Spectral Graph Theory: Graph Clustering and Partitions

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1 Introduction

In this paper I will discuss spectral graph theory and how it can be used to find graph partitions and clusters within a graph. Spectral theory stems from linear algebra and analyzes the eigenvalues and eigenvectors of a matrix. Spectral graph theory relies on the use of matrix representations of graphs, particularly it asks how the eigenvectors and eigenvalues of the graph can be used to interpret structural graph properties. I will discuss one particularly important eigenvector, the Fiedler vector, and how the Fiedler vector can be used to find graph partitions and graph clusters. This can be applied for community detection in the real world.

2 Laplacian Matrix

Since spectral theory is focused mainly on analyzing the eigenvectors and eigenvalues of a matrix, often called the spectrum, we need a suitable matrix representation of a graph to analyze. For the purposes of this paper, we will utilize the Laplacian matrix.

The Laplacian matrix of a graph G is $L_G = D_G - A_G$ where D_G is the degree matrix of G and A_G is the adjacency matrix of G. As we shall see, the Laplacian matrix serves as a very useful tool for the study of graph clusters and partitions.

2.1 Adjacency Matrix

Given a simple undirected graph $G = (V, E)$, the adjacency matrix A_G is a $|V| \times |V|$ matrix whose entries follow the the rule:

$$a_{i,j} = \begin{cases} 1 & \text{If } (v_i, v_j) \in E \\ 0 & \text{If } (v_i, v_j) \notin E. \end{cases}$$

The result will be a symmetric matrix whose i, j entry will be a 1 if v_i and v_j are connected for vertices $v_i, v_j \in V$ and entry 0 if v_i is not connected with vertex v_j. What is of note is that since this is a **simple** undirected graph, $(v_i, v_i) \notin E$ since there are no loops in simple graphs. This means that the entries along the diagonal of the adjacency matrix are all 0.

2.2 Degree Matrix

Given a simple undirected graph $G = (V, E)$, the degree matrix D_G is a $|V| \times |V|$ matrix whose entries follow the rule:

$$d_{i,j} = \begin{cases} deg(v_i) & \text{If } i = j \\ 0 & \text{Else.} \end{cases}$$

The degree matrix merely has the degree of every vertex along its diagonal.

3 Eigenvalues and Eigenvectors of the Laplacian Matrix

In this section, I will prove certain properties regarding the eigenvalues and eigenvectors of the Laplacian matrix. For the purposes of this paper, we will assume that all eigenvectors are normalized, meaning their magnitude is 1.

3.1 Positive Semi-Definiteness of L_G

We say that a matrix M is positive semi-definite if $x^T M x$ is zero or a positive number for any real valued vector x.

Theorem: The Laplacian matrix of any simple undirected graph G, L_G, is positive semi-definite.

Proof (Jiang, 2012): Let $G = (V, E)$ be a simple undirected graph.

First let us reframe the definition of the Laplacian matrix. Recall that $L_G = D_G - A_G$, we will use an alternate definition of L_G. Let $L_{G_{\{u,v\}}}$ be an $n \times n$ matrix whose entries are defined as:

$$l_{G_{\{u,v\}}}(i,j) = \begin{cases} 1 & \text{If } i = j \text{ and } i \in \{u, v\} \\ -1 & \text{If } i = u \text{ and } j = v, \text{ or vice versa,} \\ 0 & \text{Else} \end{cases}$$

Note that with this definition, $\sum_{(u,v)\in E} L_{G_{\{u,v\}}} = L_G$. Next, note that for $x \in \mathbb{R}^n$,

$$L_{G_{\{u,v\}}} x = \begin{bmatrix} 0 \\ \vdots \\ x_u - x_v \\ \vdots \\ -x_u + x_v \\ \vdots \\ 0 \end{bmatrix}$$

where x_u, x_v represent real values entries at position u, v. Next,

$$x^T L_{G_{\{u,v\}}} x = \begin{bmatrix} x_1 & x_2 & \ldots & x_u & \ldots & x_v & \ldots & x_{n-1} & x_n \end{bmatrix} \begin{bmatrix} 0 \\ \vdots \\ x_u - x_v \\ \vdots \\ -x_u + x_v \\ \vdots \\ 0 \end{bmatrix}$$
$$= x_u^2 - x_u x_v - x_u x_v + x_v^2 = (x_u - x_v)^2.$$

Since $(x_u - x_v)^2 \geq 0$ for any $x_u, x_v \in \mathbb{R}$, we can see that $x^T L_{G_{\{u,v\}}} x \geq 0$ for any $x \in \mathbb{R}^n$. Thus, using the alternate definition, $\sum_{(u,v)\in E} x^T L_{G_{\{u,v\}}} x == x^T L_G x$. Since $x^T L_{G_{\{u,v\}}} x \geq 0$, the sum over all $(u, v) \in E$ will still be greater than or equal to 0. Thus, $x^T L_G x \geq 0$ which means that the Laplacian matrix is positive semi-definite.

The following corollary follows from the previous theorem.

Corollary: The Laplacian matrix of any simple undirected graph G, L_G, will have non-negative eigenvalues.

Proof: Counting multiplicity, for a given $n \times n$ Laplacian matrix, there will be n eigenvectors and eigenvalues for L_G. For an arbitrary eigenvalue λ, we know that there is an eigenvector z such that $L_G z = \lambda z$. If we left multiply both sides by z^T,

$$z^T L_G z = z^T \lambda z = \lambda z^T z.$$

As we have seen, $z^T L_G z \geq 0$ and it is easily shown that $z^T z > 0$ for non-zero z. Then $\lambda \geq 0$. So, all eigenvalues for L_G are non-negative.

Commentary: Let $\lambda_1, \lambda_2, ..., \lambda_n$ be the eigenvalues of an $n \times n$ Laplacian matrix. Since our eigenvalues are real non-negative values, we can assume an order for the eigenvalues of L_G where

$$0 \leq \lambda_1 \leq \lambda_2 \leq ... \leq \lambda_n.$$

3.2 Multiplicity of 0

Another interesting result of the Laplacian matrix is that the multiplicity of eigenvalues equal to 0 counts the number of connected components in the graph.

Theorem: Let $G = (V, E)$ be a graph. The multiplicity of the 0 eigenvalue is the number of connected components in G.

We will not prove this theorem, but refer to lemma 3.8 and corollary 3.10 from Jiaqi Jiang's "An Introduction to Spectral Graph Theory" for more details. This theorem however is pertinent to ensure that our method of graph partitioning functions properly. We will from now on assume our graph has only 1 connected component. Since the multiplicity of the 0 eigenvalue is equal to the number of connected components, this means that $\lambda_1 = 0 < \lambda_2$.

One may wonder why it is necessary to make this assumption. The notion of partitioning a graph which is already naturally partitioned by its lack of edges seems redundant. Of course, one can analyze how to partition a specific component of a graph, and this justifies our assumption that the graphs we are going to analyze will be connected.

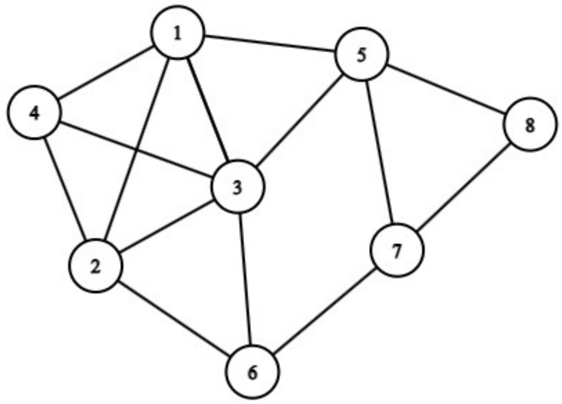
4 The Fiedler Vector

The Fiedler vector is the eigenvector that is associated with the second smallest eigenvalue. Since the smallest eigenvalue is $\lambda_1 = 0$ and we made the assumption there is only one connected component, λ_2 is the second smallest eigenvalue. What is interesting to note is that the eigenvalue λ_2 is called the "algebraic connectivity", where the greater value λ_2 is, the more well connected the graph is.

The Fiedler vector is special in that it can naturally be used to find clusters or to partition a graph. The sign value of the entries in the Fiedler vector naturally partition a graph into two clusters but there are other algorithms that you can apply to the Fiedler vector to get a more desired result.

One may naturally ask what it means for a graph to be "partitioned" or to find a "cluster". Of course, there is an intuitive sense of splitting a graph apart, but that does not give a clear idea of what is attempted here. Partitioning in a broad sense means any way to separate Let's take a look at an example.

Example: Let $G = (V, E)$ be the following graph



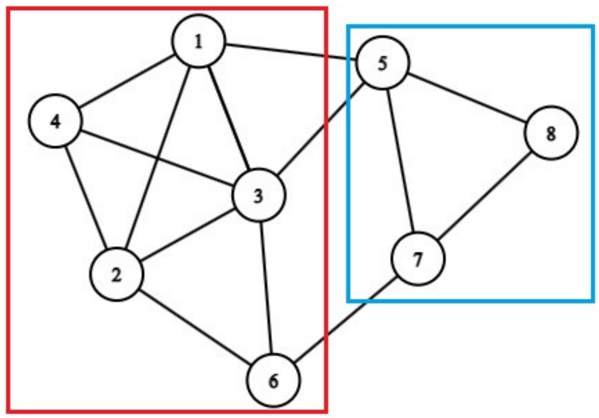
and the Laplacian matrix for this graph would be

$$\begin{bmatrix} 4 & -1 & -1 & -1 & -1 & 0 & 0 & 0 \\ -1 & 4 & -1 & -1 & 0 & -1 & 0 & 0 \\ -1 & -1 & 5 & -1 & -1 & -1 & 0 & 0 \\ -1 & -1 & -1 & 3 & 0 & 0 & 0 & 0 \\ -1 & 0 & -1 & 0 & 4 & 0 & -1 & -1 \\ 0 & -1 & -1 & 0 & 0 & 3 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & -1 & 3 & -1 \\ 0 & 0 & 0 & 0 & -1 & 0 & -1 & 2 \end{bmatrix}.$$

After calculating the eigenvalues and eigenvectors, we see that $\lambda_2 \approx 1.0659$ and the Fiedler vector is

$$\vec{F} = \begin{pmatrix} 0.2506 \\ 0.3183 \\ 0.2131 \\ 0.4043 \\ -0.2004 \\ 0.0657 \\ -0.4043 \\ -0.6473 \end{pmatrix}.$$

As we can see, the first four entries of the Fiedler vector, which correspond to the first four vertices of our graph, are solidly positive numbers while entries $5, 7, 8$ which correspond to the vertices respectively are solidly negative numbers. The sixth entry is positive but relatively closer to 0 than the other entries. Depending on the algorithm or interpretation, vertex 6 can be viewed in different ways. For now, we will group vertex 6 with vertices $1, 2, 3, 4$. Thus our partition becomes the following figure.



The Fiedler vector can be used for a very good bisection of a graph, that is partitioning a graph into two where each partition are the same size (or within one vertex difference in the case of odd number of vertices). Note that our previous partition based on signs doesn't give a perfect bisection. Since there are an even number of vertices, we should expect the partitions to have an equal number of vertices, which we do not see partitioning based only on the signs.

To address this issue, the we will use an algorithm to get a better bisection. The algorithm is as follows (Elsner, 1997):
1. Given a connected graph G, number the vertices in some way and form the Laplacian matrix L_G.

2. Calculate the eigenvector u associated with the second-smallest eigenvalue λ_2.

3. Calculate the median m_u of all the components of u.

4. Choose $V_1 = \{v_i \in V : u_i < m_i\}, V_2 = \{v_i \in V : u_i > mu\}$. If some elements of u equal m_u, distribute the vertices so that the partition is balanced.

Calculating the median to be 0.1394 and applying the algorithm, we see a bisection of the graph to be $V_1 = \{1, 2, 3, 4\}, V_2 = \{5, 6, 7, 8\}$.

5 Understanding the Fiedler Vector

It seems almost magical that such a vector is able to so effortlessly capture information such as the connectedness of vertices. Let us begin to make sense of the Fiedler vector.

First note that our ordering of the eigenvalues will come in very handy here. Since we know that the Laplacian matrix is positive semi-definite, we can write the eigenvalues λ in the form

$$\lambda = \frac{x^T Lx}{x^T x}.$$

5.1 Understanding $x^T Lx$

Let us first interpret $x^T Lx$. We can rewrite this in summation form as

$$x^T Lx = \sum_{i=1}^{n} \sum_{j=1}^{n} L_{i,j} x_j x_i = \sum_{i,j=1}^{n} L_{i,j} x_j x_i.$$

Recall our original definition of the Laplacian matrix as $L_G = D_G - A_G$. Thus,

$$\sum_{i,j=1}^{n} L_{i,j} x_j x_i = \sum_{i,j=1}^{n} (D_{i,j} - A_{i,j}) x_j x_i = \sum_{i,j=1}^{n} D_{i,j} x_j x_i - A_{i,j} x_j x_i.$$

Let us examine $D_{i,j}$ first. Since the entries of a degree matrix is 0 unless $i = j$, we can write

$$\sum_{i,j=1}^{n} D_{i,j} x_j x_i = \sum_{i=1}^{n} D_{i,i} x_i^2.$$

Note that this sum is telling us to multiply x_i^2 by the degree of the vertex v_i and add up over all vertices. Taking the sum over $x_i^2 + x_j^2$ for $(i, j) \in E$ is the same. This is because for a given x_i^2, if we sum over all edges connected to the vertex v_i, it will count exactly the degree of v_i. Thus, summing over all edges in the graph will give us the exact same sum. Thus,

$$\sum_{i=1}^{n} D_{i,i}x_i^2 = \sum_{(i,j)\in E} (x_i^2 + x_j^2).$$

Next, analyzing $A_{i,j}$. Recall that for a given entry $a_{i,j}$, the entry will be 0 if $(v_i, v_j) \notin E$ and 1 if $(v_i, v_j) \in E$. Thus, if v_i, v_j are not connected, then $A_{i,j}x_jx_i = 0$. If they are connected, then $A_{i,j}x_jx_i = x_jx_i$ Then, by summing over all i, j, we are double counting. Thus,

$$\sum_{i,j=1}^{n} A_{i,j}x_jx_i = \sum_{(i,j)\in E} 2x_ix_j.$$

Given this rewriting of the sums, we can see that

$$\sum_{i,j=1}^{n} D_{i,j}x_jx_i - A_{i,j}x_jx_i = \sum_{(i,j)\in E} (x_i^2 + x_j^2) - 2x_ix_j = \sum_{(i,j)\in E} (x_i - x_j)^2 \tag{1}$$

5.2 Understanding x^Tx

Now let us taking a look at x^Tx. It is simple to see that

$$x^Tx = \sum_{i=1}^{n} x_i^2.$$

Since we had made the assumption that all eigenvectors are normalized, $\sum_{i=1}^{n} x_i^2 = 1$.

5.3 Putting it together

Taking our original form for the eigenvalue, we are able to rewrite it

$$\lambda = \frac{x^TLx}{x^Tx} = \frac{\sum_{(i,j)\in E}(x_i - x_j)^2}{\sum_{i=1}^{n} x_i^2} = \sum_{(i,j)\in E} (x_i - x_j)^2.$$

Using this formulation, it is abundantly clear that any vector whose components are all equal will result in the 0 eigenvalue.

Here is where our ordering of the eigenvalues becomes useful. In order to find λ_2, the second **smallest** eigenvalue, we want to minimize this sum as much as possible without it becoming 0. In order to help us to that end, we will cite the following theorem.

Theorem: If A is a symmetric matrix, then any two distinct eigenvectors are orthogonal.

The Laplacian matrix is of course, symmetric. The theorem is then applicable in this situation. Given that two eigenvectors x, y are orthogonal, then $\sum_i x_i y_i = 0$. We have just noted that the vector of all the same components is an eigenvector. To make our calculations easier we can simply use $\vec{1}$ the $n \times 1$ vector of all 1s. Then, for any eigenvector x of the Laplacian matrix, $\sum_i x_i(1) = \sum_i x_i = 0$. Since our vector's components must sum to 0, our vector will contain both positive and negative components.

So, we want to find the eigenvector x that minimizes our sum in order to get the second smallest eigenvalue. Our sum,

$$\lambda_2 = \min \sum_{(i,j) \in E} (x_i - x_j)^2$$

increases when vertices with negative values are well connected with vertices of positive values.

Consider what happens if a graph's vertices are all well connected. Without loss of generality, let us assign a positive value to an arbitrary vertex. Since it is well connected, it is more likely to be connected with vertices assigned with a negative value. This will cause the sum will grow, resulting in a larger value for λ_2.

Consider instead, if a graph has an obvious 'choke point', a certain subset of vertices which are not well connected, which naturally partitions a graph. Assign positive values to one side of the partition and negative values to the other side. Since the boundary region between the two partitions are not well connected, this partition will not increase the sum by much in comparison.

References

Elsner, U. (1997). Graph partitioning-a survey.

Jiang, J. (2012). *An introduction to spectral graph theory.*