Spectral Graph Theory and its Applications

Lillian Dai
October 20, 2004

I. Introduction

The study of eigenvalues and eigenvectors of various matrices associated with graphs play a central role in our understanding of graphs. The set of graph eigenvalues are termed the *spectrum* of the graph. Over the past thirty years or so, many interesting discoveries have been made regarding the relationship between various graph properties and the spectrum of the associated matrices. The goal of these studies is to deduce characteristic properties or structures of graphs from its spectrum as well to use spectral techniques to aid in the design of useful algorithms.

This report first presents a brief survey of some of the results and applications of spectral graph theory. A significant portion of the report is then devoted to a discussion of using spectral techniques in solving graph partitioning problems where graph vertices are partitioned into two disjoint sets of similar sizes while the number of edges between the two sets is minimized. This problem has been shown to be NP-complete. It has been found that partitioning a graph based on its spectrum and eigenvectors provides a good heuristic for this problem. Indeed, spectral partitioning techniques are widely used in practice and work well on a large set of graphs. It is intriguing and not obvious why the spectral technique works at all. In this report, I summarize three papers [1], [2], and [3] that discuss the quality of spectral partitioning and try to gain some insights on why this technique works well on some graphs but not on others.

II. Preliminaries

A graph $G=(V,E)$ is specified by its vertex set V and edge set E. Let $V=\{1,...,n\}$ and $|E|=m$. In this report, all graphs are undirected and finite, without self-loops, and without multiple edges between two nodes.

There are several associated matrices of interest:

<u>Adjacency matrix</u> A_G: $n \times n$ matrix whose entries $a_{i,j}$ are given by $a_{i,j}=\begin{cases}1 & \text{if } (i,j)\in E \\ 0 & \text{otherwise}\end{cases}$

<u>Degree matrix</u> D_G: $n \times n$ matrix whose entries $d_{i,j}$ are given by $d_{i,j}=\begin{cases}d_i & \text{if } i=j \\ 0 & \text{otherwise}\end{cases}$, where d_i is the degree of vertex i.

<u>Incidency matrix</u> B_G: $n \times m$ matrix. Each column of B_G corresponds to an edge $(i,j)\in E$. In that column, the entry is 1 in the i^{th} row, -1 in the j^{th} row, and 0 in all other rows.

Laplacian matrix L_G : $n \times n$ matrix given by $D_G - A_G$. The entries $l_{i,j}$ are expressed explicitly by $l_{i,j} = \begin{cases} -1 & \text{if } (i,j) \in E \\ d_i & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$, where d_i is the degree of vertex i.

Since L_G is a symmetric matrix, all of its eigenvalues are real and eigenvectors corresponding to different eigenvalues are orthogonal. The Laplacian matrix is closely related to the incidency matrix since $L_G = B_G B_G{}^T$ (where T denotes transpose). Take a vector $x = (x_1, x_2, \ldots, x_n) \in \mathbb{R}^n$, then $x^T L_G x = x^T B_G B_G{}^T x = \left(x^T B_G\right)\left(x^T B_G\right)^T = \sum_{(i,j)\in E} \left(x_i - x_j\right)^2 \geq 0$. Hence the Laplacian matrix of every graph is positive semidefinite and its eigenvalues are non-negative real numbers. Since each row of L_G sums to 0, the matrix is singular with at least one eigenvalue equal to 0 and the corresponding eigenvector equal to $(1,1,\ldots,1)^T$. Let $(u_1, u_2, \ldots, u_n)^T$ be the eigenvector corresponding to a non-zero eigenvalue, then since eigenvectors of symmetric matrices are orthogonal, $\sum_{i=1}^{n} u_i = 0$.

III. Some Properties and Applications of Graph Spectra

A. Connectedness of Graphs

The second smallest eigenvalue of the Laplacian matrix indicates the connectedness of a graph.

Theorem III.1. Let $G = (V, E)$ be a connected graph and let $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$ be the eigenvalues of its Laplacian matrix. Then $\lambda_2 > 0$.

Proof: Since L_G is a symmetric matrix, it is orthogonally diagonalizable and has n linearly independent eigenvectors. Let $\vec{x}$ be an eigenvector of L_G corresponding to an eigenvalue of 0. Then $L_G \vec{x} = 0$ and $\vec{x}^T L_G \vec{x} = \sum_{(i,j)\in E} \left(x_i - x_j\right)^2 = 0$. This implies $x_i = x_j$ for every $(i,j) \in E$. Since the graph is connected, this means that $x_1 = x_2 = \ldots = x_n$. Therefore, for connected graphs, the eigenspace of 0 has dimension 1 for connected graphs.

□

The magnitude of λ_2 has been considered as a measure of how well-connected a graph is [4]. λ_2 is called the *Fiedler value* of a graph and the corresponding eigenvector, $\vec{v}$, is termed *Fielder vector*.

Define the Rayleigh quotient to be $\phi_x = \frac{\vec{x}^T L_G \vec{x}}{\vec{x}^T \vec{x}} = \frac{\sum_{(i,j)\in E} \left(x_i - x_j\right)^2}{\sum x_i^2}$, where $\vec{x} \in \mathbb{R}^n$. Observe the Fiedler value satisfies $\lambda_2 = \min_{\vec{x} \perp (1,\ldots,1)} \phi_x$ with the minimum occurring only when $\vec{x}$ is a Fiedler vector.

Corollary III.1. The spectrum of the Laplacian of an unconnected graph is the union of the spectra of the disconnected components. The multiplicity of the 0 eigenvalue equals to the number of connected components of G.

B. Testing Graph Isomorphism

Two graphs $G=(V,E)$ and $H=(V,F)$ are isomorphic if there is a way of re-labeling the vertices that makes the two graphs the same. If the spectra of G and H are different, then the two graphs are non-isomorphic. However this does not determine graph isomorphism since there are non-isomorpic graphs with the same spectra. As shown in [5], the eigenvectors of the adjacency matrix can be used to test for isomorphism. They construct polynomial time algorithms which test isomorphism of graphs whose eigenvalues associated with the adjacency matrix have bounded multiplicity.

C. Graph coloring

The goal in graph coloring problems is to assign a color to each vertex, selected from a minimum set of colors, such that each edge connects vertices of different colors (ie. finding the *chromatic number* χ_G of a graph G). Several results indicate that the spectral properties of a graph provide some information on its chromatic number. Let $\lambda_1 \le \lambda_2 \le \ldots \le \lambda_n$ be the eigenvalues of a graph's adjacency matrix, then $1-\frac{\lambda_n}{\lambda_1} \le \chi_G \le 1+\lambda_n$ [6]. In [6], the authors designed a polynomial time algorithm that colors optimally with high probability for random 3-colorable graphs based on spectral techniques.

***D. Expander Graphs* [7, 8, 9]**

Consider a sequence of graphs G_n, one for each n. A sequence of *d*-regular graphs is a family of expander graphs if there exists a constant c such that $\lambda_2(G_n) \ge c$ for all n. It is known that randomly chosen *d*-regular graphs are expanders with high probability. Good constructions of expanders exist and they enable good constructions of error-correcting codes and pseudo-random generators. In [7], the authors present an asymptotically good family of linear error-correcting codes that can be decoded in linear time. These codes are derived from expander graphs and are termed "expander codes". Expander codes belong to the class of low density parity check codes.

Among the various applications of expander graphs, those in communication networks have the longest history and can be traced to the early development of switching networks. [9] shows the construction of a nonblocking network using Ramanujan graphs which are a family of expander graphs.

***F. Paths, Flows, and Routing* [9]**

Flows and routes are useful in providing lower bounds for eigenvalues. For a *d*-regular graph on n vertices, suppose there is a set of $\binom{n}{2}$ paths joining all pairs of vertices such that each path has length at most l and each edge of G is contained in at most m paths, then $\lambda_2 \ge \frac{n}{kml}$, where λ_2 is the second-smallest eigenvalue of the normalized Laplacian matrix. [9] also shows that for graphs with good eigenvalue lower bounds, short routes and effective routing schemes exist with small congestion.

IV. GRAPH PARTITIONING

In general graph partition problems, the goal is to find a partition of the vertices into two disjoint subsets, S and $\bar{S}$, such that some conditions on the number of edges between the sets and the size of the sets are met. Two common variations of this problem are the *bisection* and *ratio-partition* problems. Let $E\left(S,\bar{S}\right)$ be the set of edges with one endpoint in S and the other in $\bar{S}$. The *cut size* of the partition $\left(S,\bar{S}\right)$ is $\left|E\left(S,\bar{S}\right)\right|$. In the *bisection* problem, the cut size is minimized subject to the constraint that $|S|$ and $|\bar{S}|$ differ by at most 1. Finding the best value of $\left|E\left(S,\bar{S}\right)\right|$ for this problem is NP-complete [10]. In the *ratio-partition* problem, the objective is to minimize the *cut ratio*, which is defined as $\phi_G(S)=\dfrac{\left|E\left(S,\bar{S}\right)\right|}{\min\left(|S|,|\bar{S}|\right)}$. This also has the effect of finding a partition with a small cut size while balancing the number of nodes in each subset. The minimum value $\phi_G=\min_{S\subset V}\phi_G(S)$ is called the *isoperimetric* number of a graph. Note that G is connected iff $\phi_G>0$.

The graph partitioning problem arises in a variety of parallel computing problems, including sparse matrix-vector multiplication, solving PDEs, optimizing VLSI layout, telephone network design, and sparse Gaussian elimination [11].

A. Spectral Partitioning

There are a variety of algorithms for the bisection problem, including greedy search algorithms, randomized algorithms, and spectral methods. For a discussion, see [12]. Spectral methods are widely used to compute graph separators. It is first suggested by Donath and Hoffman in 1972. Typically, the Laplacian matrix is used. The eigenvector $\vec{v}$ of L_G corresponding to λ_2 is computed and is treated as a one-dimensional drawing of the graph G (ie. map the vertices to their corresponding entries in $\vec{v}$). Choose some real number s and consider the partition of the vertices given by $V_L=\{i:v_i\le s\}$ and $V_L=\{i:v_i>s\}$. For the bisection problem, s is the median of $\{v_1,\ldots v_n\}$. For the ratio-partitioning problem, s is the value that gives the best cut ratio.

The spectral bisection technique is best illustrated by an example. Consider the graph in Figure 1. The Fiedler vector is [-0.2887 -0.5774 -0.2887 0.2887 0.5774 0.2887]. Hence vertices $\{1,2,3\}$ are mapped with negative entries in the vector and $\{4,5,6\}$ are mapped with positive entries. In this example, s = -0.2887 or 0.2887. This bisects the graph into $\{1,2,3\}$ and $\{4,5,6\}$ as shown in Figure 1 and is the optimal bisection.

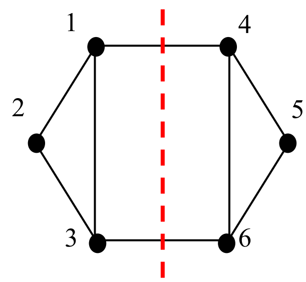


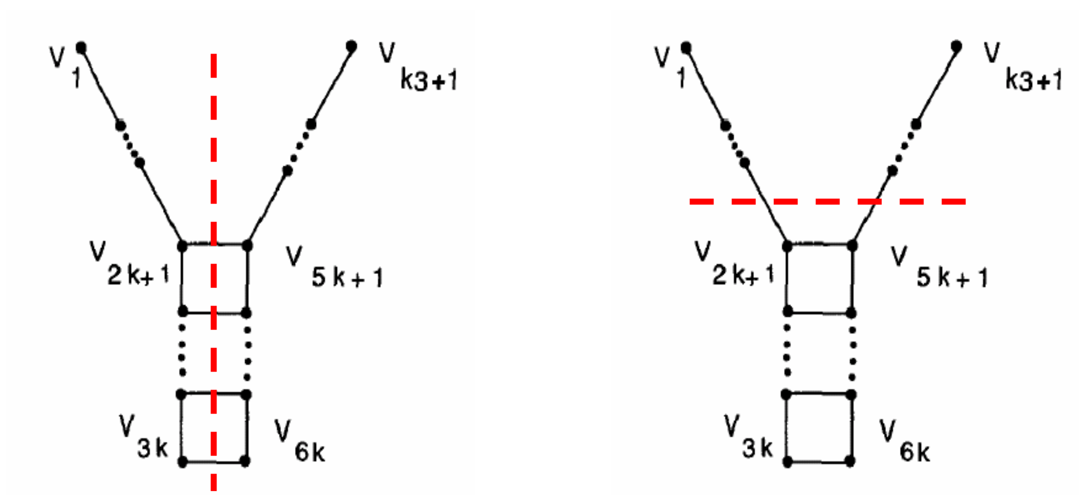
Figure 1. Sample Graph

B. Theoretical Results

Although spectral partitioning is used extensively in practice, there is little work on how well these methods work. In 1995, Guattery and Miller first attempted to provide some theoretical basis for this problem [1]. They showed that naïve applications of spectral partitioning, such as simple spectral bisection, will fail on some graphs that could arise in practice. In 1996, Spielman and Teng showed that for bounded-degree planar graphs and finite element meshes, spectral partitioning works quite well. In particular, they showed that bounded-degree planar graphs have Fiedler value at most $O(1/n)$, which implies that spectral techniques can be used to find bisectors of size at most $O\left(\sqrt{n}\right)$ in these graphs. These bounds are the best possible for planar graphs [2]. Recently in 2004, Kelner extended these results to graphs with bounded genus [3]. I summarize some of the main results of these papers below with more focus on the theorems developed in [2].

Performance of Spectral Graph Partitioning (Guattery and Miller) [1]

An example of a graph where simple spectral bisection yields poor results is shown in Figure 2. Let there be n nodes with a ladder shaped bottom and the top 2/3 of the rungs kicked out. The simple bisection method suggests partitioning the graph along the rungs which clearly yields poor results for $k \geq 3$.



Simple Spectral Bisection Optimal Bisection

Figure 2. Bisecting the Roach Graph

Let G_k be the Roach Graph parameterized by k.

Theorem IV. 1. The simple spectral bisection method produces cut size of $\Theta(n)$ for G_k, for any k.

As we will show next, there are algorithms that produce cut size of $O\left(\sqrt{n}\right)$ for bounded degree planar graphs. Hence the simple spectral method performs poorly on the family of Roach Graphs.

Spectral Method Works for Planar Graphs (Spielman and Teng) [2, 10]

There are two equivalent definitions of *planar graphs*. For concreteness, planar graphs of $n \le 4$ is shown in Figure 3.

Definition 1. A graph is planar if there exists an embedding of the vertices in $\mathbb{R}^2$, $f: V \to \mathbb{R}^2$ and a mapping of edges $e \in E$ to simple curves in $\mathbb{R}^2$, $f_e:[0,1] \to \mathbb{R}^2$ such that the endpoints of the curves are the vertices at the endpoints of the edge, and no two curve intersect in their interiors.

Definition 2. A graph is planar if there exists an embedding of the vertices in $\mathbb{R}^2$, $f: V \to \mathbb{R}^2$, such that for all pairs of edges (a,b) and (c,d) in E, with a,b,c,d distinct, the line segment from $f(a)$ and $f(b)$ does not cross the line segment from $f(c)$ and $f(d)$.

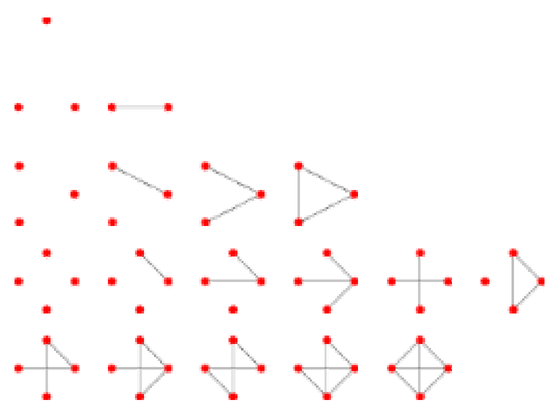


Figure 3. Planar Graphs of $n \le 4$, [6]

Lemma IV.2 (Embedding Lemma). For any dimension $d \ge 1$,

$$\lambda_2 = \min\left\{ \frac{\sum_{(i,j)\in E} \left\|\vec{x}_i - \vec{x}_j\right\|^2}{\sum \left\|\vec{x}_i\right\|^2} : \vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d, \sum_{i=1}^{n} \vec{x}_i = \vec{0} \right\}.$$

Proof: For $d = 1$, this is the standard characterization $\lambda_2 = \min_{\sum x_i = 0} \frac{\sum_{(i,j)\in E}(x_i - x_j)^2}{\sum x_i^2}$. Apply this component-wise. For $d > 1$ and all $\{\vec{x}_1, ..., \vec{x}_n\}$ such that $\sum_{i=1}^{n} \vec{x}_i = 0$,

$$\frac{\sum_{(i,j)\in E}\left\|\vec{x}_i - \vec{x}_j\right\|^2}{\sum\left\|\vec{x}_i\right\|^2} = \frac{\sum_{(i,j)\in E}\sum_{k=1}^{d}(x_{i,k} - x_{j,k})^2}{\sum_{i=1}^{n}\sum_{k=1}^{d} x_{i,k}^{\ 2}} \geq \min_k \frac{\sum_{(i,j)\in E}(x_{i,k} - x_{j,k})^2}{\sum_{i=1}^{n} x_{i,k}^{\ 2}} \geq \lambda_2 .$$

□

Theorem IV.3 (Koebe-Andreev-Thurston). Let G be a planar graph. Then, there exist a set of disks $\{D_1, ..., D_n\}$ in the plane with disjoint interiors such that D_i touches D_j iff $(i, j) \in E$.

Such an embedding is called a *kissing disk* embedding of G. An example of kissing disk embedding is shown in Figure 4.

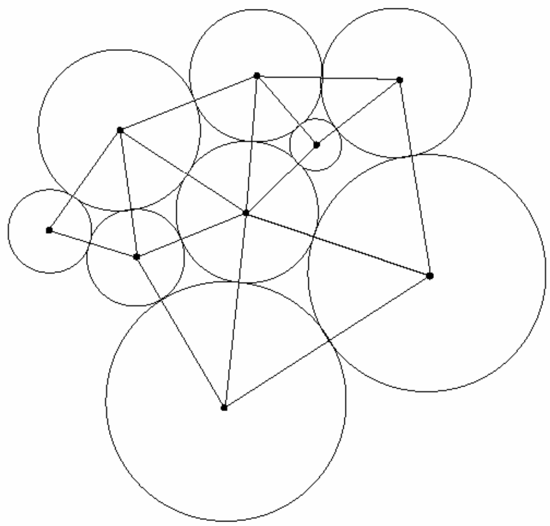


Figure 4. Kissing Disk Embedding of Planar Graphs

The analogue of a disk on the sphere is a *cap*. A cap is given by the intersection of a half-space with the sphere, and its boundary is a circle. To bound the eigenvalue, Spielman and Teng lift the disk embedding to a unit sphere in $\mathbb{R}^3$ by applying the *stereographic projection*.

Definition (Stereographic Projection). Consider a plane and a unit sphere touching the plane in its origin. Call this point on the sphere the south pole, and the point on the sphere farthest away from the plane the north pole. For a point $x \in \mathbb{R}^2$, consider the line passing through x and the north pole. Define $\pi(x)$ to be the other point x' where this line intersects the sphere.

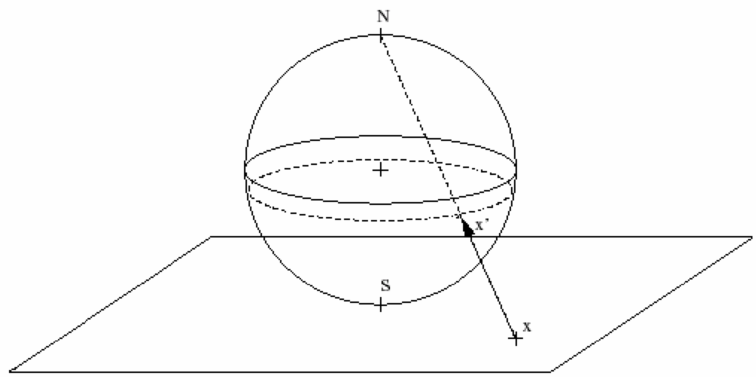


Figure 5. Stereographic Projection

Circles in the plane are mapped onto circles on the sphere. Thus the projection can lift the disk embedding $\{D_1,...,D_n\}$ to obtain a disk embedding $\{\pi(D_1),...,\pi(D_n)\}$ on the sphere. It still holds that $\pi(D_i)\cap\pi(D_j)\neq\varnothing$ iff (i,j) is an edge.

Theorem IV.4. For all planar graphs G with n vertices and maximum degree Δ, $\lambda_2 \le \frac{8\Delta}{n}$.

Proof: Let $\vec{x}_i$ be the center of $\pi(D_i)$ on the sphere. It can be shown that $\sum \vec{x}_i = 0$. Then $\|\vec{x}_i\| = 1$, $\sum_{i=1}^{n}\|\vec{x}_i\|^2 = n$. Let r_i be the radius of the cap $\pi(D_i)$, measured in a straight line from $\vec{x}_i$ to the boundary of $\pi(D_i)$. If $(i,j)\in E$, the two caps touch, and therefore $\|\vec{x}_i - \vec{x}_j\|^2 \le (r_i + r_j)^2 \le 2(r_i^2 + r_j^2)$. On the other hand, the caps are interior-disjoint and the sum of their areas does not exceed the area of the sphere, therefore $\sum \pi r_i^2 \le 4\pi$. Hence, $\sum_{(i,j)\in E}\|\vec{x}_i - \vec{x}_j\|^2 \le 2\sum_{(i,j)\in E}(r_i^2 + r_j^2) \le 2\sum_i d_i r_i^2 \le 8\Delta$. For the Fiedler value, we get $\lambda_2 \le \frac{\sum_{(i,j)\in E}\|\vec{x}_i - \vec{x}_j\|^2}{\sum\|\vec{x}_i\|^2} \le \frac{8\Delta}{n}$. Hence the Fiedler value of every bounded degree planar graph is $O(1/n)$.

□

Theorem IV.5 (Mihail). Let G be a graph of maximum degree Δ, and let $\vec{x} \perp (1,...,1)$, then $\phi_G \le \sqrt{2\Delta\frac{\vec{x}^T L_G \vec{x}}{\vec{x}^T \vec{x}}}$.

Combined with the bound on λ_2 for planar graphs, this yields a cut of ratio $\phi_G \le \sqrt{2\Delta\lambda_2} \le \frac{4\Delta}{\sqrt{n}}$ for planar graphs. Hence planar graphs have Fiedler cuts of ratio $O\left(1/\sqrt{n}\right)$.

Theorem IV.6 (Lipton-Tarjan). For any planar graph with n vertices and degrees $\vec{\Delta}_i$, there exists a bisection $\left(S,\bar{S}\right)$ with $E\left(S,\bar{S}\right) \le O\left(\sqrt{\left\|\vec{\Delta}_i\right\|^2}\right) \le \Delta\sqrt{n}$.

Now it can be shown through the following lemma that bisector of size $O\left(\sqrt{n}\right)$ can be found by repeatedly applying Fiedler ratio-partitions. Note that this recursive algorithm produces much better results than the simple spectral bisection algorithm used to partition the Roach Graph at the expense of increased complexity.

Lemma IV.7. Assume that we are given an algorithm that will find a cut of ratio at most $\phi(k)$ in every k-node subgraph of G, for some monotonically decreasing function ϕ. Then repeated application of this algorithm can be used to find a bisection of G of size at most $\int_{x=1}^{n} \phi(x)dx$.

If $\phi(x) = x^{-1/2}$, then $\int_{x=1}^{n} \phi(x)dx = 2\left(\sqrt{n}-1\right)$, giving a bisector of size $O\left(\sqrt{n}\right)$.

Spectral Partitioning for Graphs with Bounded Genus (Kelner) [3]

The genus g of a graph G is the smallest integer such that G can be embedded on a surface of genus g without any of its edges crossing one another. A sphere, disc, and annulus all have genus zero. A torus has genus one. The genus of a planar graph is 0 since it can be drawn on a sphere without self-crossing.

Kelner shows that a graph of genus g and bounded degree have Fiedler value $\lambda_2 \le O(g/n)$. This is asymptotically tight. Furthermore, he shows that there is a spectral algorithm that produces cuts of ratio $O\left(\sqrt{g/n}\right)$ and vertex bisectors of size $O\left(\sqrt{gn}\right)$. Both of these values are optimal.

REFERENCES

[1] S. Guttery and G. Miller, "On the Performance of Spectral Graph Partitioning Methods," *Proceedings of the Second Annual ACM-SIAM Symposium on Discrete Algorithms*, pp 233 – 242, 1995.

[2] D. Spielman and S.H. Teng, "Spectral Partitioning Works: Planar Graphs and Finite Element Meshes," http://math.mit.edu/~spielman/Research/spect.html, Extended abstract appeared in *IEEE Symposium on Foundations of Computer Science*, pp. 96 – 105, 1996.

[3] J. Kelner, "Spectral Paritioning, Eigenvalue Bounds, and Circle Packing for Graphs of Bounded Genus," *Proceedings of the Thirty-Sixth Annual ACM Symposium on Theory of Computing*, pp. 455 – 464, 2004.

[4] M. Fiedler, "Algebraic Connectivity of Graphs," *Czechoslovak Mathematical Journal*, 23(98):298-305, 1973.

[5] L. Babai, D. Grigoryev, and D. Mount, "Isomorphism of Graphs with Bounded Eigenvalue Multiplicity," *Proceedings of the Fourteenth Annual ACM Symposium on Theory of Computing*, pp. 310 – 324, 1982.

[6] N. Alon, "Spectral Techniques in Graph Algorithms," Lecture Notes in Computer Science 1380, Sringer, Berlin, pp. 206-215, 1998.
http://www.math.tau.ac.il/~nogaa/PDFS/spectalg.pdf

[7] M. Sipser and D. Spielman, "Expander Codes," IEEE Transactions on Information Theory, vol. 42, no. 6, pp. 1710 – 1722, Nov. 1996.

[8] N. Linial and A. Wigderson, Expander Graphs and their Applications, Lecture notes, Hebrew University, Israel, http://www.math.ias.edu/~avi/TALKS/expander_course.pdf, Jan. 2003.

[9] F. Chung, Spectral Graph Theory, American Mathematical Society, 1997.

[10] Daniel Spielman, "Spectral Graph Theory and its Applications," class notes, http://www-math.mit.edu/~spielman/eigs/, 2004.

[11] Graph Partitioning,
http://http.cs.berkeley.edu/~demmel/cs267/lecture18/lecture18.html, CS 267 Lecture notes, University of California at Berkeley, Apr. 1996.

[12] A. Ferencz, et. al., "Graph Bisection,", CS 270 Final Report, University of California at Berkeley, http://www.cs.berkeley.edu/~szewczyk/cs270/ , May 1999.