SPECTRAL GRAPH THEORY

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Abstract.
Spectral Graph Theory studies the properties of eigenvalues of different matrices related to graphs. In this paper, we consider a few basic properties before understanding the relation between the eigenvalues of a graph and its chromatic number.

1. Introduction

Spectral graph theory relates the algebraic properties of matrices (particularly eigenvalues) to their related graphs. The theory was first developed in the 1950s by graph theorists; at the same time, similar problems and questions were being pursued in the field of quantum chemistry. The field became fully formalized around 1980. In this paper we will look into some basic definitions, and then look more closely into an application of the theory to graph coloring.

2. Graphs

Definition 2.1. An *undirected graph* is a pair $G = (V, E)$ consisting of a vertex set $V = \{1, 2, \dots, |V|\}$ and an edge set $E \subseteq V \times V$ of unordered pairs.

Definition 2.2. A *directed graph* is a pair $G = (V, E)$ consisting of a vertex set $V = \{1, 2, \dots, |V|\}$ and an edge set $E \subseteq V \times V$ of ordered pairs. In other words, we give each edge an orientation.

We generally let $n = |V|$ and $m = |E|$; this notation will be used to describe graphs throughout this paper.

Definition 2.3. We say a graph is *weighted* if the edge set consists of triples (i, j, w_{ij}), where $w_{ij} \geq 0$ is the weight of an edge between i and j.

Definition 2.4. The *degree* d_i of a vertex i in an undirected graph is the number of pairs $(j, k) \in E$ such that $k = i$ or $j = i$.

In other words, this is the number of vertices that are directly connected to i.

Definition 2.5. The *adjacency matrix* of a graph is an $n \times n$ matrix A such that $a_{ij} = 1$ if there is an edge starting at i and ending at j, and 0 otherwise (in the weighted case, we let $a_{ij} = w_{ij}$ if an edge exists). Note that $a_{ij} = a_{ji}$ in undirected graphs.

Definition 2.6. The *incidence matrix* of a graph is an $n \times m$ matrix (where the graph has m edges) Q such that $q_{ij} = 0$ if the j-th edge does not contain i, $q_{ij} = -1$ if the j-th edge starts at i, and $q_{ij} = 1$ if the j-th edge ends at i (in the weighted case, we have $q_{ij} = -\sqrt{w_{ij}}$ if the jth edge starts at i and $q_{ij} = \sqrt{w_{ij}}$ if it ends at i).

Note that for undirected graphs we choose the start and end of an edge arbitrarily.

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3. The Laplacian

Definition 3.1. The *Laplacian* of a graph is the matrix L such that $L_{ii} = d_i$ for all $1 \le i \le n$, and $L_{ij} = -1$ if there is an edge between i and j (and 0 otherwise). Note that in weighted graphs, we let $L_{ii} = \sum_{j \neq i} a_{ij}$ and $L_{ij} = -w_{ij}$. We denote the Laplacian of a graph G by L_G.

Remark 3.2. For an arbitrary graph G, $L_G = QQ^T$ where Q is the incidence matrix of G.

For example, consider the cycle C_3 on 3 vertices. Its Laplacian is

$$QQ^T = \begin{pmatrix} -1 & 0 & 1 \\ 1 & -1 & 0 \\ 0 & 1 & -1 \end{pmatrix} \begin{pmatrix} -1 & 1 & 0 \\ 0 & -1 & 1 \\ 1 & 0 & -1 \end{pmatrix} = \begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix}.$$

This agrees with our definition for the Laplacian, as every vertex has degree 2 and is adjacent to every other vertex ($C_3 = K_3$).

Definition 3.3. With regards to a graph G, we denote the eigenvalues of its adjacency matrix as

$$\alpha_1 \ge \alpha_2 \ge \ldots \ge \alpha_n,$$

and the eigenvalues of its Laplacian as

$$0 = \lambda_1 \ge \lambda_2 \ge \ldots \ge \lambda_n.$$

At this point we can introduce some properties of the eigenvalues.

Theorem 3.4. *The multiplicity of* 0 *as an eigenvalue of* L_G *is the number of connected components of the graph.*

Proof. First, consider the column vector $\mathbf{c}_i$ consisting of $c_{i1}, \ldots, c_{in}$ such that $c_{ij} = 1$ if j is in the i-th connected component (which we denote by C_i) and 0 otherwise. We will show that $\mathbf{c}_i$ is an eigenvector of L_G with eigenvalue 0 for all i. Note that the j-th entry of $L_G\mathbf{c}_i$ is

$$c_{ij} = \sum_{j \in C_i} d_j + 2 \cdot \sum_{j,k \in C_i} -1 = 0.$$

Now assume $\mathbf{v}$ is a vector such that $L_G\mathbf{v} = 0$. Then

$$L_G\mathbf{v} = \mathbf{v}^T L_G \mathbf{v} = \sum_{\{i,j\} \in E(G)} (v_i - v_j)^2 = 0,$$

meaning that $v_i = v_j$ when i, j are in the same connected component. Thus $\mathbf{v}$ can be written as a linear combination of our $\mathbf{c}_i$s, so we are done. ■

Theorem 3.5 (Perron-Frobenius)**.** *For any connected weighted graph* G, $\alpha_1 \ge -\alpha_n$ *and* α_1 *has a strictly positive eigenvector.* [Spi15]

Remark 3.6. Note that an unweighted graph is simply a special case of a weighted graph where all weights are equal to 1, so this theorem holds for the unweighted case as well.

We state a few important theorems and lemmas for the proof.

Theorem 3.7 (Spectral Theorem)**.** *Let* V *be a finite-dimensional real/complex inner product space, and let* $T : V \to V$ *be a self-adjoint operator on* V. *Then all the eigenvalues of* T *are real, and there exists an orthonormal basis of* V *consisting of eigenvectors of* T.

We will not prove the Spectral Theorem here, but interested readers are encouraged to view a proof in [Li16].

Lemma 3.8. *Let A be a symmetric matrix with orthonormal eigenvectors $\mathbf{v}_1, \dots \mathbf{v}_n$ and corresponding eigenvalues $\alpha_1 \geq \dots \geq \alpha_n$. Then*

$$\alpha_1 = \max_{\mathbf{x}} \frac{\mathbf{x}^T A \mathbf{x}}{\mathbf{x}^T \mathbf{x}}.$$

Proof. By Theorem 3.7, we know that the eigenvectors form an orthonormal basis, so we can write

$$\mathbf{x} = \sum_i c_i \mathbf{v}_i$$

where $c_i = \mathbf{v}_i^T \mathbf{x}$. Then we have

$$\begin{aligned} \mathbf{x}^T A \mathbf{x} &= \left(\sum_i c_i \mathbf{v}_i \right)^T A \left(\sum_i c_i \mathbf{v}_i \right) \\ &= \left(\sum_i c_i \mathbf{v}_i \right)^T \left(\sum_i \alpha_i c_i \mathbf{v}_i \right) \\ &= \sum_i c_i^2 \alpha_i. \end{aligned}$$

Similarly, we find

$$\mathbf{x}^T \mathbf{x} = c_i^2.$$

Then

$$\frac{\mathbf{x}^T A \mathbf{x}}{\mathbf{x}^T \mathbf{x}} = \frac{\sum_i c_i^2 \alpha_i}{\sum_i c_i^2} \leq \frac{\sum_i c_i^2 \alpha_1}{\sum_i c_i^2} = \alpha_1,$$

and since we can choose $\mathbf{x} = \mathbf{v}_1$ to obtain equality, we are done. ∎

We now have the tools required to prove the Perron-Frobenius theorem.

Proof of Theorem 3.5. We first prove that $\alpha_1 \geq -\alpha_n$. Let $\boldsymbol{\phi}_n$ be the eigenvector corresponding to α_n, and let $\mathbf{x}$ satisfy $x_i = |\left(\phi_n\right)_i|$. Then

$$|\alpha_n| = |\boldsymbol{\phi}_n A \boldsymbol{\phi}_n| \leq \sum_{u,v} A_{uv} \mathbf{x}_u \mathbf{x}_v \leq \alpha_1 \mathbf{x}^T \mathbf{x} = \alpha_1,$$

so $\alpha_1 \geq -\alpha_n$.

Now let $\boldsymbol{\phi}_1$ be an eigenvector of α_1, and let $\mathbf{x}$ satisfy $x_i = \left(\phi_1\right)_i$ for all i. Then $\mathbf{x}^T \mathbf{x} = \boldsymbol{\phi}_1^T \boldsymbol{\phi}$, so

$$\mathbf{x}^T A \mathbf{x} = \sum_{u,v} A_{uv} |\left(\phi_1\right)_u| |\left(\phi_1\right)_v| \geq \sum_{u,v} A_{uv} \left(\phi_1\right)_u \left(\phi_1\right)_v = \boldsymbol{\phi}_1^T A \boldsymbol{\phi} = \alpha_1.$$

Now, note that

$$\alpha_1 \leq \frac{\mathbf{x}^T A \mathbf{x}}{\mathbf{x}^T \mathbf{x}},$$

so

$$\alpha_1 = \frac{\mathbf{x}^T A \mathbf{x}}{\mathbf{x}^T \mathbf{x}}$$

and thus $\mathbf{x}$ is an eigenvector of α_1. Then $\mathbf{x}$ is strictly positive. ■

Theorem 3.9. *For a graph G, $\alpha_n = -\alpha_1$ if and only if it is bipartite.*

Proof. First, assume that the graph is bipartite, or that there are sets X and Y such that every edge has $i \in X$ and $j \in Y$ or vice versa. Let $\boldsymbol{\phi}_1$ be an eigenvector corresponding to α_1. Then take $\mathbf{x}$ such that $x_i = (\phi_1)_i$ if $i \in U$ and $x_i = -(\phi_1)_i$ otherwise. Then $\mathbf{x}$ is an eigenvector of eigenvalue $-\alpha_1$.

Similarly, assume $\alpha_n = -\alpha_1$, and construct $\mathbf{x}$ in the same way as described above. Then

$$|\alpha_n| = |\boldsymbol{\phi}_n A \boldsymbol{\phi}_n| = \left| \sum_{u,v} A_{uv} (\phi_n)_u (\phi_n)_v \right| \leq \sum_{u,v} A_{uv} x_u x_v \leq \alpha_1 \mathbf{x}^T \mathbf{x} = \alpha_1.$$

For equality we must have $\mathbf{x} = c\boldsymbol{\phi}_1$. Note that to have equality of the third and fourth terms, $\text{sgn}((\phi_n)_u (\phi_n)_v)$ must be constant across terms. Here it is negative, so each edge is between a vertex such that $(\phi_n)_u > 0$ and a vertex such that $(\phi_n)_v) < 0$. This gives a valid partition into two sets, so the graph is bipartite. ■

4. Graph Coloring

Definition 4.1. A *coloring* of a graph consists of an assignment of a color to each vertex such that no adjacent vertices share the same color. The *chromatic number* $\chi(G)$ of a graph is the minimum number of colors necessary for a valid coloring of G to exist.

Theorem 4.2 (Wilf)**.** $\chi(G) \leq \alpha_1 + 1$.

We omit this proof, but it can be found in [Wil67].

Theorem 4.3. *If $|E| \neq 0$, $\chi(G) \geq 1 - \frac{\alpha_1}{\alpha_n}$.* [CB20]

To prove this theorem, we first need to state the following lemma:

Lemma 4.4. *Let $k \geq 2$ be an integer. Define*

$$A = \begin{pmatrix} A_{1,1} & A_{1,2} & \dots & A_{1,k} \\ A_{1,2}^T & A_{2,2} & \dots & A_{2,k} \\ \vdots & \vdots & \ddots & \vdots \\ A_{1,k}^T & A_{2,k}^T & \dots & A_{k,k} \end{pmatrix}$$

to be a block-partitioned symmetric matrix. Then

$$(k-1)\lambda_{min}(A) + \lambda_{max}(A) \leq \sum_i \lambda_{max}(A_{i,i}).$$

We will not prove this lemma here, but it is necessary for the proof of Theorem 4.3. We are now ready to prove our theorem.

Proof of Theorem 4.3. Assume that G is a k-colorable graph. Then its adjacency matrix A can be written as follows:

$$A = \begin{pmatrix} \mathbf{0} & A_{1,2} & \dots & A_{1,k} \\ A_{1,2}^T & \mathbf{0} & \dots & A_{2,k} \\ \vdots & \vdots & \ddots & \vdots \\ A_{1,k}^T & A_{2,k}^T & \dots & \mathbf{0} \end{pmatrix}$$

where each block corresponds to some color used in the coloring. By Lemma 4.4, we have

$$(k-1)\lambda_{\min}(A) + \lambda_{\max}(A) \leq 0.$$

In addition, we know that $\lambda_{\min}(A) = \alpha_n < 0$ and $\lambda_{\max}(A) = \alpha_1$, so we have

$$k \geq \frac{\lambda_{\max}(A) - \lambda_{\min}(A)}{-\lambda_{\min}(A)} = \frac{\alpha_1 - \alpha_n}{-\alpha_n} = 1 - \frac{\alpha_1}{\alpha_n}$$

as desired.

■

5. Conclusion

Spectral graph theory allows us to use the algebraic properties of the adjacency matrix and other related matrices to observe properties of the graphs themselves. Other applications of the theory include calculating the number of spanning trees of a graph, finding structural properties of random graphs, and related problems.

References

[CB20] Omid Sadeghi Catherine Babecki, Kevin Liu. A brief introduction to spectral graph theory. 2020.

[Li16] Jenny Li. A brief introduction to spectral graph theory. 2016.

[Spi15] Dan Spielman. The adjacency matrix and graph coloring. 2015.

[Wil67] Herbert S. Wilf. The eigenvalues of a graph and its chromatic number. *Journal of The London Mathematical Society-second Series*, 1967.