IMPROVEMENTS ON SPECTRAL BISECTION

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Abstract. We investigate combinatorial properties of certain configurations of a graph partition which are related to the minimality of a cut. We show that such configurations are related to the third eigenvector of the Laplacian matrix. It is well known that the second eigenvector encodes structural information, and that can be used to approximate a minimum bisection. In this paper, we show that the third eigenvector carries structural information as well. We then provide a new spectral bisection algorithm using both eigenvectors. The new algorithm is guaranteed to return a cut that is smaller or equal to the one returned by the classic spectral bisection. Also, we provide a spectral algorithm that can refine a given partition and produce a smaller cut.

1. Introduction

The classic problem of finding a minimum cut of a graph is known to be NP-hard. Nevertheless, the problem has direct applications in VLSI design, data-mining, finite elements and communication in parallel computing, etc. In practice, given the importance of the problem, the solution is generally approximated using heuristic algorithms. The problem is to separate the vertices of a graph in two parts, such that the number of edges connecting vertices in different parts is minimized. Such partition, also known as a cut, is called a balanced cut or a bisection whenever both parts have the same size.

In many applications it is desired to obtain the smallest possible cut at a cost of having a partition that is not balanced, but acceptable in the sense both parts have almost the same size. However, even for those cases efficient algorithms that approximates balanced cuts up to a constant factor do not exist. In fact, this approximation problem is NP-hard [1].

Spectral techniques are well-known approaches to this problem and they have its roots in the work of Fiedler [6] and Donath and Hoffman [4, 5]. These spectral methods are known to provide good answers, and they are broadly used in several problems [12, 13, 14]. Spectral partitioning algorithms recover global structural information and connectivity of a graph by means of the eigenvector of the second eigenvalue of the Laplacian matrix of the graph.

In [16], Spielman and Ten provided a recursive spectral bisection algorithm and showed that spectral partitioning methods work well on bounded-degree planar graphs. In [8] Guattery and Miller, perform an analysis of the quality of the separators produced by such methods. Papers [16] and [8] discuss the difference between
guarantees on the size of a balanced cut versus its optimality. Hendrickson and Le-land [12] extend the spectral approach to partition a graph into four or eight parts by using multiple eigenvectors.

In this paper, instead of using structural information provided by multiple eigenvectors to partition graphs into multiple parts, we develop an approach that uses multiple eigenvectors to create a bisection of the graphs. It is well known that the second eigenvector encodes structural information, and that can be used to approximate a minimum bisection. In this paper, we show that the third eigenvector carries structural information as well, which enable us to apply that information in the bisection problem. We then provide a new spectral bisection algorithm using both eigenvectors.

From a more general perspective, there are several heuristics for the graph partitioning problem, and they can be classified as either:

- Geometric - based solely on the coordinate information of the vertices;
- Combinatorial - which attempt to group together highly connected vertices;
- Spectral - formulate the problem as the optimization of a discrete quadratic function. The relaxed counterpart of the discrete problem becomes a continuous one, which can be solved by computing the second eigenvector of the discrete Laplacian of the graph;
- Multilevel methods - a sequence of smaller graphs is constructed in order to produce a similar coarser graph. The initial bisection is performed on the smallest of these graphs. Finally, the graph is uncoarse and partition refinement is performed on each of the coarse graph.

Each method has its advantages and disadvantages, and many of them are described in [15], where we can find a detailed description of several different methods in each of these classes. Combining those methods is a common strategy to overcome the disadvantages. For instance, spectral schemes can use eigenvectors to produce coordinate information for vertices. Geometric methods can then use these coordinates to partition the graph. Usually, for each application it is unclear which method is better. There are many factors to be considered: degree of parallelism, run time, quality of the cut produced. In [10], the author evaluate different aspects for many combinations of methods. In general, it is agreed that spectral methods are good, specially multilevel spectral bisection.

In this paper, we aggregate more information present in the spectra to improve the tradition spectral bisection algorithm (SB) and produce a new graph bisection algorithm. While SB makes use of one eigenvector only, the new algorithm uses two eigenvectors, which allows us to returns a partition with cut size smaller or equal to the SB cut size. Besides, the additional running time of computing an extra eigenvector is rather small compared to the overall running time of SB.

One one hand, we are specially concerned with the theoretical relations of eigenvectors and cuts on graphs, and also show there still more to be understood about these relations. Therefore, we do not intend to make an extensive comparison between different classes of algorithms and the new one, since the new algorithm is guaranteed to return a cut that is not worse than the one of SB, at a cost of a rather small running time. Nevertheless, we present some numerical results comparing the quality of the cut between the new algorithm and SB. It is worth it to mention that there is no restriction on using the new algorithm in combination with
other methods, and we expect that the new algorithm improves the existing mixed methods that make use of the traditional SB.

To reach our goal, we investigate properties of certain configurations of a graph partition which are related to the minimality of a cut and the structure of the graph, and we prove several results on that. Such configurations, that we call organized partitions, are shown in this paper to be related to eigenvectors of the Laplacian matrix. Turns out that organized partitions are relate to the maximum cut problem as well, as we will show in section 2.

Finally, we combine the organized partition, the third, and the second eigenvector to construct an algorithm that approximates a minimum graph bisection. For this algorithm, it is proven that the resulting partition has number of edges smaller or equal than the classical spectral bisection algorithm. Besides, we provide a second algorithm that can produce a smaller cut, given a known cut, a procedure known as refining a partition. There are several multilevel algorithms [2, 3, 9, 11] that further refine the partition during the uncoarsening phase. The second algorithm presented in this paper refines the partition by making use the information about the organized partition present in the third eigenvector.

The rest of the paper is organized as follow: properties of organized partitions are investigated on section 2 and related to minimum and maximum cuts on graphs. In section 3 we connect organized partitions with spectral properties of graphs, and we prove bounds on the minimum cut in terms of these properties. In section 4 we derive both algorithms, the first improving SB, and the second producing a smaller cut based on a given one. In section 5 we present some experimental results comparing the quality of partitions returned by SB and the new algorithm.

2. Organized Partitions

Let $G = (V, E)$ be a connected graph with $4n$ vertices. Consider a cut $\{A, B\}$ of the vertex set $V$ such that $|A| = |B|$. Such cut is also known as a balanced cut or a bisection. In this paper we deal only with balanced cuts, thus from now on we will simply refer to it simply as a cut. Let $A = A_1 \cup A_2$ and $B = B_1 \cup B_2$. Now create a new partition of vertices $C = \{A_1, A_2, B_1, B_2\}$. Here $E(X, Y)$ denotes the number of edges between the set of vertices $X$ and $Y$. We say that the partition $C$ is organized whenever

\begin{equation}
E(A_1, A_2) + E(B_1, B_2) - E(A_1, B_1) - E(A_2, B_2)
\end{equation}

is minimum among all subsets with $|A_1| = |A_2| = |B_1| = |B_2|$. See Figure 2.1 which depicts the partition in question.
It is worth mentioning that saying $C$ is organized is equivalent to say that

$$E(A_1, B_2) + E(A_2, B_1) + E(A_1, A_2) + E(B_1, B_2)$$

is minimum among the prescribed sets. To see that, we notice that

$$E(A_1, B_2) + E(A_2, B_1) + E(A_1, A_2) + E(B_1, B_2) = E(A, B) + E(A_1, A_2) + E(B_1, B_2) - E(A_1, B_1) - E(A_2, B_2).$$

Since $A$ and $B$ are fixed, we know that $E(A, B)$ is fixed too. Thus the same subsets that minimize (2.1) also minimize (2.2). We will show later how organized partitions relate to minimum and maximum cuts of graphs.

In this paper, we tacitly assume that any partition $C$ has $|A| = |B|$ and $|A_1| = |A_2| = |B_1| = |B_2|$. Now, given a cut $\{A, B\}$ we can compute the quantity

$$D_C = \min_{A=A_1 \cup A_2, B=B_1 \cup B_2 \atop |A_1|=|A_2|, |B_1|=|B_2|} E(\tilde{A}_1, \tilde{A}_2) + E(\tilde{B}_1, \tilde{B}_2) - E(\tilde{A}_1, \tilde{B}_1) - E(\tilde{A}_2, \tilde{B}_2).$$

In this notation the solution of the optimization problem $C = \{A_1, A_2, B_1, B_2\}$ is an organized partition for $\{A, B\}$.

We say that $C$ is a minimum cut whenever $E(A, B)$ is minimum among all choices of $A$ and $B$ with $|A| = |B|$. In section 3 we will see that the quantity $D_C$ relates with the eigenvalues of the Laplacian matrix whenever $C$ is a minimum cut.

The next Theorem provides a necessary condition for a cut to be minimum or maximum from the perspective of its organized partition.

**Theorem 1.** Let $\{A, B\}$ be any cut with organized partition $C$. If $D_C < 0$, then $\{A, B\}$ is not a minimum cut. If $D_C > 0$, then $\{A, B\}$ is not a maximum cut.

**Proof.** Let $C = \{A_1, A_2, B_1, B_2\}$. Notice that

$$E(A, B) = E(A_1, B_1) + E(A_1, B_2) + E(A_2, B_1) + E(A_2, B_2).$$

Besides,

$$E(A_1 \cup B_1, A_2 \cup B_2) = E(A_1, A_2) + E(B_1, B_2) + E(A_1, B_1) + E(A_2, B_2).$$

Now, if $D_C < 0$ and from its the definition, we have

$$E(A_1, A_2) + E(B_1, B_2) < E(A_1, B_1) + E(A_2, B_2).$$
This together with (2.3) and (2.4), gives us
\[
E(A_1 \cup B_1, A_2 \cup B_2) \ < \ E(A_1, B_1) + E(A_2, B_2) + E(A_2, B_1) + E(A_2, B_2) \\
= \ E(A, B).
\]
Therefore, \( \{A, B\} \) is not a minimum cut.
If \( D_C > 0 \), then
\[
E(A_1, A_2) + E(B_1, B_2) > E(A_1, B_1) + E(A_2, B_2).
\]
Similarly as before, that gives us
\[
E(A_1 \cup B_1, A_2 \cup B_2) > E(A, B).
\]
Thus, \( \{A, B\} \) is not a maximum cut. That finishes the proof. \( \square \)

In fact, the proof reveals a way to construct a better cut. That is one of the fundamental ideas behind the algorithm we provide in section 4. We explicit this construction in the form of Corollary.

**Corollary 2.** If a cut \( \{A, B\} \) has \( D_C < 0 \), then \( E(A_1 \cup B_1, A_2 \cup B_2) < E(A, B) \).
If \( D_C > 0 \), then \( E(A_1 \cup B_1, A_2 \cup B_2) > E(A, B) \).

The next result gives some insights on how the organized partition of a minimum/maximum cut looks like.

**Theorem 3.** If \( \{A, B\} \) is a minimum cut, then its organized partition satisfies
\[
E(A_1, A_2) + E(B_1, B_2) \neq 0.
\]
If \( \{A, B\} \) is a maximum cut, then its organized partition satisfies
\[
E(A_1, B_1) + E(A_2, B_2) \neq 0.
\]

**Proof.** Let \( \{A, B\} \) be a minimum cut and assume by contradiction that \( E(A_1, A_2) + E(B_1, B_2) = 0 \). We can assume that \( E(A_1, B_1) + E(A_2, B_2) \neq 0 \), otherwise the graph would be disconnected. Thus
\[
D_C = E(A_1, A_2) + E(B_1, B_2) - E(A_1, B_1) - E(A_2, B_2) < 0.
\]
Therefore, Theorem 1 implies that \( \{A, B\} \) is not a minimum cut, which is a contradiction.

If \( \{A, B\} \) is a maximum cut, assume by contradiction that \( E(A_1, B_1) + E(A_2, B_2) = 0 \). If \( E(A_1, A_2) + E(B_1, B_2) = 0 \), then the graph would be disconnected. Thus \( E(A_1, B_1) + E(A_2, B_2) \neq 0 \), and that gives us
\[
D_C = E(A_1, A_2) + E(B_1, B_2) - E(A_1, B_1) - E(A_2, B_2) > 0.
\]
Finally, Theorem 1 implies that \( \{A, B\} \) is not a maximum cut, which is a contradiction. That finishes the proof. \( \square \)

Organized partitions also indicate conditions for which a graph has more than one minimum or maximum cut and, if that is the case, how to construct them.

**Theorem 4.** Let \( \{A, B\} \) be any cut with organized partition \( C = \{A_1, A_2, B_1, B_2\} \). If \( D_C = 0 \), then \( E(A, B) = E(A_1 \cup B_1, A_2 \cup B_2) \).

**Proof.** From the definition of \( D_C \), we have
\[
E(A_1, A_2) + E(B_1, B_2) = E(A_1, B_1) + E(A_2, B_2).
\]
Thus, we can write
\[
E(A_1 \cup B_1, A_2 \cup B_2) = E(A_1, B_1) + E(A_2, B_2) + E(A_2, B_1) + E(A_2, B_2) = E(A, B).
\]
That finishes the proof. □

**Corollary 5.** Let \( \{A, B\} \) be a minimum or a maximum cut. If \( D_C = 0 \), then it is not unique.

Thus, in some cases finding an organized partition can be useful to construct a different minimum bisection whenever it is not unique. On the other hand, for a graph with a unique minimum bisection, the organized partition can be used to bound the size of the second minimum bisection. As the next Theorem shows, a second minimum bisection is not too far from the minimum whenever \( D_C \) is small.

**Theorem 6.** Let \( \{A, B\} \) be a unique minimum cut and \( C = \{A_1, A_2, B_1, B_2\} \) its organized partition. Let \( \{R, S\} \) be a second minimum cut. Then

\[
E(R, S) - E(A, B) \leq D_C + 1.
\]

**Proof.** By Theorem \([1]\), \( D_C \geq 0 \). Form a new graph \( G^* \) by adding \( D_C + 1 \) edges between \( A_1 \) and \( B_1 \). For this new graph it still holds that \( C = \{A_1, A_2, B_1, B_2\} \) is an organized partition. Similarly, denoting by \( D^*_C \) and \( E^*(A, B) \) the corresponding quantities in the graph \( G^* \), it holds that \( D^*_C = -1 \) and \( E^*(A, B) = E(A, B) + D_C + 1 \).

Now, assume by contradiction that \( E^*(R, S) > E(R, S) > E^*(A, B) \). If we consider any cut \( \{X, Y\} \) different than \( \{A, B\} \), it holds that

\[
E^*(X, Y) \geq E(X, Y) \geq E(R, S) > E^*(A, B),
\]

since \( \{R, S\} \) is a second minimum cut. This implies that \( \{A, B\} \) is a minimum cut for \( G^* \) as well. By Theorem \([1]\), this minimum cut satisfy \( D^*_C \geq 0 \). That is a contradiction with \( D^*_C = -1 \). Therefore, \( E(R, S) \leq D_C + E(A, B) + 1 \), which finishes the proof. □

### 3. Integer Program Formulation

This section is dedicated to relate organized partitions with spectral properties of the graph. We prove bounds on the minimum cut in terms of these properties. In the next Theorem, we show how to construct the organized partition of given cut. Turns out it suffices to solve an integer program in terms of the Laplacian matrix of the graph.

**Theorem 7.** Let \( \{A, B\} \) be any bisection of a graph \( G \) and denote by \( y \) be the vector with entries

\[
y_i = \begin{cases} 
\frac{1}{\sqrt{n}} & \text{if } i \in A \\
-\frac{1}{\sqrt{n}} & \text{if } i \in B.
\end{cases}
\]

Let \( L \) be the Laplacian matrix of the \( G \). Then

\[
\frac{4}{n} (E(A, B) + D_C) = \min_{\substack{x^T 1 = 0 \\ \|x\|_1 = 1 \\ y^T x = 0}} x^T L x.
\]

Furthermore, each solution \( \bar{x} \) of \((3.1)\) prescribes an organized partition for \( \{A, B\} \) as follow

\[
\bar{x}_i = \begin{cases} 
\frac{1}{\sqrt{n}} & i \in A_1 \cup B_1 \\
-\frac{1}{\sqrt{n}} & i \in A_2 \cup B_2.
\end{cases}
\]
Proof. Let $A_1, A_2, B_1$ and $B_2$ be disjoint sets such that $A_1 \cup A_2 = A$ and $B_1 \cup B_2 = B$, with $|A_1| = |A_2|$ and $|B_1| = |B_2|$. Define the vector $x$ with entries

$$x_i = \begin{cases} 1/\sqrt{n} & i \in A_1 \cup B_1 \\ -1/\sqrt{n} & i \in A_2 \cup B_2 \end{cases}.$$ 

Clearly $x^T 1 = 0$, $\|x\| = 1$, and $y^T x = 0$.

Now, we can write $x^T Lx$ in terms of the partition $\{A_1, A_2, B_1, B_2\}$ as

$$x^T Lx = \sum_{(i,j) \in E} (x_i - x_j)^2$$

$$= \sum_{i \in A_1, j \in B_1} (x_i - x_j)^2 + \sum_{i \in A_2, j \in B_2} (x_i - x_j)^2 + \sum_{i \in A_1, j \in A_2} (x_i - x_j)^2 + \sum_{i \in B_1, j \in B_2} (x_i - x_j)^2$$

$$= \frac{4}{n} (E(A_1, B_2) + E(A_2, B_1) + E(A_1, A_2) + E(B_1, B_2)),$$

since the first two sums are zero. That gives us

$$\frac{n}{4} x^T Lx = E(A, B) + E(A_1, A_2) + E(B_1, B_2) - E(A_1, B_1) - E(A_2, B_2),$$

for each choice of partition $\{A_1, A_2, B_1, B_2\}$. Therefore, in view of the definition of $D_C$, we have

$$\min_{\|x\| = 1} \frac{4}{n} (E(A, B) + D_C).$$

Besides, by the construction of the feasible set of solutions, $\tilde{x}$ indicates the organized partition of $\{A, B\}$. That finishes the proof. \(\square\)

Thus, whenever $\{A, B\}$ is a minimum cut, the minimum of (3.1) reduces to

$$\frac{4}{n} (\text{MinCut}(G) + D_C).$$

In the work of [2] the authors proved the inequality

$$\text{MinCut}(G) \geq \frac{n}{4} \lambda_2.$$ 

In light of the concept of organized partitions we can go further on the relation between minimum cuts and eigenvalues of the Laplacian matrix and prove the next result.

**Theorem 8.** Let $C$ be an organized partition of a minimum cut. Then

$$\text{MinCut}(G) \geq \frac{n}{8} (\lambda_2 + \lambda_3) - \frac{D_C}{2}.$$ 

**Proof.** Define the vector $y$ with entries

$$y_i = \begin{cases} 1/\sqrt{n} & i \in A \\ -1/\sqrt{n} & i \in B \end{cases}$$

(3.3)
Clearly $y^T 1 = 0$ and $\|y\| = 1$. Thus, we can write

$$y^T Ly = \sum_{(i,j) \in E} (y_i - y_j)^2 = \sum_{(i,j) \in E \atop i \in A, j \in B} (y_i - y_j)^2 + \sum_{(i,j) \in E \atop i \in A} (y_i - y_j)^2 + \sum_{(i,j) \in E \atop i \in B} (y_i - y_j)^2.$$ 

Notice the sum over the edges with both endpoints in the same set vanishes. Thus, we have

$$y^T Ly = \sum_{(i,j) \in E \atop i \in A, j \in B} (1/\sqrt{n} - (-1/\sqrt{n}))^2 = \frac{4}{n} E(A,B).$$

An important idea here is that a minimum cut is achieved if we take the minimum over all prescribed vectors, i.e.,

$$\text{MinCut}(G) = \frac{n}{4} \min_{y \in \{1/\sqrt{n}, -1/\sqrt{n}\}} y^T Ly.$$

Now, we apply Theorem 7 for the vector $\bar{y}$ that solves the minimization problem (3.4). Thus, we can solve the sum of minimization problems as

$$\min_{y^T 1 = 0, \|y\| = 1} y^T Ly + \min_{x^T 1 = 0, \|x\| = 1} x^T Lx = \frac{4}{n} (2 \text{MinCut}(G) + D_C).$$

Equivalently, we can write

$$\text{MinCut}(G) = \frac{n}{8} \min_{y \in \{1/\sqrt{n}, -1/\sqrt{n}\}} y^T Ly + \min_{x \in \{1/\sqrt{n}, -1/\sqrt{n}\}} x^T Lx - \frac{D_C}{2}.$$ 

Thus, if we drop the constraint $y_i, x_i \in \{1/\sqrt{n}, -1/\sqrt{n}\}$ and consider all $x, y \in \mathbb{R}^n$, we find the inequality

$$\text{MinCut}(G) \geq \frac{n}{8} \min_{y^T 1 = 0, \|y\| = 1} y^T Ly + \min_{x^T 1 = 0, \|x\| = 1} x^T Lx - \frac{D_C}{2}$$ 

$$= \frac{n}{8} \min_{y^T 1 = x^T 1 = 0, \|y\| = \|x\| = 1} y^T Ly + x^T Lx - \frac{D_C}{2}$$

$$= \frac{n}{8} (\lambda_2 + \lambda_3) - \frac{D_C}{2}.$$ 

That finishes the proof. \hfill \Box

It is worth mentioning that if we drop the constraint $y_i \in \{1/\sqrt{n}, -1/\sqrt{n}\}$ in the minimization problem (3.4), then we precisely obtain the lower bound (3.2) as the authors in [5]. Besides, whenever

$$D_C < \frac{n}{4} (\lambda_3 - \lambda_2),$$

Theorem 8 provides a tighter lower bound on the minimum cut of a graph. Intuitively, it means that an optimization problem that considers both $\lambda_2$ and $\lambda_3$ is more likely to reveal a minimum cut than a problem that considers only $\lambda_2$.

We finish this section with a result that summarizes all its underlying ideas.

**Theorem 9.** For a graph with Laplacian matrix $L$, the solution $(\bar{x}, \bar{y})$ of the problem

\[
\begin{align*}
\min_{y^T 1 = 0, \|y\| = 1, y_i \in \{1/\sqrt{n}, -1/\sqrt{n}\}} & y^T Ly + \\
\min_{x^T 1 = 0, \|x\| = 1, \bar{y}^T x = 0, x_i \in \{1/\sqrt{n}, -1/\sqrt{n}\}} & x^T Lx
\end{align*}
\]

constructs a minimum cut $\{A, B\}$ together with its organized partition $C = \{A_1, A_2, B_1, B_2\}$, as follow:

\[
\bar{y}_i = \begin{cases} 
1/\sqrt{n} & i \in A \\
-1/\sqrt{n} & i \in B
\end{cases} \quad \text{and} \quad \bar{x}_i = \begin{cases} 
1/\sqrt{n} & i \in A_1 \cup B_1 \\
-1/\sqrt{n} & i \in A_2 \cup B_2.
\end{cases}
\]

**Proof.** Follows from equation (3.4) and Theorem 7. \hfill \Box

### 4. Derivation of the Algorithms

In this section we provide an intuitive description of the main ideas behind our new algorithm, which turns out to arise from the theoretical background developed in the previous sections. We do that by showing how to improve the bisection provided by the traditional SB algorithm by means of properties of organized partitions. We will prove that there are infinite many solutions for the minimization problem that finds the organized partition of a cut, if we apply relaxation. Thus, these solutions constructs better candidates for a minimum cut. First, we consider some examples where SB fails to approximate a good bisection.

As an approximation algorithm, SB sometimes provides a cut that is too far from optimal. There are investigations about this phenomenon, and the best known example where SB fails is given by the roach graph, due to Guattery and Miller [8]. The roach graph consists of two path graphs with the same even size connected by a few edges, as illustrated in Figure 4.1.

![Figure 4.1. Roach graph on 16 vertices](image)

This is a very good example which seems to be taylor made to defeat SB. The roach graph is an important example not only because SB provides a cut that is far from optimal, in fact it is the prototype of many cases where this algorithm gives a very bad result. Let us look closer to what is happening with the algorithm on this kind of graph.

For a roach graph the minimum bisection consists of two edges separating the antennae - the pending paths on the right side of Figure 4.1. But that is not what SB returns. Taking a roach graph on 16 vertices, we label the upper and lower path
from 1 to 8 and 9 to 16, respectively. For this ordering, its eigenvector associated with \( \lambda_2 \) is approximately given by

\[
y = \begin{bmatrix}
-0.0028 & -0.0083 & -0.0295 & -0.1068 & -0.3869796 & -0.6270 & -0.8024 & -0.8948 \\
0.0028 & 0.0083 & 0.0295 & 0.1068 & 0.3869 & 0.6270 & 0.8024 & 0.8948
\end{bmatrix}^T.
\]

Now, we can plot the entries of \( y \) displayed in Figure 12. The upper path corresponds to the points above the origin and the lower path below it. SB will split the graph in two paths, which provides a cut with 4 edges, which is not a maximum cut. In [8] the authors showed this is true for the whole class of roach graphs, therefore showing a class of graphs where the resulting bisection from SB is far from optimal, i.e., with a bisection of order \( O(n) \).

![Figure 4.2. The y eigenvector for the roach graph](image)

This is the prototype of what happens with SB when it returns a wrong bisection. In view of this problem, it is natural to ask how to overcome this pathology on the SB algorithm. Here we show how that can be done using the concept of organized partitions.

In light of Corollary 2 if a cut has \( D_C < 0 \), then its organized partition can be used to construct a smaller cut. Thus, it would be useful to have an algorithm that approximates a minimum cut and which computes its organized partition as well. That means if we could solve both problems simultaneously, then we can obtain a better cut than the original algorithm, whenever this cut has \( D_C < 0 \).

That is the case of the roach graph and many examples of this nature. Notice that the cut provided by SB for the roach graph on 16 vertices is \( C = \{ A_1, A_2, B_1, B_2 \} \), where

\[
A_1 = \{ v_1, \ldots, v_4 \}, \quad A_2 = \{ v_5, \ldots, v_8 \}, \quad B_1 = \{ v_9, \ldots, v_{12} \}, \quad \text{and} \quad B_2 = \{ v_{13}, \ldots, v_{16} \}.
\]

Therefore, we have

\[
D_C = E(A_1, A_2) + E(B_1, B_2) - E(A_1, B_1) - E(A_2, B_2) = 1 + 1 - 4 - 0,
\]

which gives us the desired property \( D_C < 0 \). For this reason, the organized partition of this cut will provide a smaller bisection.

Now, let us see what the eigenvector of \( \lambda_3 \) tells about the organized partition. Theorem 9 constructs the organized partition based on the solution of an integer program. Theorem 8 and its proof indicate that the eigenvectors of \( \lambda_2 \) and \( \lambda_3 \) can be used to approximate the solution. Thus, if we drop the constraints on \( x \) and \( y \) putting \( x, y \in \mathbb{R}^n \), it is expected that the solution of the new program
(4.1) \[
\min_{\|y\|=\|x\|=1} y^T L y + x^T L x \]

approximates the minimum cut and its organized partition by the eigenvector \( x \) associated with \( \lambda_3 \).

For the same roach graph, that eigenvector is approximately

\[
x = \begin{bmatrix}
-0.6935 & -0.5879 & -0.3928 & -0.1379 & 0.1379 & 0.3928 & 0.5879 & 0.6935 \\
-0.6935 & -0.5879 & -0.3928 & -0.1379 & 0.1379497 & 0.3928475 & 0.5879 & 0.6935
\end{bmatrix}^T.
\]

Notice that if we use \( x \) as an approximation for the integer solution of the program in Theorem 9, then \( x \) induces the correct organized partition \( C = \{A_1, A_2, B_1, B_2\} \) as described above. Here we simply used the entries of \( x \) as an approximation for the integer solution

\[
\bar{x}_i = \begin{cases}
1/\sqrt{n} & \text{if } i \in A_1 \cup B_1 \\
-1/\sqrt{n} & \text{if } i \in A_2 \cup B_2.
\end{cases}
\]

Since \( D_C < 0 \), this implies that we can construct a smaller bisection than the one provided by SB by using the eigenvector \( x \). More precise, by Corollary 2 the partition \( \{A_1 \cup B_1, A_2 \cup B_2\} \) gives a smaller bisection. In fact, this is the minimum bisection for the roach graph.

Figure 4.3. Roach graph with \( x \) and \( y \) as embedding

Figure 4.3 depicts the underlying idea behind the proof of Theorem 8. We plotted points using the entries of both eigenvectors of the roach graph \( x \) and \( y \) as coordinates. There, each point corresponds to a vertex. It is clear to see that if we separate the vertices by the signs of the coordinates in \( x \), then we would get the minimum cut.

The previous discussion suggests to consider both eigenvectors in a new algorithm, in the sense either \( x \) or \( y \) will approximate a minimum cut. Essentially, when \( y \) gives a cut with \( D_C < 0 \), we can appeal to the cut provided by \( x \). Thus it would suffices to check which one gives a better cut. Actually, this neat idea can be taken further when we look from the perspective of integer programming.
As we will see in the next Theorem, certain specific linear combinations of \(x\) and \(y\) are solutions for \((4.1)\) as well. Thus, those new solutions can be used to approximate a minimum bisection.

**Theorem 10.** Let \(x\) and \(y\) be a solution of \((4.1)\). Let \(\theta \in [0, 2\pi)\) and let \(u = \cos \theta x + \sin \theta y\) and \(v = \sin \theta x - \cos \theta y\). Then \(u\) and \(v\) is a solution of \((4.1)\).

**Proof.** We proceed by showing that
\[
x^T L x + y^T L y = u^T L u + v^T L v.
\]
Hence, we write
\[
u^T L u = (\cos \theta x + \sin \theta y)^T L (\cos \theta x + \sin \theta y)
= \cos \theta x^T L \cos \theta x + \sin \theta y^T L \sin \theta y + 2 \sin \theta y^T L \cos \theta x.
\]
Also, we can write
\[
v^T L v = (\sin \theta x - \cos \theta y)^T L (\sin \theta x - \cos \theta y)
= \sin \theta x^T L \sin \theta x + \cos \theta y^T L \cos \theta y - 2 \sin \theta y^T L \cos \theta x.
\]
Therefore, we obtain
\[
u^T L u + v^T L v = \cos \theta x^T L \cos \theta x + \sin \theta y^T L \sin \theta y + 2 \sin \theta y^T L \cos \theta x + \sin \theta x^T L \sin \theta x + \cos \theta y^T L \cos \theta y - 2 \sin \theta y^T L \cos \theta x
= \cos^2 \theta x^T L x + \sin^2 \theta y^T L y + \sin^2 \theta x^T L x + \cos^2 \theta y^T L y
= (\cos^2 \theta + \sin^2 \theta)(x^T L x + y^T L y)
= x^T L x + y^T L y.
\]

It follows that \(u\) and \(v\) is also a minimizer of \((4.1)\).

It remains to verify that \(u\) and \(v\) satisfy the constraints \(u^T 1 = 0\), \(v^T 1 = 0\), \(\|u\| = \|v\| = 1\) and \(u^T v = 0\). To see that \(u^T 1 = 0\), we notice that \(u^T 1 = \cos \theta x^T 1 + \sin \theta y^T 1 = 0\). Now, using the fact that \(x^T x = y^T y = 1\) and \(y^T x = 0\), we can write
\[
u^T u = (\cos \theta x + \sin \theta y)^T (\cos \theta x + \sin \theta y)
= \cos^2 \theta x^T x + \sin^2 \theta y^T y + 2 \sin \theta \cos \theta y^T x
= \cos^2 \theta + \sin^2 \theta = 1,
\]
which implies \(\|u\| = 1\). Similarly, we obtain \(v^T 1 = 0\) and \(\|v\| = 1\).

To show \(u^T v = 0\), again we use the fact that \(x^T x = y^T y = 1\) and \(y^T x = 0\)
\[
u^T v = (\cos \theta x + \sin \theta y)^T (\sin \theta x - \cos \theta y)
= \cos \sin \theta x^T x - \cos^2 \theta x^T y + \sin^2 \theta x^T y - \sin \theta \cos \theta y^T y
= \cos \sin \theta x^T x - \sin \theta \cos \theta y^T y = 0.
\]

This concludes the proof. \(\square\)

By constructing a infinite set of solutions for the problem \((4.1)\), the last Theorem introduces a degree of freedom in the solutions of \((4.1)\). We can explore this degree of freedom in order to create different bisections. As discussed before, solutions of \((4.1)\) can be used to approximate a minimum bisection and its organized partition. However, there are infinite \(u\) and \(v\) described in the last Theorem. Naturally, all of them can be used to approximate a minimum bisection. That is a key idea in the algorithm presented next. The next Theorem show how to construct different \(n\) different bisections based on the solutions of solutions of \((4.1)\).
Theorem 11. Let $x$ and $y$ be solutions of (4.1). For each pair $x_i$ and $y_i$, $i = 1, \ldots, n$, define the vector $u = \frac{x_i}{\sqrt{x_i^2 + y_i^2}} x + \frac{y_i}{\sqrt{x_i^2 + y_i^2}} y$. Then $u$ induces a bisection that approximates the vector $\bar{u}_i$ with entries
\[
\bar{u}_i = \begin{cases} 
\frac{1}{\sqrt{n}} & i \in A \\
-\frac{1}{\sqrt{n}} & i \in B 
\end{cases}.
\]

Proof. In order to construct different bisections using Theorem 10 we need to choose $\theta \in [0, 2\pi)$, then define $u$ and $v$, and finally define a new partition $\{A, B\}$ based on $u$ and $v$. To this end, consider the set of euclidean points $(x_i, y_i)$ given by the corresponding entries of the eigenvectors $x$ and $y$. Choose a point $(x_i, y_i)$, and let $\theta_i$ be the angle between the point $(x_i, y_i)$ and the abscissa. Now define $u$ and $v$ as in Theorem 10 and let $(u_i, v_i)$ be points defined by the corresponding entries of $u$ and $v$. The point $(u_i, v_i)$ is simply a rotation of angle $\theta_i$ for the point $(x_i, y_i)$.

Now using the solution of (4.1), we can approximate the solution of the integer program in Theorem (9). By Theorem (9), its solution defines a minimum cut, and we can define the cut $\{A, B\}$ using the entries of $u$ as an approximation for
\[
\bar{u}_i = \begin{cases} 
\frac{1}{\sqrt{n}} & i \in A \\
-\frac{1}{\sqrt{n}} & i \in B 
\end{cases}.
\]

Finally, to simplify the computation of $u$ we can calculate $\cos \theta$ and $\sin \theta$ instead of $\theta$. That follows straightforward from
\[
\cos \theta = \frac{x_i}{\sqrt{x_i^2 + y_i^2}} \quad \text{and} \quad \sin \theta = \frac{y_i}{\sqrt{x_i^2 + y_i^2}}.
\]

That finishes the proof. \qed

Algorithm 1 Graph Bisection.

Require: $G=(V,E)$

Compute $y$ and $x$, the second and third smallest eigenvector of $L$.
Set $A$ with the $n/2$ vertices with largest $y_i$ and $B$ with the remaining vertices.
for $i = 1, \ldots, n$ do
\[
u = \frac{x_i}{\sqrt{x_i^2 + y_i^2}} x + \frac{y_i}{\sqrt{x_i^2 + y_i^2}} y
\]
Set $R$ with the $n/2$ vertices with largest $u_j$ and $S$ with the remaining vertices.
if $E(R, S) < E(A, B)$ then
\[
A = R \\
B = S
\]
end if
end for
return $\{A, B\}$

As an illustration of Algorithm 1 Figures 4.4a and 4.4b show the same graph embedded on the coordinates given by the second and the third eigenvalue. Figure 4.4a depicts the SB algorithm choosing a set of vertices based on a Fiedler vector only. The straight line has the same direction of the Fiedler vector. Since SB sorts
the vertices based on the this vector and chooses the top largest to construct the bisection, it is clear that it is simply a projection of points along the straight line. As more linear combinations of the Fiedler vector and the third eigenvector are considered, different cuts are created. Figure 4.4 depicts the optimal choice of vertices induced by one of those linear combinations.

(a) SB chooses vertices from a Fiedler vector
(b) Algorithm 1 considers both, the Fiedler vector and the third eigenvector to choose vertices

Figure 4.4. Different lines induce different bisections

Notice that the cut induced by $x$, the standard spectral bisection solution, is among the possible cuts $\{R, S\}$ constructed by Algorithm 1. Therefore, the number of edges in the partition provided by Algorithm 1 is not larger than the one in the partition returned by SB, which leads us to the next Theorem.

**Theorem 12.** The cut returned by Algorithm 1 has number of edges smaller or equal than the number of edges in the SB partition.

For any roach graph its eigenvectors have the same shape of the previous example with 16 vertices. That leads us to the next Theorem.

**Theorem 13.** For any roach graph, Algorithm 1 returns a minimum cut.

**Proof.** By Lemma 5.1 of [8], the third eigenvector of a roach graph induces a cut separating the pending paths of the roach graph, which is a minimum cut. This cut is among the possible cuts constructed by Algorithm 1. That finishes the proof.

Now we will turn our attention to the derivation of an algorithm that refines a given bisection. Since an organized partition can be used to construct a better bisection, the next algorithm constructs an approximation for an organized partition of a given bisection. In the same fashion as in Algorithm 1 these approximations are candidates for a smaller cut.
Theorem 7 provides us with a way to construct the organized partition of a given cut. If \( \{A, B\} \) is the cut in question, we can denote by \( y \) be the vector with entries

\[
y_i = \begin{cases} 
1/\sqrt{n} & \text{if } i \in A \\
-1/\sqrt{n} & \text{if } i \in B.
\end{cases}
\]

Now, if we use relaxation on the set of solutions of the integer program (3.1) and drop the constraint \( x_i \in \{1/\sqrt{n}, -1/\sqrt{n}\} \), we obtain the following program

\[
\min_{x^T1 = 0, \|x\| = 1, y^Tx = 0} x^T L x.
\]

The minimization problem (4.2) is not an eigenvalue problem anymore, because the vector \( y \) is not necessarily an eigenvector of the matrix \( L \). However, it is easy to transform problem (4.2) into a standard eigenvalue problem, as shown in [7] by Gene and Golub. Therefore, the solution of program (4.2) can be used as an approximation for the organized partition: the half largest entries of \( x \) indicate the vertices in the set \( A_1 \cup B_1 \) of the organized partition, and the other half indicates the remaining vertices in the organized partition. Again, we can use linear combinations of \( x \) and \( y \) to construct different approximations for the organized partition. The algorithm can be described as follows.

**Algorithm 2 Spectral Bisection Refinement.**

**Require:** \( G = (V, E), y \)

Set \( A \) with the \( n/2 \) vertices with largest \( y_i \) and \( B \) with the remaining vertices.

Compute \( x \), the solution of \( \min_{x^T1 = 0, \|x\| = 1, y^Tx = 0} x^T L x \) for \( i = 1, \ldots, n \) do

\[
u = \frac{y_i}{\sqrt{x_i^2 + y_i^2}} x + \frac{x_i}{\sqrt{x_i^2 + y_i^2}} y
\]

Set \( R \) with the \( n/2 \) vertices with largest \( u_j \) and \( S \) with the remaining vertices.

if \( E(R, S) < E(A, B) \) then

\[
A = R \\
B = S
\]

end if

end for

return \( \{A, B\} \)

5. Experimental results

We compared the quality of partitions returned by SB and Algorithm 1 on a wide range of graph matrices. The matrices represent graphs arising in different application domains found in Matrix Market. Table 1 describes the characteristics of these matrices and the comparison between cut sizes of both algorithms.

The last column of Table 1 indicates percentage of improvement of Algorithm 1 over SB. We highlight the best results.

Next, we compared the quality of partitions for several random graphs by computing the average gain of Algorithm 1 over SB. Here, a random graphs with \( n \)
vertices follows the Erdős–Rényi model, where an edge is present between two vertices uniformly with probability $p$. For different combinations of probabilities and number of vertices, we sampled 1000 random graphs and calculated the average gain. The experiments discarded graphs that are disconnected. Table 2 shows the resulting ratio of improvement, where each column corresponds to a given number of vertices $n$ and each row to a given probability $p$.

| $p$ | $n$ | 100 | 500 | 1000 |
|-----|-----|-----|-----|------|
| 0.1 | 7.68% | 1.87% | 1.01% |
| 0.2 | 4.67% | 0.90% | 0.46% |
| 0.3 | 3.29% | 0.61% | 0.30% |
| 0.4 | 2.73% | 0.64% | 0.32% |
| 0.5 | 2.62% | 1.10% | 0.82% |
| 0.6 | 2.91% | 1.20% | 0.68% |
| 0.7 | 1.98% | 0.39% | 0.19% |
| 0.8 | 1.00% | 0.19% | 0.09% |
| 0.9 | 0.57% | 0.15% | 0.07% |

Table 2. Average gain for 1000 random graphs

The expected number of edges of these random graphs is $pn(n - 1)/2$. Thus, Table 2 indicates that Algorithm 1 performs better for sparse graphs than for dense graphs. We highlighted three best results for each column of Table 2. We notice that in multilevel algorithms, the coarsest graph is usually small, with 100 vertices or less. Putting $p = 0.1$ we obtain on the average 495 edges for random graphs with 100 vertices. Table 2 indicates a good improvement ratio for those graphs, with
average of 7.6%. That suggests that very often the new algorithm provides better cuts for the initial partition in multilevel algorithms.

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