To appear in *Linear and Multilinear Algebra*
Vol. 00, No. 00, Month 20XX, 1–9

On the Maximal Error of Spectral Approximation of Graph Bisection

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(*Received 00 Month 20XX; final version received 00 Month 20XX*)

Spectral graph bisections are a popular heuristic aimed at approximating the solution of the NP-complete graph bisection problem. This technique, however, does not always provide a robust tool for graph partitioning. Using a special class of graphs, we prove that the standard spectral graph bisection can produce bisections that are far from optimal. In particular, we show that the maximum error in the spectral approximation of the optimal bisection (partition sizes exactly equal) cut for such graphs is bounded below by a constant multiple of the order of the graph squared.

Keywords: graph Laplacian; Fiedler vector; spectral bisection

AMS Subject Classification: 05C40, 05C50

1. Introduction and preliminaries

A graph bisection is a partition of the vertex set into two parts of equal order, thereby creating two subgraphs. A bisection is considered good if the number of edges between the two partitions is small. Finding the graph bisection that minimizes the number of edges between the two partitions is NP-complete [7]. Despite this, graph bisections have found application in scientific computing, VLSI design, and task scheduling [10, 11]. A variety of heuristic algorithms have been implemented in an attempt to approximate the optimal graph bisection. One of the most popular techniques approximates the optimal cut via the zero level set of the discrete Laplacian eigenvector corresponding to the smallest non-zero eigenvalue. Naturally, such technique is called a spectral bisection. The efficient construction and the properties of spectral bisections is and has been an active area of research [19, 20, 22]. Experiments have shown that this technique works well in practice, and it has been proven that spectral bisection works well on bounded degree planar graphs and finite element meshes [21]. For general graphs, however, this is not the case, and, in what follows, we show that spectral bisection is not a robust technique for approximating the optimal cut. In particular, we construct a special class of

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†The work of this author was supported in part by NSF DMS-1217142 and NSF DMS-1418843.

graphs for which the maximum error in the spectral approximation of the optimal bisection is bounded below by a constant multiple of the order squared.

We begin the technical discussion by briefly introducing notation and definitions from graph theory, referring the readers to [3] for details. Let $G = (V, E)$, $n = |V|$, $n_E = |E|$, be a simple, connected, undirected graph. The graph Laplacian associated with G is the matrix $L(G)$, defined via the following bilinear form

$$\langle L(G)u, v\rangle = \sum_{j=1}^{n} \sum_{k\in N(j)} (u_i - u_j)(v_i - v_j), \quad \forall u,\ v \in \mathbb{R}^n.$$

Here, $\langle\cdot,\cdot\rangle$ is the standard Euclidean scalar product on $\mathbb{R}^n$, and $N(i)$ is the set of neighbors of $i \in V$; namely, $N(i) = \{j \in V \mid (i,j) \in E\}$. Note that

$$[L(G)]_{ij} = -1, \text{ when } (i,j) \in E; \quad [L(G)]_{ij} = 0, \text{ when } (i,j) \notin E, \text{ and } i \neq j;$$
$$[L(G)]_{ii} = -\sum_{j\in N(i)} [L(G)]_{ij}.$$

In the following, we denote the eigenvalues of $L(G)$ by $\lambda_1(G) \le \lambda_2(G), \ldots \le \lambda_n(G)$ and the corresponding set of $\ell^2(\mathbb{R}^n)$-orthogonal eigenvectors by $\varphi_1(G), \varphi_2(G), \ldots, \varphi_n(G)$. We have that $\lambda_1 = 0$ and $\varphi_1(G) = (\underbrace{1,\ldots,1}_{n})^T =: \mathbf{1}_n$ for all graphs, and that $\lambda_2(G) > 0$ for all connected graphs G. The eigenvalue $\lambda_2(G)$ is known as the *algebraic connectivity* of G, denoted by $a(G)$. The eigenvector $\varphi_2(G)$ is known as the Fiedler vector, or *characteristic valuation* of G [4–6]. When $a(G)$ is a repeated eigenvalue of multiplicity k, the Fiedler vectors lie in the k-dimensional eigenspace corresponding to $a(G)$, denoted here by $E_{\lambda_2}[L(G)]$. When G is clear from the context, we will omit the argument "(G)" in $\lambda_k(G)$, $\varphi_k(G)$ and simply write λ_k and φ_k.

Further, by $\mathbf{1}_W$ we denote the indicator vector (function) of a set. For a subset $W \subset V$ this function is defined as follows

$$\mathbf{1}_W \in \mathbb{R}^n, \quad [\mathbf{1}_W]_k = \begin{cases} 1, & k \in W, \\ 0, & k \notin W. \end{cases}, \quad \mathbf{1}_n = \mathbf{1}_{\{1,\ldots,n\}}.$$

We recall the usual definition of a median value $M(v)$ for $v \in \mathbb{R}^n$. If w is a nondecreasing rearrangment of v, that is, there exists a permutation π such that $w = \pi v$ and $w_1 \le w_2 \le \ldots \le w_n$, then

$$M(v) = \begin{cases} w_m, & n = 2m-1, \\ \frac{1}{2}(w_m + w_{m+1}), & n = 2m. \end{cases}$$

The set of all cuts of G is identified with the set of decompositions of the set of vertices V as a union of $W \subset V$ and its complement $W^c \subset V$, isomorphic to the set of vectors $v \in \mathbb{R}^n$ such that $v_k \in \{-1, 1\}$, $k = 1 : n$. For a vector $v \in \mathbb{R}^n$, its median cut is defined as corresponding to the vector $C_M(v)$, where

$$C_M(v) = \mathbf{1}_W - \mathbf{1}_{W^c}, \quad W = \{k \mid v_k > M(v)\}.$$

Adopting notation from [21], we consider the graph partitioning problem, that is, partitioning V into two disjoint sets S and S^c, $S \cup S^c = V$, where $|S| \approxeq |S^c|$, such that the edge cut (number of the edges with one vertex in S and one in S^c) is minimized. In the notation we just introduced, this is equivalent to

$$S = \arg\min\{F(W) \mid W \subsetneq V,\ W \neq \emptyset\},$$
$$F(W) = \frac{1}{2}\langle L(G)(\mathbf{1}_W - \mathbf{1}_{W^c}), \mathbf{1}_W - \mathbf{1}_{W^c}\rangle.$$

The relation $|S| \approxeq |S^c|$ quite ambiguous, and one of the most common approaches to resolve this is to minimize over the sets $|W| = \left\lfloor \frac{n}{2} \right\rfloor$. In what follows, we will refer to this as a *bisection.* An alternative is to minimize the cut ratio function, given by

$$\phi(W) = \frac{F(W)}{\min\{|W|, |W^c|\}},$$

which we refer to as a *cut ratio partition.* Finding the minimizing bisection and cut ratio partition of a graph are both NP-complete problems [7]. In what follows, we consider solely the graph bisection problem. For more on the cut ratio partition, we refer readers to [24, 25].

Numerous techniques have been devised and aimed at approximating the optimal solution in polynomial time and are currently used in graph-partitioning software [10, 11]. Some of the techniques involve the use of a Fiedler vector of the graph Laplacian [19, 20, 22]. Miroslav Fiedler, [4–6], proved many results about algebraic connectivity and its associated eigenvector. General results regarding the graph Laplacian and its spectrum can be found in [13–18]. Following Fiedler [4, 5], for $x \in \mathbb{R}^n$ we define

$$i_+(x) := \{i | x_i > 0\}, \quad i_-(x) := \{i | x_i < 0\}, \quad i_0(x) = \{i | x_i = 0\}.$$

For a graph G, $i_0(\varphi_2 - M(\varphi_2)\mathbf{1}) = \emptyset$, the bisection via a Fiedler vector φ_2 is given by

$$S = i_+(\varphi_2 - M(\varphi_2)\mathbf{1}), \quad S^c = i_-(\varphi_2 - M(\varphi_2)\mathbf{1}).$$

Techniques of this form are called spectral bisections. The approximation can be seen by noting that minimizing the Rayleigh quotient of the Laplacian over integer vectors is equivalent to minimizing the edge cut of the corresponding partition (see, e.g. [1, 12]). We note that the case when $i_0(\varphi_2 - M(\varphi_2)\mathbf{1})$ is non-empty is more complicated and still provides a bisection, depending on how the zero valuated vertices in $(\varphi_2 - M(\varphi_2)\mathbf{1})$ are distributed between S and S^c. For more details on such special cases, we refer to [23].

2. Comparison: spectral bisection and optimal bisection

In this section we show how far from optimal a spectral bisection can be. We note that the area of cut quality has been studied previously. Spielman and Teng showed that spectral partitioning performs well for bounded degree planar graphs [21]. Guattery and Miller produced a class of graphs for which the error in cut quality of a spectral bisection is bounded below by a constant multiple of the order of the graph. In addition, they found estimates for how poorly spectral techniques can perform in the cut ratio partition [8, 9]. By contrast, our focus is solely on the bisection problem, and we aim to produce a lower bound of a constant multiple of the order squared.

We introduce a special graph Laplacian and calculate a spectral decomposition for it. Given $n = 4m$, $m > 0$, we define

$$L_* = \begin{pmatrix} I & -I & 0 & 0 \\ -I & (m+1)I & -\mathbf{1}\mathbf{1}^T & 0 \\ 0 & -\mathbf{1}\mathbf{1}^T & (m+1)I & -I \\ 0 & 0 & -I & I \end{pmatrix}.$$

To avoid the proliferation of indices here and in what follows, we set $\mathbf{1} = \mathbf{1}_m$. To describe the eigenbasis of L_*, we use the tensor product, defined as follows:

$$\mathrm{I\!R}^{pr\times qs} \ni a \otimes b = \begin{pmatrix} a_{11}b & \dots & a_{1q}b \\ \vdots & \vdots & \vdots \\ a_{p1}b & \dots & a_{pq}b \end{pmatrix}, \quad a \in \mathrm{I\!R}^{p\times q}, \quad b \in \mathrm{I\!R}^{r\times s}.$$

Simple calculations show that the eigen-decomposition for L_* is as follows:

1. One simple 0 eigenvalue with eigenvector $\mathbf{1}_n = (1,1,1,1)^T \otimes \mathbf{1}$.
2. Two simple eigenvalues $\lambda_\pm = m + 1 \pm \sqrt{m^2+1}$ with eigenvectors

$$\phi_\pm = (1, (1-\lambda_\pm), (\lambda_\pm - 1), -1)^T \otimes \mathbf{1}.$$

3. Two repeated eigenvalues $\mu_\pm = \dfrac{m}{2} + 1 \pm \sqrt{\left(\dfrac{m}{2}\right)^2 + 1}$, each of which has a eigenspace of dimension $(2m-2)$ with a basis

$$\begin{aligned} \psi_k^- &= (1, (1-\mu_-), 0, 0)^T \otimes \xi_k, \quad k = 1:m-1, \\ \psi_{k+m-1}^- &= (0, 0, (1-\mu_-), 1)^T \otimes \xi_k, \quad k = 1:m-1, \\ \psi_k^+ &= (1, (1-\mu_+), 0, 0)^T \otimes \xi_k, \quad k = 1:m-1, \\ \psi_{k+m-1}^+ &= (0, 0, (1-\mu_+), 1)^T \otimes \xi_k, \quad k = 1:m-1. \end{aligned}$$

   Here $\{\xi_k\}_{k=1}^{m-1}$ is a basis in $[\mathrm{span}\{\mathbf{1}\}]^\perp$.
4. One eigenvalue equal to 2 with eigenvector

$$\phi_2 = (1, -1, -1, 1)^T \otimes \mathbf{1}.$$

We now consider a family of graphs for which the cut produced by spectral bisection and the optimal bisection are "far" from each other. We consider four connected undirected graphs, G_k, $k = 1:4$, each with m vertices and corresponding graph Laplacians L_k, $k = 1:4$. Let $G_0 = G_1 + G_2 + G_3 + G_4$ be the disjoint union of these graphs and note that G_0 is a disconnected graph. Let L_0 be the graph Laplacian associated with G_0. We now consider the graph G (see Figure 1) with Laplacian

$$L = L_0 + L_* = \begin{pmatrix} L_1 + I & -I & 0 & 0 \\ -I & L_2 + (m+1)I & -\mathbf{1}\mathbf{1}^T & 0 \\ 0 & -\mathbf{1}\mathbf{1}^T & L_3 + (m+1)I & -I \\ 0 & 0 & -I & L_4 + I \end{pmatrix}. \quad (1)$$

The key concept in the construction of G is that the obvious best choice of $(1,-1,-1,1)^T \otimes \mathbf{1}$ results in a bisection in which one of the resulting graphs is disconnected. A main result of Fiedler shows that graphs generated by $i_+(\varphi_2) \cup i_0(\varphi_2)$ and $i_-(\varphi_2) \cup i_0(\varphi_2)$ are necessarily connected [5, 23]. This result implies that $(1,-1,-1,1)^T \otimes \mathbf{1}$ cannot be induced by a Fiedler vector.

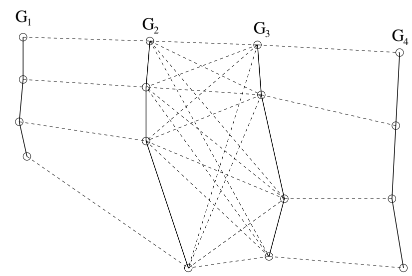

Figure 1. Example of 4 graphs connected using G_*

We note that we have $\mathrm{Ker}(L_0) = \mathcal{W}_0 \oplus \mathrm{span}\{\mathbf{1}_n\}$, where

$$\mathcal{W}_0 = \mathrm{span}\{\phi_-, \phi_+, \phi_2\}.$$

We then have the decomposition

$$\mathbb{R}^n = \mathrm{span}\{\mathbf{1}_n\} \oplus \mathcal{W}_0 \oplus \mathcal{W}_1,$$

where

$$\mathcal{W}_1 = \mathrm{span}\{\psi_k^-, \psi_k^+\}_{k=1}^{2m-2} = \mathrm{Ker}(L_0)^\perp.$$

Obviously, we have that $\mathrm{Ker}(L)^\perp = \mathcal{W}_0 \oplus \mathcal{W}_1$ and that $\mathcal{W}_0$ and $\mathcal{W}_1$ are orthogonal. The following lemma relates the algebraic connectivity $a(G)$ and the eigenvalues of L_* under certain conditions.

Lemma 2.1 *Let $a(G_k)$ be the algebraic connectivity of G_k, $k = 1:4$. Assume that $a(G_k) \geq \lambda_- - \mu_-$ for all $k = 1:4$. Then $a(G) = \lambda_-$, and the corresponding Fiedler vector is ϕ_-.*

Proof. Because $\mathcal{W}_0$ and $\mathcal{W}_1$ are invariant subspaces, we necessarily have that the subspace of Fiedler vectors is contained in exactly one of the two spaces. We have that

$$\begin{aligned} \min_{\varphi \in \mathcal{W}_1} \frac{\langle L\varphi, \varphi \rangle}{\langle \varphi, \varphi \rangle} &\geq \min_{\varphi \in \mathcal{W}_1} \frac{\langle L_0\varphi, \varphi \rangle}{\langle \varphi, \varphi \rangle} + \min_{\varphi \in \mathcal{W}_1} \frac{\langle L_*\varphi, \varphi \rangle}{\langle \varphi, \varphi \rangle} \\ &\geq [\min_{1 \leq k \leq 4} a(G_k)] + \mu_- > \lambda_- - \mu_- + \mu_- = \lambda_-. \end{aligned}$$

Noting that

$$\min_{\varphi \in \mathcal{W}_0} \frac{\langle L\varphi, \varphi \rangle}{\langle \varphi, \varphi \rangle} = \min_{\varphi \in \mathcal{W}_0} \frac{\langle L_* \varphi, \varphi \rangle}{\langle \varphi, \varphi \rangle} = \lambda_-,$$

the desired result follows. □

It is easy to estimate that for $m \geq 2$

$$0 < \lambda_- - \mu_- \leq \sqrt{\frac{m^2}{4} + 1} - \frac{m}{2} = \frac{1}{\sqrt{\frac{m^2}{4} + 1} + \frac{m}{2}} < \frac{1}{m}.$$

There are many examples of graphs for which $a(G) \geq \frac{1}{m}$, including the path graph P_m, the cycle graph C_m, the complete graph K_m, the bipartite complete graph $K_{p,q}$, and the n-dimensional cube Q_m [2]. We give the following lemma, which can be quickly verified and will be useful in proving the main theorem of the paper.

LEMMA 2.2 *Let L be the Laplacian of some simple, connected, undirected graph $G = (V, E)$, with eigenvalues λ_k and eigenvectors φ_k, $k = 1, \ldots, n$. Let $\widehat{G} = (\widehat{V}, \widehat{E})$ be the graph obtained from G by adding one vertex to V and connecting it with every vertex in G, namely, $\widehat{V} = V \cup \{n+1\}$ and $\widehat{E} = E \cup \{(1, n+1), \ldots, (n, n+1)\}$. Then $L(\widehat{G})$ has eigenvalues $\widehat{\lambda}_1 = 0$, $\widehat{\lambda}_k = \lambda_k + 1$, $k = 2, \ldots, n$, $\widehat{\lambda}_{n+1} = n + 1$ and the corresponding eigenvectors are $\widehat{\varphi}_1 = \begin{pmatrix} \varphi_1 \\ 1 \end{pmatrix}$, $\widehat{\varphi}_k = \begin{pmatrix} \varphi_k \\ 0 \end{pmatrix}$, $k = 2, \ldots, n$, and $\widehat{\varphi}_{n+1} = \begin{pmatrix} \varphi_1 \\ -n \end{pmatrix}$.*

Proof. By construction, the graph Laplacian corresponding to $\widehat{G}$ is

$$\widehat{L} = \begin{pmatrix} L + I & -\mathbf{1} \\ -\mathbf{1}^T & \langle \mathbf{1}, \mathbf{1} \rangle \end{pmatrix}.$$

Verifying that $\widehat{L}\widehat{\varphi}_k = \widehat{\lambda}_k \widehat{\varphi}_k$ for $k = 1, \ldots, (n+1)$ is rather straightforward. This concludes the proof. □

From Lemmas 2.1 and 2.2, the following theorem regarding maximum spectral approximation error quickly follows.

THEOREM 2.3 *Let $\mathcal{G}_n$ be the set of simple, connected, undirected graphs of order n, $n > 48$. Then the maximum spectral approximation error over all graphs $G \in \mathcal{G}_n$ of the bisection has bounds*

$$\frac{n^2}{384} < \max_{G \in \mathcal{G}_n} \Big| \min_{y \in E_{\lambda_2}[L]} F(i_+(y - M(y)\mathbf{1})) - \min_{A \subset V, |A| = \lfloor \frac{n}{2} \rfloor} F(A) \Big| < \frac{n^2}{2}.$$

Proof. Suppose we have $n = 4m$ for some integer m. Let us choose $G \in \mathcal{G}_n$ such that $L(G)$ corresponds to the Laplacian $L = L_0 + L_*$, with $a(G_k) \geq \lambda_- - \mu_-$, $k = 1:4$. This gives us $a(G) = m+1-\sqrt{m^2+1}$, with corresponding Fiedler vector $y = (1, (1-a(G)), (a(G)-1), -1)^T \otimes \mathbf{1}$. We have

$$F(i_+(y - M(y)\mathbf{1})) = F(i_+(y)) = m^2 = \frac{n^2}{16}.$$

We now consider the bisection induced by the vector $v = (1, -1, -1, 1)^T \otimes \mathbf{1}$. We have

$$F(i_+(v - M(v)\mathbf{1})) = F(i_+(v)) = 2m = \frac{n}{2}.$$

Now suppose $n \neq 4m$ for some integer m. Let $k = n \mod 4$, so that $n = 4m + k$. Using the same graph $G \in \mathcal{G}_{4m}$ as before, let us now add k vertices sequentially, with each addition adjacent to every current vertex in the graph, as in Lemma 2.2. By Lemma 2.2, the Fiedler vector remains unchanged, with zeros in the entries of the added vertices.

In this case we have $i_0(y)$ non-empty. However, irrespective of how we choose to distribute these vertices, we still have similar bounds on the cut. The cut with respect to y must necessarily increase. For the vector $\tilde{v} = \begin{pmatrix} v \\ 0 \end{pmatrix}$, we have the upper bound

$$F(i_+(\tilde{v}) \cup U) < \frac{(k+1)n}{2} \leq 2n,$$

where $U \subset i_0(\tilde{v})$.

Looking at both cases together, with $\tilde{v} = v$ for $k = 0$, we have

$$\begin{aligned} |F(i_+(y) \cup U_1) - \min_{A \subset V, |A| = \lfloor \frac{n}{2} \rfloor} F(A)| &\geq |F(i_+(y) \cup U_1) - F(i_+(\tilde{v}) \cup \tilde{U}_1)| \\ &\geq |\frac{n^2}{16} - 2n| > |\frac{n^2}{16} - \frac{n^2}{24}| = \frac{n^2}{384} \end{aligned}$$

for any $U_1 \subset i_0(y)$, $\tilde{U}_1 \subset i_0(\tilde{v})$. That completes the lower bound. The upper bound results from considering an upper bound on the size of the graph. □

Acknowledgments

The authors would like to thank Louisa Thomas for improving the style of presentation.

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