and obtain the partition by clustering those points (usually through k-means) in \mathbb{R}^k . A justification for this idea is the following equivalence form of the relaxed problem (1.2):

54 (1.3)
$$\min_{U \in \mathbb{R}^{n \times k}} \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} ||U_{i\cdot} - U_{j\cdot}||_{2}^{2} \quad \text{s.t. } U^{T}U = I_{k}.$$

Hence U_i and U_j tend to be close in \mathbb{R}^k if v_i and v_j are strongly connected in G. For this reason we call U the Laplacian eigenmap of G. Spectral clustering, which consists of the Laplacian eigenmap and a rounding step, is shown in Algorithm 1.1.

In this paper we try to answer the fundamental question: under what condition is Algorithm 1.1, a relaxation of the minimum ratio cut problem (1.1), able to find the global minimum of (1.1)?

Algorithm 1.1 Spectral clustering

- 1: Input: Weighted adjacency matrix W and the number of clusters k.
- 2: Compute the graph Laplacian L = D W.
- 3: Compute $U \in \mathbb{R}^{n \times k}$ whose columns are the eigenvectors correspond to the k smallest eigenvalues of L.
- 4: Treat U_i as the embedding of vertex v_i in \mathbb{R}^k and apply clustering method (k-means etc.,) on the points $\{U_i\}_{i=1}^n$.
- 5: Obtain the partition $\{V_i\}_{i=1}^k$ of V based on the result form step 4.

1.1. Related work. Spectral clustering is a popular graph partition method. We refer the 61 readers to [22] for an excellent survey on this subject, whose topics include basic properties of 62the graph Laplacian, variants of spectral clustering methods, constructing similarity graphs 63 from non-graph data, different perspectives of spectral clustering, etc. Even though we have 64 yet to fully understand the mechanism of spectral clustering, some excellent research has been 65 done about its theoretical analysis. One of the most prominent ones is the work on (higher-66 order) Cheeger-type inequalities [6, 13]. Another closely related work is [16] which gives 67 performance guarantees for a SDP relaxation to (1.1). In fact our Theorem 2.2 is a direct 68 improvement to their work. For an analysis of the spectral clustering method on random 69 graphs we refer to [10, 9, 14, 20, 21, 1]. 70

The technical tool we use is the invariant subspace perturbation theory which studies the change to the invariant subspace of a self-adjoint matrix after the matrix is perturbed. One of the most celebrated works is the classic Davis-Kahan theorem [8] which bounds the invariant subspace perturbation in term of canonical angle. Recent years have witnessed a surge of research on the two-to-infinity norm bound of the invariant subspace perturbation, which is more suitable in many applications. The result we use for this paper is from the remarkable paper by A. Damle and Y. Sun [7]. Other related work on this topic includes [1, 11, 10, 5].

1.2. Notation. We introduce some notation which will be used throughout this paper. For 78any matrix $M \in \mathbb{C}^{n \times m}$, we denote by M_{i} and M_{i} its *i*th row vector and *i*th column vector 79 respectively. Moreover, $||M||_2$ denotes the $\ell^2 \to \ell^2$ induced norm, $||M||_{\infty} = \max_i ||M_i||_1$ 80 denotes the $\ell^{\infty} \to \ell^{\infty}$ induced norm and $||M||_{2,\infty} = \max_i ||M_i||_2$ is the $\ell^2 \to \ell^{\infty}$ induced 81 norm. We denote by $\mathbb{1}_n$ the vector of length n with all entries being 1 and let $J_{n \times m} = \mathbb{1}_n \mathbb{1}_m^\top$ 82 be the $n \times m$ matrix of all ones. If S is a subset of the vertex set V, then $\mathbb{1}_S$ is the indicator 83 vector such that $(\mathbb{1}_S)_i = 1$ if $v_i \in S$ and $(\mathbb{1}_S)_i = 0$ if $v_i \notin S$. If $M \in \mathbb{C}^{n \times n}$ is self-adjoint, then 84 we arrange its eigenvalues in increasing order: 85

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$$\lambda_1(M) \le \lambda_2(M) \le \dots \le \lambda_n(M).$$

87 **2. Main results.**

2.1. Certifying the global minimum of ratio cut. Suppose the partition $\{V_i\}_{i=1}^k$ achieves the minimum ratio cut. If we see each V_i as a planted cluster, then the connectivity within each cluster should be strong and the connections between them should be weak. To quantify this, let $L_i \in \mathbb{R}^{|V_i| \times |V_i|}$ be the graph Laplacian of the induced subgraph $G[V_i]$. We measure the connectivity of $G[V_i]$ by $\lambda_2(L_i)$, which is the second smallest eigenvalue of L_i . The second smallest eigenvalue of a graph Laplacian is also called the algebraic connectivity of the graph. The larger it is, the stronger the graph is connected. In the case the graph is disconnected, the algebraic connectivity drops to 0. One way to interpret the algebraic connectivity is that it provides a lower bound for the edge density of the graph (see Lemma 2.1 below). The proof of this result and subsequent results will be presented in Section 4.

98 Lemma 2.1. Let G be a weighted undirected graph with vertex set V. Let L be the graph 99 Laplacian of G. Let S be a subset of V. Then

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$$Cut(S, V - S) \ge \lambda_2(L) \frac{|S| \cdot |V - S|}{|V|}.$$

101 To measure the inter-cluster connectivity, we define for each vertex v_i ,

102
$$d_{\delta}^{(i)} = \sum_{v_k \in V_i^c} w_{ik}$$

where V_j is the cluster that contains v_i . In other words, $d_{\delta}^{(i)}$ is the total weight between v_i and outside clusters. With such definitions for intra- and inter-cluster connectivity, we are able to certify when a partition is optimal.

106 Theorem 2.2. Suppose a partition $\{V_i\}_{i=1}^k$ satisfies

107 (2.1)
$$\max_{1 \le i \le n} d_{\delta}^{(i)} \le \frac{1}{2} \min_{1 \le i \le k} \lambda_2(L_i),$$

then $\{V_i\}_{i=1}^k$ achieves the minimum ratio cut among all k-way partitions of V. If (2.1) holds with the strict inequality, then $\{V_i\}_{i=1}^k$ is also the unique partition (up to relabeling) that achieves the minimum ratio cut.

Theorem 2.2 is a direct improvement of the result in [16], which has a constant $\frac{1}{4}$ instead of $\frac{1}{2}$. The following example shows that the constant $\frac{1}{2}$ cannot be further improved.

113 Example 2.3. Let $W \in \mathbb{R}^{4n \times 4n}$,

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$$W = \begin{pmatrix} J_{n \times n} & J_{n \times n} & cJ_{n \times n} & 0\\ J_{n \times n} & J_{n \times n} & 0 & cJ_{n \times n}\\ cJ_{n \times n} & 0 & J_{n \times n} & J_{n \times n}\\ 0 & cJ_{n \times n} & J_{n \times n} & J_{n \times n} \end{pmatrix} - I_{4n}.$$

115 Consider the partition $V_1 = \{v_1, \dots, v_{2n}\}, V_2 = \{v_{2n+1}, \dots, v_{4n}\}$. The corresponding

116
$$\min_{1 \le i \le 2} \lambda_2(L_i) = 2n \quad \text{and} \quad \max_{1 \le i \le 4n} d_{\delta}^{(i)} = cn.$$

117 If c > 1 then the condition in Theorem 2.2 is violated for this partition. One can check that 118 in this case a different partition $V^{(1)} = \{v_1, \dots, v_n, v_{2n+1}, \dots, v_{3n}\}, V^{(2)} = V - V^{(1)}$ has a 119 smaller ratio cut.

Theorem 2.2 is algorithm independent and can be useful in many ways. For example one can use it to check in polynomial time if a given partition is optimal. It can also serve as a benchmark for comparing different algorithms. In [16] the authors propose a SDP relaxation

to the minimum ratio cut problem (1.1) and show that it is able to find the optimal partition if it satisfies $\max_{1 \le i \le n} d_{\delta}^{(i)} < \frac{1}{4} \min_{1 \le i \le k} \lambda_2(L_i)$. In this paper we prove that Algorithm 1.1 is able to find the optimal partition if $\max_{1 \le i \le n} d_{\delta}^{(i)} \lesssim \frac{1}{\ln n} \min_{1 \le i \le k} \lambda_2(L_i)$. The notation " \lesssim "

126 hides a term that does not depend on n.

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127 **2.2.** A two-to-infinity norm bound for the Laplacian eigenmap. Algorithm 1.1 can be 128 understood from a perturbation perspective. Suppose we try to recover the planted partition 129 $\{V_i\}_{i=1}^k$. Let W_i , D_i , L_i denote the weighted adjacency matrix, degree matrix and graph 130 Laplacian of the induced subgraph $G[V_i]$ respectively. Let

$$W_{\rm iso} = \begin{pmatrix} W_1 & & & \\ & W_2 & & \\ & & \ddots & \\ & & & \ddots & \\ & & & & W_k \end{pmatrix}, W_{\delta} = W - W_{\rm iso}$$

Let D_{iso} , L_{iso} , D_{δ} , L_{δ} be the corresponding degree matrices or graph Laplacians (here we suppose $\lambda_{k+1}(L_{iso}) > 0$). Let $U(U_{iso})$ be a matrix with orthonormal columns whose range is the invariant subspace of $L(L_{iso})$ that corresponds to the k smallest eigenvalues. Then the ksmallest eigenvalues of L_{iso} are 0 and U_{iso} , up to a multiplication of orthogonal matrix from the right, is

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$$U_{\rm iso} = \left(\frac{1}{\sqrt{|V_1|}} \mathbb{1}_{V_1} \quad \frac{1}{\sqrt{|V_2|}} \mathbb{1}_{V_2} \quad \cdots \quad \frac{1}{\sqrt{|V_k|}} \mathbb{1}_{V_k}\right).$$

Hence the rows of U_{iso} reduce to k different points in \mathbb{R}^k with one cluster at each point. Any rounding method will recover the planted clusters perfectly. Here we also point out that a multiplication of orthogonal matrix from the right transforms all the rows simultaneously and thus preserves the geometry of the embedding. If W_{δ} is small, then U should be close to U_{iso} . A reasonable measurement for the closeness is

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$$\min_{V \in \mathbf{O}^{k}} ||UV - U_{iso}||_{2,\infty} = \min_{V \in \mathbf{O}^{k}} \max_{1 \le i \le n} ||(UV - U_{iso})_{i}||_{2},$$

where the minimization is taken over all $k \times k$ orthogonal matrices. This error measures the maximum distance of a point U_i away from its origin $(U_{iso})_i$ after some global orthogonal transformation. If this error is small enough then the rounding step should be able to recover the planted clusters perfectly. We present our bound for $\min_{V \in \mathbf{O}^k} ||UV - U_{iso}||_{2,\infty}$ in Theorem 2.4 below. The result is stated in terms of $||U\tilde{V} - U_{iso}||_{2,\infty}$ where \tilde{V} solves the orthogonal Procrustes problem

150
$$\tilde{V} = \arg\min_{V \in \mathbf{O}^k} ||UV - U_{\rm iso}||_F.$$

151 Note that $\min_{V \in \mathbf{O}^k} ||UV - U_{iso}||_{2,\infty} \leq ||U\tilde{V} - U_{iso}||_{2,\infty}$. The matrices V and \tilde{V} are only 152 defined for the sake of analysis and are not required by the actual algorithm. 153 Theorem 2.4. Suppose each $|V_i| \ge 3$. Let

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$$c = \max_{1 \le i \le k} \frac{n}{|V_i|} \quad and \quad r = \frac{\max_{1 \le i \le n} d_{\delta}^{(i)}}{\min_{1 \le i \le k} \lambda_2(L_i)}$$

155 be the unbalanceness and the perturbation/eigengap ratio respectively. If $r \leq \frac{1}{16(1+c)\ln n}$, then

156
$$\left| \left| U\tilde{V} - U_{iso} \right| \right|_{2,\infty} \le 32\sqrt{c} \left(r^2 + r \ln n \right) \frac{1}{\sqrt{n}}.$$

The rest of this section is dedicated to the technical details of the proof. Discussions and applications regarding this bound are deferred to Section 3. The tool we use is Corollary 3.3 in [7] which gives a two-to-infinity norm perturbation bound for the invariant subspace. We cite this result in Lemma 2.5 below. The definition of the separation of two matrices (denoted by *sep*) that arises in Lemma 2.5, is stated below the lemma.

162 Lemma 2.5. Let $L_{iso} = U_{iso}\Lambda_1 U_{iso}^T + U_2\Lambda_2 U_2^T$ be the spectral decomposition of L_{iso} where 163 $\Lambda_1 \in \mathbb{R}^{k \times k}$ is a zero matrix and $\Lambda_2 \in \mathbb{R}^{(n-k) \times (n-k)}$ whose diagonal contains all the posi-164 tive eigenvalues of L_{iso} . Let gap = min $\left\{ \operatorname{sep}_2(\Lambda_1, \Lambda_2), \operatorname{sep}_{(2,\infty), U_2}(\Lambda_1, U_2\Lambda_2 U_2^T) \right\}$ and $\mu =$ 165 $\sqrt{n} ||U_{iso}||_{2,\infty}$. If $||L_{\delta}||_2 \leq \frac{\operatorname{gap}}{5}$ and $||L_{\delta}||_{\infty} \leq \operatorname{gap}/(4 + 4\mu^2)$ then

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$$\left| \left| U\tilde{V} - U_{iso} \right| \right|_{2,\infty} \le 8 \left| |U_{iso}| \right|_{2,\infty} \left(\frac{||L_{\delta}||_2}{\sup_2(\Lambda_1, \Lambda_2)} \right)^2 + 4 \frac{\left| |U_2 U_2^T L_{\delta} U_{iso}| \right|_{2,\infty}}{\operatorname{gap}} \right)^2 + 4 \frac{||U_2 U_2^T L_{\delta} U_{iso}||_{2,\infty}}{\operatorname{gap}}$$

167 Classical perturbation theory like Davis-Kahan usually bounds the invariant subspace per-168 turbation in terms of the perturbation/eigengap ratio. Lemma 2.5 is similar but with the 169 classical eigengap replaced by the gap term defined therein. Here the separation of two ma-170 trices is defined as

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$$\operatorname{sep}_{*,W}(B,C) = \inf\left\{||ZB - CZ||_* : Z \in \mathbb{R}^{m \times l}, \operatorname{ran} Z \subseteq \operatorname{ran} W, ||Z||_* = 1\right\}$$

172 where $B \in \mathbb{R}^{l \times l}$, $C \in \mathbb{R}^{m \times m}$, ran W is a linear subspace of \mathbb{R}^m and $|| \cdot ||_*$ is a norm on $\mathbb{R}^{m \times l}$.

173 When ran $W = \mathbb{R}^m$ we denote $\sup_{*}(B, C) = \sup_{*,W}(B, C)$. $||L_{\delta}||_2$ and $||L_{\delta}||_{\infty}$ in Lemma 2.5

174 can be bounded by $2 \max_{1 \le i \le n} d_{\delta}^{(i)}$. Moreover, the two matrix separation terms $\operatorname{sep}_2(\Lambda_1, \Lambda_2)$ 175 and $\operatorname{sep}_{(2,\infty),U_2}(\Lambda_1, U_2\Lambda_2 U_2^T)$ are closely related to the eigengap $\min_{1 \le i \le k} \lambda_2(L_i)$. In fact,

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$$\operatorname{sep}_{2}(\Lambda_{1},\Lambda_{2}) = \inf\left\{||Z\Lambda_{1} - \Lambda_{2}Z||_{2} : Z \in \mathbb{R}^{(n-k) \times k}, ||Z||_{2} = 1\right\}$$

177
$$= \inf \left\{ ||\Lambda_2 Z||_2 : Z \in \mathbb{R}^{(n-k) \times k}, ||Z||_2 = 1 \right\}$$

178 (2.2)
$$= \min_{1 \le i \le k} \lambda_2(L_i)$$

180 is exactly the eigengap. Furthermore,

181
$$\operatorname{sep}_{(2,\infty),U_2}(\Lambda_1, U_2\Lambda_2 U_2^T) = \inf \left\{ ||0 - L_{\operatorname{iso}}Z||_{2,\infty} : Z \in \mathbb{R}^{n \times k}, \operatorname{ran} Z \subseteq \operatorname{ran} U_2, ||Z||_{2,\infty} = 1 \right\}$$

182 $= \min_{1 \le i \le k} \inf \left\{ ||L_iZ||_{2,\infty} : Z \in \mathbb{R}^{|V_i| \times k}, \operatorname{ran} Z \subseteq \left\{ \mathbb{1}_{|V_i|} \right\}^{\perp}, ||Z||_{2,\infty} = 1 \right\}$

185 can be understood as the "eigengap" in terms of the ℓ^{∞} norm. The third equality holds 186 because for any Z if we let $x \neq 0$ be the vector that $||Zx||_{\infty} = ||x||_2$, then

187
$$||L_iZ||_{2,\infty} \ge \frac{||L_iZx||_{\infty}}{||x||_2} = \frac{||L_iZx||_{\infty}}{||Zx||_{\infty}} \ge \inf_{x \perp \mathbb{1}_{|V_i|}} \frac{||L_ix||_{\infty}}{||x||_{\infty}}.$$

188 And on the other hand we can pick a \tilde{Z} such that its first column satisfies

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$$\left\| \tilde{Z}_{\cdot 1} \right\|_{\infty} = 1 , \quad \left\| L_i \tilde{Z}_{\cdot 1} \right\|_{\infty} = \inf_{x \perp \mathbb{1}_{|V_i|}} \frac{\left\| L_i x \right\|_{\infty}}{\left\| x \right\|_{\infty}}$$

190 and its other columns are 0 so that

191
$$\left| \left| L_i \tilde{Z} \right| \right|_{2,\infty} = \inf_{x \perp \mathbb{1}_{|V_i|}} \frac{\left| \left| L_i x \right| \right|_{\infty}}{\left| \left| x \right| \right|_{\infty}}$$

192 Note that we always have

$$\inf_{x \perp \mathbb{1}_{|V_i|}} \frac{||L_i x||_{\infty}}{||x||_{\infty}} \le \lambda_2(L_i).$$

194 Therefore the the gap term in Lemma 2.5 is simplified to

195 (2.3)
$$gap = \min_{1 \le i \le k} \inf_{x \perp \mathbb{1}_{|V_i|}} \frac{||L_i x||_{\infty}}{||x||_{\infty}}.$$

196 There is a trivial bound that relates gap to the eigengap:

197
$$\inf_{x \perp \mathbb{I}_{|V_i|}} \frac{||L_i x||_{\infty}}{||x||_{\infty}} \ge \frac{\lambda_2(L_i)}{\sqrt{|V_i|}}.$$

But we will show that due to the diagonally dominant structure of the graph Laplacian, the $\sqrt{|V_i|}$ factor can be improved to $\ln |V_i|$. The following theorem, which is also of independent interest, is essential in this context.

Theorem 2.6. Let B be a self-adjoint $n \times n$ matrix, $n \geq 3$ such that $B_{i,i} \geq \sum_{j \in \{1,...,n\} \setminus \{i\}} |B_{i,j}|$ for all $1 \leq i \leq n$. Let \mathcal{M} be a subspace of \mathbb{C}^n such that $B\mathcal{M} \subset \mathcal{M}$. Then

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$$||Bx||_{\infty} \ge \frac{\lambda_{\min}(B|_{\mathcal{M}})||x||_{\infty}}{2\ln n}$$

204 for all $x \in \mathcal{M}$.

Corollary 2.7. Suppose that L is the Laplacian of a graph with n vertices, $n \ge 3$. Then

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$$\frac{\lambda_2(L)}{2\ln n} \le \inf_{x \perp \mathbb{I}_n} \frac{\|Lx\|_{\infty}}{\|x\|_{\infty}} \le \frac{4M}{D}$$

where the second inequality holds for unweighted graphs with M being the maximum degree and D being the diameter. The following example shows that the $\ln n$ factor in Corollary 2.7 is necessary. However, at this point we do not know whether it must carry over to $||U\tilde{V} - U_{\rm iso}||_{2,\infty}$ as well.

211 Example 2.8. Suppose that L is the Laplacian of a d-regular Ramanujan graph with n212 vertices. This means that $\lambda_2(L) \geq d - 2\sqrt{d-1}$. Note that $n \leq (d+1)^D$ where D is the 213 diameter of the graph. This follows from the fact that for a fixed vertex u_0 , every vertex can be 214 connected to u_0 via a path of length at most D and that there are at most $1+d+d^2+\ldots+d^D \leq$ 215 $(d+1)^D$ paths of length at most D. Thus, $D \geq \frac{\ln n}{\ln(d+1)}$. By Corollary 2.7,

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$$\frac{d - 2\sqrt{d-1}}{2\ln n} \le \inf_{x \perp \mathbb{1}_n} \frac{\|Lx\|_{\infty}}{\|x\|_{\infty}} \le \frac{4d}{D} \le \frac{4d\ln(d+1)}{\ln n}.$$

217 For example, if L is the Laplacian of a 5-regular Ramanujan graph with n vertices, then

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$$\frac{1}{2\ln n} \le \inf_{x \perp \mathbb{1}_n} \frac{\|Lx\|_{\infty}}{\|x\|_{\infty}} \le \frac{36}{\ln n}.$$

For every $d \ge 3$, there exist infinitely many *d*-regular Ramanujan graphs by [19]. This shows that the $\ln n$ factor in Corollary 2.7 is necessary.

3. Discussions. Algorithm 1.1 consists of two steps: the Laplacian eigenmap and a round-221 ing step. We have bounded the Laplacian eigenmap in Theorem 2.4. The next question is 222whether the rounding step will successfully recover the planted clusters based on the embed-223ded points in \mathbb{R}^k . The answer depends on our understanding of the choice of the rounding 224method and it is beyond the scope of this paper to present a survey on this subject. But since 225the rows of $U_{\rm iso}$ have a natural magnitude of $O(1/\sqrt{n})$, if we have $\left\| U\tilde{V} - U_{\rm iso} \right\|_{2,\infty} < C/\sqrt{n}$ 226for some sufficiently small C, then it means the rows of U (after some proper global rotation) 227 228 are close enough to the ideal $U_{\rm iso}$ and thus should be nicely separable. Indeed, we will show through several examples that the condition 229

230 (3.1)
$$\left\| U\tilde{V} - U_{\rm iso} \right\|_{2,\infty} < \frac{C}{\sqrt{n}}$$

can imply successful recovery, where C depends on the specific choice of the rounding method and (possibly) the number of clusters k.

• A simple bisector for two clusters. When k = 2, the Fiedler eigenvector (i.e., the 233eigenvector $u_2(L)$ that corresponds to the second smallest eigenvalue of L) is a popular 234tool to partition the graph. One way to do this is to first put the entries of the Fiedler 235eigenvector in algebraic order. Then out of all n-1 possible linear bisections of the entries 236we pick the one that gives the smallest ratio cut. This method is equivalent to finding the 237best linear bisection of the embedded points in \mathbb{R}^2 . For this rounding method we can let 238C = 1 in (3.1). To see why, first note that \tilde{V} is the solution to an orthogonal Procrustes 239problem and therefore has a closed form solution 240

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$$\tilde{V} = V_1 V_2^T$$

where $U^T U_{\text{iso}} = V_1 \Sigma V_2^T$ is the singular value decomposition of $U^T U_{\text{iso}}$. Given that $u_1(L) = u_1(L_{\text{iso}}) = \frac{1}{\sqrt{n}} \mathbb{1}_n$, it is easy to check that

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$$\left| \left| U\tilde{V} - U_{\text{iso}} \right| \right|_{2,\infty} = \left| \left| u_2(L) - u_2(L_{\text{iso}}) \right| \right|_{\infty}$$

where the sign of $u_2(L)$ is chosen so that $\langle u_2(L_{iso}), u_2(L) \rangle > 0$. Note that the distance between the two embedded unperturbed clusters is $\sqrt{1/|V_1| + 1/|V_2|}$. To ensure the separation of the two clusters in $u_2(L)$ we require

$$||u_2(L) - u_2(L_{iso})||_{\infty} < \frac{1}{2}\sqrt{\frac{1}{|V_1|} + \frac{1}{|V_2|}},$$

which is guaranteed by $\left\| U\tilde{V} - U_{iso} \right\|_{2,\infty} < 1/\sqrt{n}$. • An SDP type of k-means algorithm. The k-means algorithms are a family of algorithms

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• An SDP type of k-means algorithm. The k-means algorithms are a family of algorithms that seek the k-way partition $\{\Gamma_i\}_{i=1}^k$ of n points in \mathbb{R}^d by minimizing the following k-means objective function:

253
$$\min_{\{\Gamma_i\}_{i=1}^k} \sum_{i=1}^k \sum_{x \in \Gamma_i} ||x - \mu_i||_2^2$$

where μ_i is the mean of points in Γ_i . Note that the optimization is shown to be NP-254hard ([18, 2]) so no polynomial-time algorithm is guaranteed to find the optimal partition 255in general. The most famous and widely used k-means algorithm is the Lloyd's algorithm 256257([17]). But its heuristic nature and random initial starts make the analysis of exact recovery difficult. Here we consider a SDP type of k-means algorithm proposed in [15]. The proposed 258algorithm comes with a proximity condition for the planted partition under which the 259algorithm is guaranteed to recover the planted partition. Let $n_i = |\Gamma_i|$ and $X_i \in \mathbb{R}^{n_i \times d}$ be 260the data matrix of the *i*-th cluster with each row being a point in Γ_i . Let $\overline{X}_i = X_i - \mathbb{1}_{n_i} \mu_i^T$ 261be the centered data matrix of the *i*-th cluster. For each pair of $i \neq j$, let $M_{i,j}$ denote the 262bisecting hyperplane that passes through $\frac{\mu_i + \mu_j}{2}$ and is perpendicular to the line segment 263that joins μ_i and μ_j . The proximity condition is then stated as follows: for all $i \neq j$, (i) Γ_i 264and Γ_j are separated by $M_{i,j}$ and (ii) 265

266
$$\xi_{i,j} > \frac{1}{2} \sqrt{\sum_{i=1}^{k} \left| \left| \overline{X}_i \right| \right|_2^2 \left(\frac{1}{n_i} + \frac{1}{n_j} \right)}$$

where $\xi_{i,j} = \text{dist} \{M_{i,j}, \Gamma_i \cup \Gamma_j\}$ is the margin between the clusters and the bisecting hyperplane (see also Figure 1). We now claim that if C = 1/5 in (3.1) then the SDP k-means algorithm is guaranteed to recover the planted partition. To see why, note that (3.1) implies the points in Γ_i and Γ_j , together with their means, are confined within two balls of radius C/\sqrt{n} whose centers are $\sqrt{\frac{1}{n_i} + \frac{1}{n_j}}$ apart. By Lemma 4.3 in Section 4.3 we have

272
$$\xi_{i,j} > \frac{1}{2}\sqrt{\frac{1}{n_i} + \frac{1}{n_j}} - \frac{3C}{\sqrt{n}} \ge \frac{1 - 3C}{2}\sqrt{\frac{1}{n_i} + \frac{1}{n_j}}.$$

And on the other hand

$$\sum_{i=1}^{k} \left| \left| \overline{X}_{i} \right| \right|_{2}^{2} \le \sum_{i=1}^{k} \left| \left| \overline{X}_{i} \right| \right|_{F}^{2} < 4C^{2}$$

Therefore, if $C \leq 1/5$ then the proximity condition is satisfied.



Figure 1: Proximity condition for the SDP k-means algorithm. If the partition satisfies the proximity condition, then each pair of clusters Γ_i and Γ_j are separated by and sufficiently bounded away from the bisecting hyperplane of the line segment that joins μ_i and μ_j .

• Two projective k-means algorithms. In [12] and [3] two projective k-means algorithms are proposed which consist of an SVD-based projection followed by iterative Lloyd steps with informed initial starts. By our notation, the algorithm in [12] is guaranteed to recover the planted partition if for any $i \neq j$,

281
$$\xi_{i,j} > \tilde{C}k\left(\frac{1}{\sqrt{n_i}} + \frac{1}{\sqrt{n_j}}\right) \left|\left|\overline{W}\right|\right|_2$$

where $\tilde{C} > 0$ is an absolute constant and $\overline{W} = [\overline{X}_1^T, \cdots, \overline{X}_k^T]^T$. The algorithm in [3] is guaranteed to recover the planted partition if for any $i \neq j$,

284
$$\xi_{i,j} > \frac{1}{2}\tilde{C}\left(\frac{1}{\sqrt{n_i}} + \frac{1}{\sqrt{n_j}}\right) \left|\left|\overline{W}\right|\right|_2$$

285 and

286
$$||\mu_i - \mu_j||_2 > \tilde{C}\sqrt{k} \left(\frac{1}{\sqrt{n_i}} + \frac{1}{\sqrt{n_j}}\right) ||\overline{W}||_2.$$

287 Then C in (3.1) can be similarly derived for both methods.

Thus, by Theorem 2.4 and the discussion above, Algorithm 1.1 finds the planted partition if $r \leq 1/\ln n$ where the hidden term depends on k and the unbalanceness term c. By Theorem 2.2 when $r \leq 1/2$, we can certify that the planted partition is optimal. Therefore we may claim that Algorithm 1.1 finds the optimal partition when $r \leq 1/\ln n$.

274

Note that when the unbalanceness term c gets arbitrarily large, Theorem 2.4 gets arbi-292 trarily bad. This is to be expected. We illustrate the effect of unbalanceness on the Laplacian 293eigenmap using a simple numerical example. Consider $|V_1| = 3$ and $|V_2| = |V_3| = 300$. Let 294 $W_i = J_{|V_i| \times |V_i|} / |V_i|$ so $\lambda_2(L_i) = 1$ for $1 \le i \le 3$. We perturb the graph by adding a weight 0.5 295between a vertex in V_1 and a vertex in V_2 . We then add another weight 0.5 between a vertex 296 in V_3 and another vertex in V_2 . The Laplacian eigenmap of both the unperturbed and the 297 perturbed graphs are shown in Figure 2. As seen from the figure, $\min_{V \in \mathbf{O}^k} ||UV - U_{iso}||_{2,\infty}$ 298 is large and will be even more so as the clusters get more unbalanced. Despite the error 299being large, the Laplacian eigenmap still separates the three clusters well. The reason is that 300 $\min_{V \in \mathbf{O}^k} ||UV - U_{iso}||_{2,\infty}$ only measures the magnitude and thus ignores the directions of the 301 perturbation. A more refined analysis on the Laplacian eigenmap should consider the direc-302 tion of the perturbation as well as the magnitude. It remains an open problem whether there 303 304 exists a constant C such that $r \leq C$ implies successful recovery of the planted clusters by Algorithm 1.1. The constant C should only depend on k or, better yet, not even on k.

11



Figure 2: Laplacian eigenmap for both the unperturbed and the perturbed graphs. The embedded points live on a common plane in \mathbb{R}^3 so we can visualize them in \mathbb{R}^2 . The four empty circles are the four perturbed vertices.

305

4. Proofs.

4.1. Proofs for Section 2.1.

308 **Proof of Lemma 2.1.** Consider $M = L - \lambda_2(L)P$ where $P = I - \frac{1}{|V|}J_{|V|\times|V|}$. Then M309 is positive semi-definite. Therefore

$$\mathbb{1}_{S}^{T}M\mathbb{1}_{S} = \mathbb{1}_{S}^{T}L\mathbb{1}_{S} - \lambda_{2}(L)\mathbb{1}_{S}^{T}P\mathbb{1}_{S} = \operatorname{Cut}\left(S, V - S\right) - \lambda_{2}(L)\frac{|S| \cdot |V - S|}{|V|} \ge 0$$

³¹¹ **Proof of Theorem 2.2.** Suppose without loss of generality that the partition $\{V_i\}_{i=1}^k$ ³¹² satisfies

313
$$\max_{1 \le i \le n} d_{\delta}^{(i)} \le \frac{1}{2} \quad \text{and} \quad \min_{1 \le i \le k} \lambda_2(L_i) \ge 1$$

314 Let $\{V^{(j)}\}_{j=1}^k$ be another partition of V. We aim to show

315
$$\operatorname{RatioCut}\left(\{V_i\}_{i=1}^k\right) \leq \operatorname{RatioCut}\left(\left\{V^{(j)}\right\}_{j=1}^k\right)$$

316 Let $n_i = |V_i|$, $n^{(j)} = |V^{(j)}|$ and $m_i^{(j)} = |V_i \cap V^{(j)}|$. We have

317
$$\sum_{i} m_{i}^{(j)} = n^{(j)}, \quad \sum_{j} m_{i}^{(j)} = n_{i}.$$

318 Let

319
$$W_{i,i'}^{(j,j')} = \sum_{v_k \in V_i \cap V^{(j)}, v_l \in V_{i'} \cap V^{(j')}} w_{kl}.$$

Thus we have divided the weighted adjacency matrix W into $k^2 \times k^2$ rectangular areas and $W_{i,i'}^{(j,j')}$ is the total weight in one of the areas. Lemma 2.1 gives

322 (4.1)
$$\sum_{j' \neq j} W_{i,i}^{(j,j')} \ge \min_{1 \le a \le k} \lambda_2(L_a) \frac{m_i^{(j)}(n_i - m_i^{(j)})}{n_i} \ge \frac{m_i^{(j)}(n_i - m_i^{(j)})}{n_i}$$

323 for all i, j. We also know each $d_{\delta}^{(i)}$ is at most 1/2. This implies

324 (4.2)
$$\sum_{i'\neq i} W_{i,i'}^{(j,j)} + \sum_{j'\neq j} \sum_{i'\neq i} W_{i,i'}^{(j,j')} = \sum_{j'} \sum_{i'\neq i} W_{i,i'}^{(j,j')} \le \frac{1}{2} m_i^{(j)}$$

325 for all i, j. Moreover

326 (4.3)
$$\sum_{i' \neq i} W_{i,i'}^{(j,j)} \le \frac{1}{2} \min\{m_i^{(j)}, n^{(j)} - m_i^{(j)}\}$$

for all i, j because the summands together represent a rectangular area in W with length $m_i^{(j)}$ and width $n^{(j)} - m_i^{(j)}$. Therefore we need to show

329 RatioCut
$$\left(\{V_i\}_{i=1}^k\right)$$
 – RatioCut $\left(\left\{V^{(j)}\right\}_{j=1}^k\right)$
330 $=\sum_j \sum_{j'} \sum_i \sum_{i' \neq i} \frac{1}{n_i} W^{(j,j')}_{i,i'} - \sum_i \sum_{j'} \sum_j \sum_{j' \neq j} \frac{1}{n^{(j)}} W^{(j,j')}_{i,i'}$
331 $=\sum_i \sum_j \sum_{i' \neq i} \frac{1}{n_i} W^{(j,j)}_{i,i'} + \sum_i \sum_j \left(\frac{1}{n_i} - \frac{1}{n^{(j)}}\right) \left(\sum_{j' \neq j} \sum_{i' \neq i} W^{(j,j')}_{i,i'}\right) - \sum_i \sum_j \sum_{j' \neq j} \frac{1}{n^{(j)}} W^{(j,j')}_{i,i'}$

$$332 = A_1 + A_2 - A_3 \le 0$$

For A_1 , 334

335

335
$$A_{1} = \sum_{i} \sum_{j} \sum_{i' \neq i} \frac{1}{n_{i}} W_{i,i'}^{(j,j)}$$
$$= \sum_{i} \sum_{j} \sum_{i' \neq i} \frac{1}{n_{i}} W_{i,i'}^{(j,j)} - \frac{1}{2} \sum_{i' \neq i} \sum_{n} \frac{1}{n_{i}} \min\{m_{i}^{(j)}, n^{(j)} - m_{i}^{(j)}\}$$

7
$$-\frac{1}{i} - \frac{1}{j} \frac{1}{i' \neq i} n_i + \frac{1}{2} \sum_{i} \sum_{j} \frac{1}{m_i} \min\{m_i^{(j)}, n^{(j)} - m_i^{(j)}\}$$

337
$$+ \frac{1}{2} \sum_{i} \sum_{j} \frac{1}{n_i} \min\{m_i^{(j)}, n^{(j)} - m_i^{(j)}\}$$

$$=A_{11} - A_{12} + A_{13}.$$

For A_2 , when $\frac{1}{n_i} - \frac{1}{n^{(j)}} \leq 0$, the summand is upper bounded by 0. When $\frac{1}{n_i} - \frac{1}{n^{(j)}} > 0$, the summand is upper bounded by (by using (4.2))

342
$$\left(\frac{1}{n_i} - \frac{1}{n^{(j)}}\right) \left(\sum_{j' \neq j} \sum_{i' \neq i} W_{i,i'}^{(j,j')}\right) \le \left(\frac{1}{n_i} - \frac{1}{n^{(j)}}\right) \left(\frac{1}{2} m_i^{(j)} - \sum_{i' \neq i} W_{i,i'}^{(j,j)}\right).$$

Therefore we can bound A_2 by 343

$$\begin{aligned} 344 \quad A_2 &= \sum_{i} \sum_{j} \left(\frac{1}{n_i} - \frac{1}{n^{(j)}} \right) \left(\sum_{j' \neq j} \sum_{i' \neq i} W_{i,i'}^{(j,j')} \right) \\ 345 \qquad \leq \sum_{i} \sum_{j} \max\left\{ \frac{1}{n_i} - \frac{1}{n^{(j)}}, 0 \right\} \left(\frac{1}{2} m_i^{(j)} - \sum_{i' \neq i} W_{i,i'}^{(j,j)} \right) \\ 346 \qquad = \sum_{i} \sum_{j} \left(\frac{1}{n_i} - \min\left\{ \frac{1}{n^{(j)}}, \frac{1}{n_i} \right\} \right) \left(\frac{1}{2} m_i^{(j)} - \sum_{i' \neq i} W_{i,i'}^{(j,j)} \right) \\ 347 \qquad \leq \frac{1}{2} \sum_{i} \sum_{j} \frac{1}{n_i} m_i^{(j)} - \sum_{i} \sum_{j} \sum_{i' \neq i} \frac{1}{n_i} W_{i,i'}^{(j,j)} - \frac{1}{2} \sum_{i} \sum_{j} \min\left\{ \frac{1}{n^{(j)}}, \frac{1}{n_i} \right\} \max\left\{ 0, 2m_i^{(j)} - n^{(j)} \right\} \end{aligned}$$

$$349 \qquad = A_{21} - A_{22} - A_{23},$$

where in the last step we used (4.3). For A_3 , we use (4.1): 350

351
$$A_3 = \sum_i \sum_j \sum_{j' \neq j} \frac{1}{n^{(j)}} W_{i,i}^{(j,j')} \ge \sum_i \sum_j \min_{1 \le a \le k} \lambda_2(L_a) \frac{m_i^{(j)}(n_i - m_i^{(j)})}{n_i n^{(j)}}$$

352 (4.4)
353
$$\geq \sum_{i} \sum_{j} \frac{m_{i}^{(j)}(n_{i} - m_{i}^{(j)})}{n_{i}n^{(j)}}.$$

Therefore (here we introduce the shorthand notation min^{*} for min $\{m_i^{(j)}, n^{(j)} - m_i^{(j)}\}$ and max^{*} 354

355 for $\max\{m_i^{(j)}, n^{(j)} - m_i^{(j)}\})$

356
$$A_{12} - A_3 \leq \sum_i \sum_j \left(\frac{1}{2n_i} \min\{m_i^{(j)}, n^{(j)} - m_i^{(j)}\} - \frac{m_i^{(j)}(n_i - m_i^{(j)})}{n_i n^{(j)}} \right)$$

357
$$= \sum_i \sum_j \left(\frac{\min^*(\min^* + \max^*)}{2n_i n^{(j)}} - \frac{m_i^{(j)}(n_i - m_i^{(j)})}{n_i n^{(j)}} \right)$$

358
$$= \sum_{i} \sum_{j} \left(\frac{\min^{*} \max^{*}}{n_{i} n^{(j)}} - \frac{\min^{*} (\max^{*} - \min^{*})}{2n_{i} n^{(j)}} - \frac{m_{i}^{(j)} (n_{i} - m_{i}^{(j)})}{n_{i} n^{(j)}} \right)$$

359
$$= \sum_{i} \sum_{j} \left(\frac{m_i^{(j)}(n^{(j)} - m_i^{(j)})}{n_i n^{(j)}} - \frac{m_i^{(j)}(n_i - m_i^{(j)})}{n_i n^{(j)}} \right) - \frac{1}{2} \sum_{i} \sum_{j} \frac{\min^*(\max^* - \min^*)}{n_i n^{(j)}}$$

360
$$= \sum_{i} \sum_{j} \left(\frac{m_i^{(j)}(n^{(j)} - n_i)}{n_i n^{(j)}} \right) - A_4$$

361
$$= \sum_{i} \sum_{j} \frac{m_i^{(j)}}{n_i} - \sum_{j} \sum_{i} \frac{m_i^{(j)}}{n^{(j)}} - A_4$$

 $= k - k - A_4 = -A_4.$

The cancellation above is the reason why the constant in the condition (2.1) is 1/2. We also 364have $A_{11} - A_{22} = 0$. Finally 365

$$\begin{aligned} &A_{1} + A_{2} - A_{3} \\ &\leq A_{21} - A_{12} - A_{4} - A_{23} \\ &aext{367} &\leq A_{21} - A_{12} - A_{4} - A_{23} \\ &aext{368} &= \frac{1}{2} \sum_{i} \sum_{j} \left(\frac{m_{i}^{(j)}}{n_{i}} - \frac{\min^{*}(\max^{*} - \min^{*})}{n_{i}} - \frac{\min^{*}(\max^{*} - \min^{*})}{n_{i}n^{(j)}} - \min\left\{\frac{1}{n^{(j)}}, \frac{1}{n_{i}}\right\} \max\left\{0, 2m_{i}^{(j)} - n^{(j)}\right\} \right) \\ &aext{369} &= \frac{1}{2} \sum_{i} \sum_{j} \left(\frac{m_{i}^{(j)}}{n_{i}} - \frac{\min^{*}(\min^{*} + \max^{*})}{n_{i}n^{(j)}} - \frac{\min^{*}(\max^{*} - \min^{*})}{n_{i}n^{(j)}} - \min\left\{\frac{1}{n^{(j)}}, \frac{1}{n_{i}}\right\} \max\left\{0, 2m_{i}^{(j)} - n^{(j)}\right\} \right) \\ &aext{370} &= \frac{1}{2} \sum_{i} \sum_{j} \left(\frac{m_{i}^{(j)}}{n_{i}} - \frac{2\min^{*}\max^{*}}{n_{i}n^{(j)}} - \min\left\{\frac{1}{n^{(j)}}, \frac{1}{n_{i}}\right\} \max\left\{0, 2m_{i}^{(j)} - n^{(j)}\right\} \right) \\ &aext{371} &= \frac{1}{2} \sum_{i} \sum_{j} \left(\frac{m_{i}^{(j)}n^{(j)}}{n_{i}n^{(j)}} - \frac{2m_{i}^{(j)}(n^{(j)} - m_{i}^{(j)})}{n_{i}n^{(j)}} - \min\left\{\frac{1}{n^{(j)}}, \frac{1}{n_{i}}\right\} \max\left\{0, 2m_{i}^{(j)} - n^{(j)}\right\} \right) \\ &aext{372} &= \frac{1}{2} \sum_{i} \sum_{j} \left(\frac{m_{i}^{(j)}(2m_{i}^{(j)} - n^{(j)})}{n_{i}n^{(j)}} - \min\left\{\frac{1}{n^{(j)}}, \frac{1}{n_{i}}\right\} \max\left\{0, 2m_{i}^{(j)} - n^{(j)}\right\} \right) \\ &aext{372} &= \frac{1}{2} \sum_{i} \sum_{j} \left(\frac{m_{i}^{(j)}(2m_{i}^{(j)} - n^{(j)})}{n_{i}n^{(j)}} - \min\left\{\frac{1}{n^{(j)}}, \frac{1}{n_{i}}\right\} \max\left\{0, 2m_{i}^{(j)} - n^{(j)}\right\} \right) \\ &aext{373} &\leq 0. \end{aligned}$$

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The last step is because for each summand, 375

376
$$\frac{m_i^{(j)}}{n_i n^{(j)}} \le \min\left\{\frac{1}{n^{(j)}}, \frac{1}{n_i}\right\}$$

This concludes the proof that $\{V_i\}_{i=1}^k$ achieves the minimum ratio cut. To show that it is also 377 the unique global minimum when the strict inequality holds, we assume $\{V_i\}_{i=1}^k$ satisfies 378

379
$$\max_{1 \le i \le n} d_{\delta}^{(i)} \le \frac{1}{2} \quad \text{and} \quad \min_{1 \le i \le k} \lambda_2(L_i) > 1.$$

All claims above still hold but we will show (4.4) holds with the strict inequality. Since 380 $\min_{1 \le i \le k} \lambda_2(L_i) > 1$, the last inequality in (4.4) takes equal sign if and only if $m_i^{(j)}(n_i - m_i^{(j)}) = 0$ 3810 for all i, j. But this is impossible if $\{V^{(j)}\}_{j=1}^{k}$ is not a relabeling of $\{V_i\}_{i=1}^{k}$. Therefore if 382 $\left\{V^{(j)}\right\}_{i=1}^{k}$ is not a relabeling of $\left\{V_{i}\right\}_{i=1}^{k}$, we have 383

384
$$A_1 + A_2 - A_3 < 0$$

which concludes the proof. 385

4.2. Proofs for Section 2.2. We need the following two lemmas to prove Theorem 2.6. 386 For a linear transformation T on a finite dimensional vector space, $\lambda_{\max}(T)$ and $\lambda_{\min}(T)$ 387 denote the largest and the smallest eigenvalue of T, respectively. 388

Lemma 4.1. Let T be an $n \times n$ matrix such that $||T||_{\infty} \leq 1$. Then 389

$$||x - T^k x||_{\infty} \le k||x - Tx||_{\infty}$$

for all $x \in \mathbb{C}^n$ and $k \in \mathbb{N}$. 391

Proof. We have 392

393
$$||x - T^n x||_{\infty} \le ||x - Tx||_{\infty} + ||Tx - T^2 x||_{\infty} + \ldots + ||T^{k-1}x - T^k x||_{\infty}$$

 $\leq \|x - Tx\|_{\infty} + \|Tx - T^{2}x\|_{\infty} + \ldots + \|T^{\kappa-1}x - T^{\kappa}x\|_{\infty}$ = $\|x - Tx\|_{\infty} + \|T(x - Tx)\|_{\infty} + \ldots + \|T^{k-1}(x - Tx)\|_{\infty} \leq k\|x - Tx\|_{\infty},$ 394

where the last inequality follows from $||T||_{\infty} \leq 1$. 395

Lemma 4.2. Let T be a self-adjoint $n \times n$ matrix, $n \geq 3$, such that $||T||_{\infty} \leq 1$. Let \mathcal{M} be 396 a subspace of \mathbb{C}^n such that $T\mathcal{M} \subset \mathcal{M}$. Then 397

398
$$||x - Tx||_{\infty} \ge \frac{(1 - \lambda_{\max}(T|_{\mathcal{M}}))||x||_{\infty}}{2\ln n}$$

for all $x \in \mathcal{M}$. 399

Proof. We may assume that T is positive semidefinite. Indeed, $\frac{I+T}{2}$ is positive semidefinite, 400 and if the result holds with T being replaced by $\frac{I+T}{2}$, the result will hold for T. 401

Since T is positive semidefinite, 402

403
$$||T^k x||_2 \le \lambda_{\max}(T|_{\mathcal{M}})^k ||x||_2,$$

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for all $x \in \mathcal{M}$ and $k \in \mathbb{N}$. So $||T^k x||_{\infty} \leq \lambda_{\max}(T|_{\mathcal{M}})^k \sqrt{n} ||x||_{\infty}$ and hence, by Lemma 4.1, 404

405
$$||x||_{\infty} - \lambda_{\max}(T|_{\mathcal{M}})^k \sqrt{n} ||x||_{\infty} \le k ||x - Tx||_{\infty},$$

406

for all $x \in \mathcal{M}$ and $k \in \mathbb{N}$. If k is large enough so that $\lambda_{\max}(T|_{\mathcal{M}})^k \sqrt{n} \leq \frac{1}{2}$, then $||x - Tx||_{\infty} \geq \frac{1}{2k} ||x||_{\infty}$. Since $||T||_{\infty} \leq 1$, we have $\lambda_{\max}(T|_{\mathcal{M}}) \leq 1$. Note that $\lambda \leq e^{\lambda - 1}$ for all $\lambda \leq 1$. So 407 $\lambda_{\max}(T|_{\mathcal{M}})^k \sqrt{n} \le e^{k(\lambda_{\max}(T|_{\mathcal{M}})-1)} \sqrt{n} \le \frac{1}{2} \text{ for } k \ge \frac{\ln(2\sqrt{n})}{1-\lambda_{\max}(T|_{\mathcal{M}})}.$ Taking k to be the smallest 408 integer larger than or equal to $\frac{\ln(2\sqrt{n})}{1-\lambda_{\max}(T|_{\mathcal{M}})}$, we obtain 409

410
$$||x - Tx||_{\infty} \ge \frac{1}{2k} ||x||_{\infty} \ge \frac{(1 - \lambda_{\max}(T|_{\mathcal{M}})) ||x||_{\infty}}{2\ln n}$$

411 if $n \ge 30$. If $3 \le n \le 29$, then

412
$$||x - Tx||_{\infty} \ge \frac{1}{\sqrt{n}} ||x - Tx||_{2} \ge \frac{1}{\sqrt{n}} (1 - \lambda_{\max}(T|_{\mathcal{M}})) ||x||_{2} \ge \frac{(1 - \lambda_{\max}(T|_{\mathcal{M}})) ||x||_{\infty}}{2\ln n}$$

for all $x \in \mathcal{M}$. 413

416

Proof of Theorem 2.6. Without loss of generality, we may assume that $B_{i,i} \leq 1$ for all 414 $1 \leq i \leq n$. For every $1 \leq i \leq n$, 415

$$\sum_{j=1} |(I-B)_{i,j}| = 1 - B_{i,i} + \sum_{j \in \{1,\dots,n\} \setminus \{i\}} |B_{i,j}| \le 1 - B_{i,i} + B_{i,i} \le 1.$$

417 So $||I - B||_{\infty} \leq 1$. By Lemma 4.2, we have

n

418
$$||Bx||_{\infty} = ||x - (I - B)x||_{\infty} \ge \frac{(1 - \lambda_{\max}((I - B)|_{\mathcal{M}}))||x||_{\infty}}{2\ln n} = \frac{\lambda_{\min}(B|_{\mathcal{M}})||x||_{\infty}}{2\ln n}$$

for all $x \in \mathcal{M}$. 419

Proof of Corollary 2.7. Since $L\mathbb{1}_n = 0$ and L is self-adjoint, $L\{\mathbb{1}_n\}^{\perp} \subset \{\mathbb{1}_n\}^{\perp}$. By 420 Theorem 2.6, 421

422
$$||Lx||_{\infty} \ge \frac{\lambda_{\min}\left(L|_{\{1_n\}^{\perp}}\right)||x||_{\infty}}{2\ln n} = \frac{\lambda_2(L)||x||_{\infty}}{2\ln n},$$

for all $x \perp \mathbb{1}_n$. This proves one inequality. 423

To prove the other inequality, pick a vertex u_0 . Let $y \in \mathbb{C}^n$ be given by $y(v) = d(u_0, v)$, 424 for vertices v, where d is the graph distance. Then 425

426
$$(Ly)(v) = \deg(v)d(u_0, v) - \sum_{w \in N(v)} d(u_0, w),$$

for all vertex v, where N(v) is the set of all neighborhood vertices of v. Since $|d(u_0, v)|$ -427

 $d(u_0, w)| \leq 1$ for all $w \in N(v)$, we have $|(Ly)(v)| \leq \deg(v)$ for all vertex v. So $||Ly||_{\infty} \leq M$. 428 Let $z = y - (\frac{1}{n} \sum_{v} y(v)) \mathbb{1}_n \in \mathbb{C}^n$, where the sum is over all vertices v. It is easy to 429see that there exists a vertex w such that $d(u_0, w) \geq \frac{D}{2}$, where D is the diameter. So 430

431 $|z(w) - z(u_0)| = |y(w) - y(u_0)| = |d(u_0, w) - 0| = d(u_0, w) \ge \frac{D}{2}$. Thus, $||z||_{\infty} \ge \frac{D}{4}$. Since 432 $L\mathbb{1}_n = 0$, we have $||Lz||_{\infty} = ||Ly||_{\infty} \le M$. Therefore,

$$\inf_{x \perp \mathbb{1}_n} \frac{\|Lx\|_{\infty}}{\|x\|_{\infty}} \le \frac{M}{D/4} = \frac{4M}{D}.$$

434 The result follows.

435 With the help of Corollary 2.7, we can prove Theorem 2.4.

436 **Proof of Theorem 2.4.** We use the same notation as Lemma 2.5. Note that $||U_{iso}||_{2,\infty} =$ 437 $\max_{1 \le i \le k} 1/\sqrt{|V_i|}$ so $\mu = \sqrt{c}$. By Corollary 2.7 and (2.3) we have

438
$$\operatorname{gap} \ge \min_{1 \le i \le k} \frac{\lambda_2(L_i)}{2 \ln |V_i|} \ge \frac{\min_{1 \le i \le k} \lambda_2(L_i)}{2 \ln n}$$

439 If

433

439 II
440
$$r = \frac{\max_{1 \le i \le n} d_{\delta}^{(i)}}{\min_{1 \le i \le k} \lambda_2(L_i)} \le \frac{1}{16(1+c)\ln n},$$

441 then

442
$$||L_{\delta}||_{\infty} = 2 \max_{1 \le i \le n} d_{\delta}^{(i)} \le \frac{\text{gap}}{4(1+\mu^2)}$$

443 and

444
$$||L_{\delta}||_{2} \leq \sqrt{||L_{\delta}||_{\infty} ||L_{\delta}||_{1}} = ||L_{\delta}||_{\infty} = 2 \max_{1 \leq i \leq n} d_{\delta}^{(i)} \leq \frac{\operatorname{gap}}{5}.$$

445 Therefore by Lemma 2.5 we have

446
$$\min_{V \in \mathbf{O}^{k}} ||UV - U_{\rm iso}||_{2,\infty} \leq 8 \, ||U_{\rm iso}||_{2,\infty} \left(\frac{||L_{\delta}||_{2}}{\operatorname{sep}_{2}(\Lambda_{1},\Lambda_{2})}\right)^{2} + 4 \frac{\left|\left|U_{2}U_{2}^{T}L_{\delta}U_{\rm iso}\right|\right|_{2,\infty}}{\operatorname{gap}}$$

$$\leq 8 \sqrt{\frac{c}{c}} \left(\frac{2 \max_{1 \leq i \leq n} d_{\delta}^{(i)}}{\delta}\right)^{2} + \frac{8 \ln n \left|\left|U_{2}U_{2}^{T}L_{\delta}U_{\rm iso}\right|\right|_{2,\infty}}{8 \ln n \left|\left|U_{2}U_{2}^{T}L_{\delta}U_{\rm iso}\right|\right|_{2,\infty}}$$

447
$$\leq 8\sqrt{\frac{c}{n}} \left(\frac{2 \max_{1 \leq i \leq n} u_{\delta}}{\min_{1 \leq i \leq k} \lambda_2(L_i)}\right) + \frac{1122}{\min_{1 \leq i \leq k} \lambda_2(L_i)}$$

$$1 \qquad 8 \ln n ||U_2 U_2^T L_{\delta} U_{iso}||_2$$

448
449
$$= 32\sqrt{c}r^2 \frac{1}{\sqrt{n}} + \frac{\sin n || C_2 C_2 L_0 C_{150} ||_{2,\infty}}{\min_{1 \le i \le k} \lambda_2(L_i)},$$

450 where we have used (2.2) in the second step. Finally

451
$$\left| \left| U_2 U_2^T L_{\delta} U_{\text{iso}} \right| \right|_{2,\infty} = \left| \left| (I - U_{\text{iso}} U_{\text{iso}}^T) L_{\delta} U_{\text{iso}} \right| \right|_{2,\infty}$$

452
$$= \left| \left| L_{\delta} U_{\text{iso}} - U_{\text{iso}} U_{\text{iso}}^T L_{\delta} U_{\text{iso}} \right| \right|_{2,\infty}$$

453
$$\leq \left(\left| \left| L_{\delta} \right| \right|_{\infty} + \left| \left| U_{\text{iso}}^T L_{\delta} U_{\text{iso}} \right| \right|_2 \right) \left| \left| U_{\text{iso}} \right| \right|_{2,\infty} \right)$$

454
$$\leq (||L_{\delta}||_{\infty} + ||L_{\delta}||_{2}) ||U_{\text{iso}}||_{2,\infty}$$

$$455 \\ 456 \leq 4\sqrt{\frac{c}{n}} \max_{1 \leq i \leq n} d_{\delta}^{(i)}.$$

457 Hence

458
$$\min_{V \in \mathbf{O}^k} ||UV - U_{\rm iso}||_{2,\infty} \le 32\sqrt{c} \left(r^2 + r \ln n\right) \frac{1}{\sqrt{n}}$$

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459 **4.3. A lemma for Section 3.**

460 Lemma 4.3. Let $c_1, c_2 \in \mathbb{R}^n$ such that $||c_1 - c_2||_2 = d$. For any $x \in B_{c_1}(r)$ and $y \in$ 461 $B_{c_2}(r)$ let M be the (n-1)-dimensional bisecting hyperplane that passes through $\frac{x+y}{2}$ and is 462 perpendicular to the line segment that joins x and y. Then

463
$$\operatorname{dist} \{M, B_{c_1}(r) \cup B_{c_2}(r)\} \ge \frac{1}{2}d - 3r.$$

464 *Proof.* By symmetry, it suffices to show dist $\{M, B_{c_1}(r)\} \ge \frac{1}{2}d - 3r$. We may suppose 465 $c_1 = 0$ and d > 6r. Then it suffices to show dist $\{M, 0\} \ge \frac{1}{2}d - 2r$. For any $z \in M$ we have

466
$$\sum_{i=1}^{n} (x_i - y_i) \left(z_i - \frac{x_i + y_i}{2} \right) = 0$$

467 By the point-plane distance formula

468
$$\operatorname{dist} \{M, 0\} = \frac{\left|\sum_{i=1}^{n} (x_i^2 - y_i^2)\right|}{2\sqrt{\sum_{i=1}^{n} (x_i - y_i)^2}} = \frac{||y||_2^2 - ||x||_2^2}{2||x - y||_2}$$

469
470
471

$$\geq \frac{(d-r)^{2}-r}{2(d+2r)}$$

$$= \frac{1}{2}d - \frac{2dr}{d+2r}$$

$$\geq \frac{1}{2}d - 2r$$

$$\frac{171}{172} \ge \frac{1}{2}d - 2r.$$

473

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