陽明交通大學

百川學士學位學程

專題探索(一)專題大綱計劃書

題目:
譜圖論-探討圖與矩陣之間的關係

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**•動機**

在大一上接觸到線性代數的基本數學知識，結合在過去高中於人才培育學習到的圖論尤為深刻，又因應著現今多元領域整合應用，響應百川的理念，並透過導師介紹研究這個圖論分支的-譜圖論。

**•Abstract**

Spectral graph theory is a discipline that delves into the in-depth study of the interrelationships between graph structures and matrices. Its core concepts encompass the constituent elements of the Laplacian graph, including the Laplacian matrix, eigenvalues, and the corresponding eigenvectors.

A graph G = (V, E) consists of a set of vertices V and a set of edges E. Spectral graph theory primarily focuses on the structural properties of graphs and their associations with matrices. The Laplacian matrix, denoted as L = D - A, is a central concept in this field. It is formed by the difference between the degree matrix (D) and the adjacency matrix (A). The eigenvalues of this matrix play a crucial role in exploring properties such as clustering, connectivity, and partitioning of graphs, finding applications in various academic domains.

In the study of spectral graph theory, special attention is given to the Graph Laplacian Eigenvalue Problem (GLEP), which concentrates on simple, undirected, and connected graphs. The goal of GLEP is to compute the minimum eigenvalue of the Laplacian matrix. Researchers often employ iterative methods, such as the Shift-Invert Residual Arnoldi Method (SIRA), to approximate this objective. These methods excel in handling large sparse matrices, facilitating in-depth investigations into the eigenvalues and eigenvectors of Laplacian matrices, revealing both the geometric and algebraic structures of graphs.

Pagerank is another application area of spectral graph theory, particularly widely used in network analysis. This algorithm assesses the importance of nodes in a network based on the linking structure and weight distribution between nodes. The computed Pagerank scores are then employed for tasks such as web page ranking and recommendation, providing a powerful tool for network ranking and analysis.

Bipartite graphs represent a specific application domain within spectral graph theory. These graphs have nodes divided into two disjoint sets, with edges only existing

between the two sets. From the perspective of spectral graph theory, studying the isomorphic properties of bipartite graphs involves the analysis of Laplacian matrices and adjacency matrices to establish one-to-one mappings between different bipartite graphs.

**•Introduction**

1.linear transformation

Linear transformation is a method of describing the mapping of one vector space to another while preserving straight-line characteristics, preventing distortion, and maintaining the position of the origin. In essence, linear transformations ensure that grid lines remain parallel and equidistant, thereby preserving the properties of additivity and homogeneity in scalar multiplication.

Additivity: A(u+v)=Au+Av.
Homogeneity: A(cx)=cA(x)

In the two-dimensional vector space, we set the initial vectors as Î and ĵ, which represent the unit vectors of the x-axis and y-axis respectively. For example, Î can be expressed as (1,0) and ĵ can be expressed as (0, 1).

Suppose we want to represent a vector (2,3), which can be expressed as 2Î+3ĵ. The linear transformation tracks what these basis vectors Î and ĵ look like after transformation. For example, suppose that after linear transformation, the output of Î is (1,2), and the output of ĵ is (3,0). We can represent this transformation as a matrix:

$$\begin{matrix} 1 & 3 \\ 2 & 0 \end{matrix}$$

Therefore we can write it as a mathematical formula:

Au=b

$$\begin{matrix} a & b \\ c & d \end{matrix} \cdot \begin{matrix} x \\ y \end{matrix} = \mathrm{x} \cdot \begin{matrix} a \\ c \end{matrix} + \mathrm{y} \cdot \begin{matrix} b \\ d \end{matrix} = \begin{matrix} ax + by \\ cx + dy \end{matrix}$$

2.Eigenvalues and corresponding eigenvectors

During linear transformations, most vectors depart from their original space. However, certain specific vectors undergo only a scaling of their length without any rotation. These vectors are referred to as eigenvectors, and the scaling factor they correspond to is known as the eigenvalue. This type of linear transformation can be expressed in standard form as:

$$Av=\lambda v$$

where v is the eigenvector, and$\lambda$is the corresponding eigenvalue. This expression signifies that a specific vector, when subjected to a linear transformation, retains its original direction and experiences only a scaling change. The existence of such eigenvectors and eigenvalues allows us to comprehend linear transformations without relying on specific coordinate systems. Instead, by uncovering eigenvectors and eigenvalues, we reveal the fundamental properties of the transformation.

3.G=(V,E)

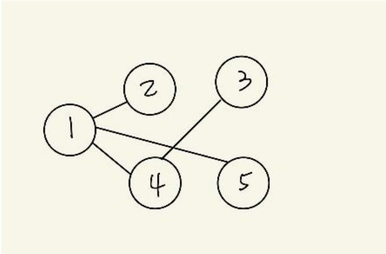
The basic structure of a graph G consists of a set of vertices V and a set of edges E. The vertex set V contains all points, while the edge set E comprises unordered pairs representing connections between points. Each edge can be represented by an unordered pair {x, y}, where x and y represent the two endpoints. This structure allows us to clearly represent and understand graphs, modeling the relationships between different entities or abstract concepts through the connections between nodes and edges.

Simple Graph:
In the edge set, there are no self-loops {x, x} connecting a point to itself, and there are no instances of two points having more than two edges.

Undirected Graph:
There is no directional relationship between nodes, meaning {x, y} is equivalent to {y, x}.

4.Laplacian graph
Consider a matrix representing a simple undirected graph, documenting the distribution of edges between each pair of vertices. The degree matrix (Figure 2) has its main diagonal recording the number of connections each vertex has with other vertices. Additionally, the adjacency matrix records how vertices are connected to each other, for example:

$$G=\{\ (1,2),\ (1,4),\ (1,5),\ (3,4)\ \}$$




Degree matrix:

The degree matrix is a diagonal matrix, where the main diagonal elements Dii, correspond to the degree of the ith node in the graph, correspond to the degree of the ith node in the graph.

$$D \begin{bmatrix} 3 & & & & \\ & 1 & & & \\ & & 1 & & \\ & & & 2 & \\ & & & & 1 \end{bmatrix}$$

Adjancency matrix:

The adjacency matrix is a symmetric matrix, where Aij equals 1 if the ith and jth nodes are connected, and it equals 0 if they are not connected.

$$A \begin{bmatrix} 0 & 1 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Laplacian matrix:

The Laplacian matrix is the difference between the degree matrix and the adjacency matrix:L=D-A.

$$L \begin{bmatrix} 3 & -1 & 0 & -1 & -1 \\ -1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 \\ -1 & 0 & -1 & 2 & 0 \\ -1 & 0 & 0 & 0 & 1 \end{bmatrix}$$

The Laplacian matrix has some properties:

Symmetric:

A=AT.

Eigenvalue are real number:

$$\begin{aligned}\lambda \|v\|^2 &= \lambda \langle v, v\rangle \\ &= \langle \lambda v, v\rangle \\ &= \langle Lv, v\rangle \\ &= \langle v, Lv\rangle \\ &= \langle v, \lambda v\rangle \\ &= \bar{\lambda} \langle v, v\rangle \\ &= \bar{\lambda} \|v\|^2\end{aligned}$$

Eigenvalue are positive:

$$(u_1, \ldots, u_n) L \begin{pmatrix} u_1 \\ \vdots \\ u_n \end{pmatrix} = \sum_{(x_i, x_j) \in E} (u_i - u_j)^2.$$

The relationship between the eigenvalues of the Laplacian matrix and the properties of a graph provides valuable insights into its structure and connectivity.

1.The smallest eigenvalue is always zero, this is because the sum of each row and each column of the matrix is zero, corresponding to an eigenvector that is a constant vector of ones. This zero eigenvalue reflects the existence of a nontrivial connected component in the graph, indicating an overall cyclic structure.

2.The corresponding eigenvector is a constant vector, this eigenvector indicates the presence of a connected component in the graph where all nodes are mutually connected.

3.The second smallest eigenvalue is positively correlated with graph connectivity, this eigenvalue provides information about the connected components in the graph, and its magnitude reflects the degree of connectivity.

4.Larger eigenvalues indicate stronger overall connectivity of the graph Larger eigenvalues of the Laplacian matrix indicate stronger overall connectivity of the graph. This implies that nodes in the graph are more interconnected, leading to a denser overall structure.

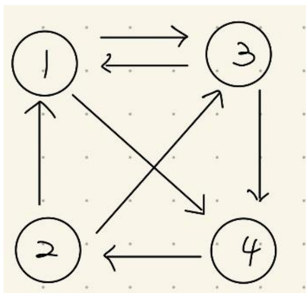
**•Application**

1.Pagerank

The core of the Pagerank algorithm lies in constructing a transition probability matrix, treating each website as a node and employing the concept of a weighted graph. In this transition probability matrix, each row and column represent a website, and matrix elements indicate the probability of transitioning from one website to another through hyperlinks.

The construction of this probability matrix is based on the hyperlink structure between web pages, where each hyperlink is regarded as an edge between websites. The concept of a weighted graph is introduced to distinguish the weights of different hyperlinks, representing the weight passed through a hyperlink.

The goal of the Pagerank algorithm is to find a steady state, a specific state where the transition probability matrix, when acting on this steady state, results in each element of a row being equal to the corresponding element of that row, i.e., Ax=x. This steady state reflects the ranking of each website, with higher-ranked websites having greater weight in this state, thus considered more important.
For example:




Then we can write the relationship:

$$X1=\frac{1}{2}X2+\frac{1}{2}X3$$

$$X2=X4$$

$$X3=\frac{1}{2}X1+\frac{1}{2}X2$$

$$X4=\frac{1}{2}X1+\frac{1}{2}X3$$

And the corresponding matrix is:

$$Av=v$$

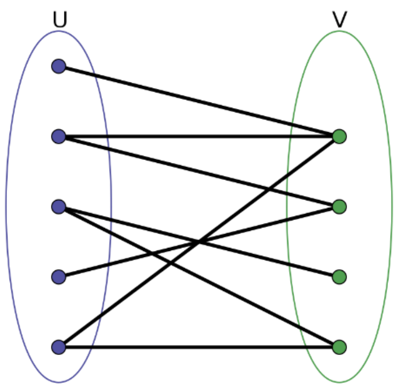
$$A=\begin{bmatrix} 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 1 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 \end{bmatrix}, v=\begin{matrix} X1 \\ X2 \\ X3 \\ X4 \end{matrix}$$

Find that the answer $v=\begin{matrix} 1 \\ 1 \\ 1 \\ 1 \end{matrix}$, show that the four websites score are even.

2.bipartitie

In graph theory, if there exist two mutually exclusive independent sets U and V, we can represent this as a bipartite graph in the form G = (U, V, E). The adjacency matrix of a bipartite graph has a diagonal matrix structure, and its eigenvalues and eigenvectors provide information about the graph's partitioning and connectivity.

Through spectral decomposition, the adjacency matrix of a bipartite graph can be decomposed into the form of a diagonal matrix, representing the existence of two independent sets in the graph. The eigenvalues and eigenvectors reflect the graph's partitioning and reveal characteristics of connectivity. By examining the strength of connections through the formation of corresponding eigenvectors, we can use them to determine the strength of relationships between two distinct groups.




•Conclusion

In conclusion, the applications of spectral graph theory extend beyond the realms of linear transformations, eigenvalues, and Laplacian matrices, permeating diverse fields such as biology, social network analysis, recommendation systems, and ecology.

In the field of biology, spectral graph theory finds application in bioinformatics, where graphs model biological interactions and relationships. Analyzing biological networks using Laplacian matrices can reveal crucial information about the functional connectivity of biomolecular entities, aiding in the identification of key components and understanding complex biological processes.

Social network analysis leverages spectral graph theory to unravel patterns and structures within social interactions. By representing individuals as nodes and relationships as edges, spectral methods provide insights into community detection, identifying influential individuals, and understanding the overall structure of social networks.

Pagerank, as a manifestation of spectral graph theory, plays a pivotal role in web page ranking and recommendation systems. The algorithm, rooted in the properties of the transition probability matrix, reflects the importance of web pages based on their connectivity. This concept extends to recommendation systems, where the connectivity of items or users is harnessed to provide personalized recommendations.

Bipartite graphs, as explored in the context of spectral graph theory, have implications in ecological studies. Representing interactions between species or different ecological components, the eigenvalues and eigenvectors of the adjacency matrix can reveal underlying patterns in species associations, aiding in the understanding of ecological networks and the dynamics of ecosystems.

In essence, the versatility of spectral graph theory allows for a nuanced exploration of structural relationships in various domains. Whether unraveling biological complexities, deciphering social structures, enhancing recommendation systems, or understanding ecological interdependencies, the application of spectral graph theory offers a powerful analytical framework with broad implications across interdisciplinary research.

**•目前進度/心得/未來展望**

在這次的數學研究中，我重新認識到數學具有除了理論層面外的多種應用面向。這包括從各種資料中找到與其他領域結合的應用，雖然我目前的理論知識還遠未達論文水平，只能簡單闡述理論的基本應用。對於一些術語如聯通性或

分群的實際含義，我還沒有足夠深入的了解。因此，這次的專題注重在已知知識的基礎上進一步延伸，並探討特徵值的多重涵義。

在和老師的討論中，我了解到譜圖論的應用仍有許多創新的可能性，而在許多領域中的實際應用我目前並沒有足夠的基礎來應對。在下次的專題中，我將更加著重於特徵值在各種應用中的地位，並期望能夠結合程式開發不同的應用，以呈現出更為豐富的報告內容。

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