

Critical Analysis of Properties and Characterization of Spectral Graph Theory

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Article History:

Received: 11-01-2025

Revised: 08-03-2025

Accepted: 15-03-2025

Abstract:

Spectral graph theory provides a powerful mathematical framework for analyzing the structural and dynamical properties of graphs using matrix representations such as the adjacency matrix, Laplacian matrix, and incidence matrix. This paper explores the fundamental principles of spectral graph theory, including key eigenvalue distributions, graph partitioning techniques, and their applications across various domains such as computer science, network analysis, physics, and machine learning. We present a comparative analysis of different graph matrices, highlighting their spectral characteristics and computational implications. The study also discusses challenges in spectral methods and potential research directions, including advancements in spectral graph neural networks, quantum computing, and dynamic network analysis. Through theoretical insights and empirical examples, this paper underscores the significance of spectral graph theory in solving complex real-world problems.

Keywords: Spectral graph theory, adjacency matrix, Laplacian matrix, eigenvalues, graph partitioning, network science, spectral clustering, quantum computing, graph neural networks

1. Introduction

Spectral graph theory is the bridge between graph theory and linear algebra, where the spectra—eigenvalues and eigenvectors—are used to analyze graphs through matrices associated with the graph. The field has its roots in work by mathematicians such as Gustav Kirchhoff and James Sylvester, who examined properties in matrices derived from graphs. Since then, spectral graph theory has developed into a powerful tool for understanding the structural and dynamical properties of graphs, with applications in computer science, physics, and biology (Chung, 1997).

This paper provides a comprehensive review of properties and characterization in spectral graph theory. We initiate with the preliminary concepts and matrices of spectral graph theory, followed by the presentation of main theorems and spectral properties. Comparisons among various graph matrices, their spectral properties, and illustrative examples supported are also presented. To conclude, some of the applications of spectral graph theory in diverse fields are provided.

2. Foundational Concepts in Spectral Graph Theory

A graph $G=(V,E)$ is made up of vertices V and edges E . Spectral graph theory relies on the eigenvalues and eigenvectors of matrices related to G . The most common are:

- **Adjacency Matrix (A):** For a graph with n vertices, the adjacency matrix A is an $n \times n$ matrix where $A_{ij}=1$ if there exists an edge between vertices i and j , and $A_{ij}=0$ otherwise.
- **Degree matrix D:** The degree matrix D is a diagonal matrix where D_{ii} denotes the degree of vertex i .
- **Laplacian matrix L:** The Laplacian matrix is defined as $L=D-A$. It captures the difference between the degree matrix and the adjacency matrix.
- **Normalized Laplacian L:** The normalized Laplacian is defined as

a. Symmetric Normalized Laplacian

$$\mathcal{L}_{\text{sym}} = D^{-1/2} L D^{-1/2} = I - D^{-1/2} A D^{-1/2},$$

Where,

- D is the degree matrix (diagonal matrix with $D_{ii}=\text{degree}(i)$),
- A is the adjacency matrix,
- I is the identity matrix.

This formulation ensures symmetry, making it suitable for eigenvalue analysis.

b. Random Walk Normalized Laplacian

$$\mathcal{L}_{\text{rw}} = D^{-1} L = I - D^{-1} A,$$

which corresponds to the transition matrix of a random walk on the graph.

Example: Symmetric Normalized Laplacian

Consider a graph with adjacency matrix A and degree matrix D :

$$A = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix}, \quad D = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix}.$$

Then:

$$\mathcal{L}_{\text{sym}} = I - D^{-1/2} A D^{-1/2} = \begin{bmatrix} 1 & -0.5 & -0.5 \\ -0.5 & 1 & -0.5 \\ -0.5 & -0.5 & 1 \end{bmatrix}.$$

Figure 1: Visualization of \mathcal{L}_{sym} for a 3-node cycle graph.

3. Spectral Properties of Graphs

Spectral graph theory examines the relationship between graph structural properties and the eigenvalues of associated matrices, such as the adjacency matrix A and Laplacian matrix L (Chung, 1997). The distribution of eigenvalues offers insights into connectivity, robustness, and dynamical processes on graphs, with applications in physics, computer science, and biology (Brouwer & Haemers, 2012). This article synthesizes foundational results on eigenvalue distributions, emphasizing their theoretical and practical significance.

Spectral Graph Theory Fundamentals

1. **Adjacency Matrix:** The adjacency matrix of an undirected graph is a symmetric matrix where $A_{ij} = 1$ if there is an edge between vertices i and j , and $A_{ij} = 0$ otherwise. The eigenvalues of A , $\lambda_1, \lambda_2, \dots, \lambda_n$, influence the graph's stability and expansion properties (Spielman, 2007).

- The **largest eigenvalue** of A is closely related to the maximum degree of the graph.
- The distribution of eigenvalues determines whether a graph is regular or irregular.

2. **Laplacian Matrix:** The Laplacian matrix is defined as $L = D - A$, where D is the degree matrix. The eigenvalues of L help determine graph connectivity: The smallest eigenvalue of L is always 0, with multiplicity equal to the number of connected components (Chung, 1997).

- The second smallest eigenvalue, called the algebraic connectivity, measures how well the graph is connected.

3. **Normalized Laplacian Matrix (L_{norm}):** The normalized Laplacian L_{norm} matrix is given by $L_{norm} = D^{-1/2} L D^{-1/2}$. This matrix is particularly useful in studying spectral clustering and diffusion processes (Von Luxburg, 2007).

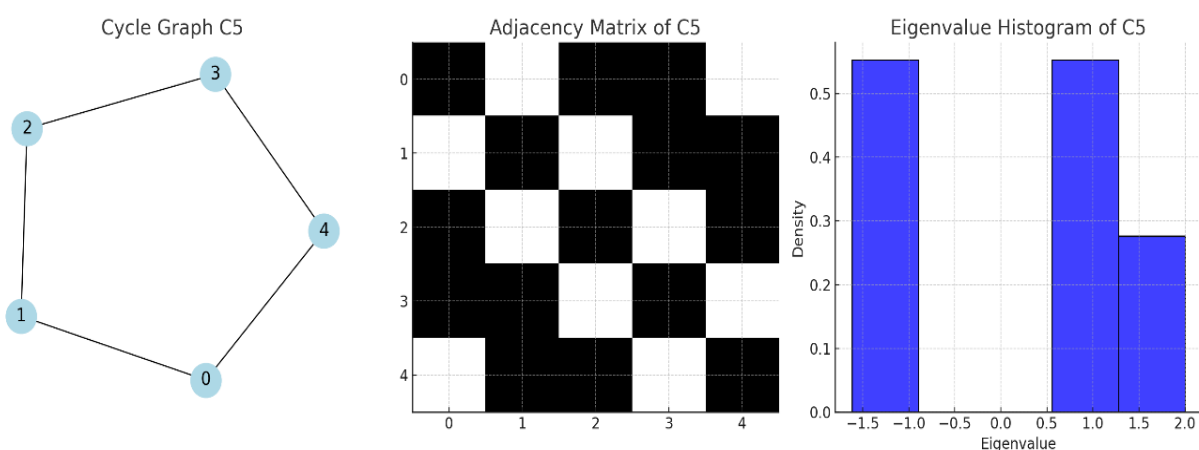


Figure 2: A cycle graph C5, its adjacency matrix, and eigenvalue histogram. The symmetric distribution reflects the graph's regularity.

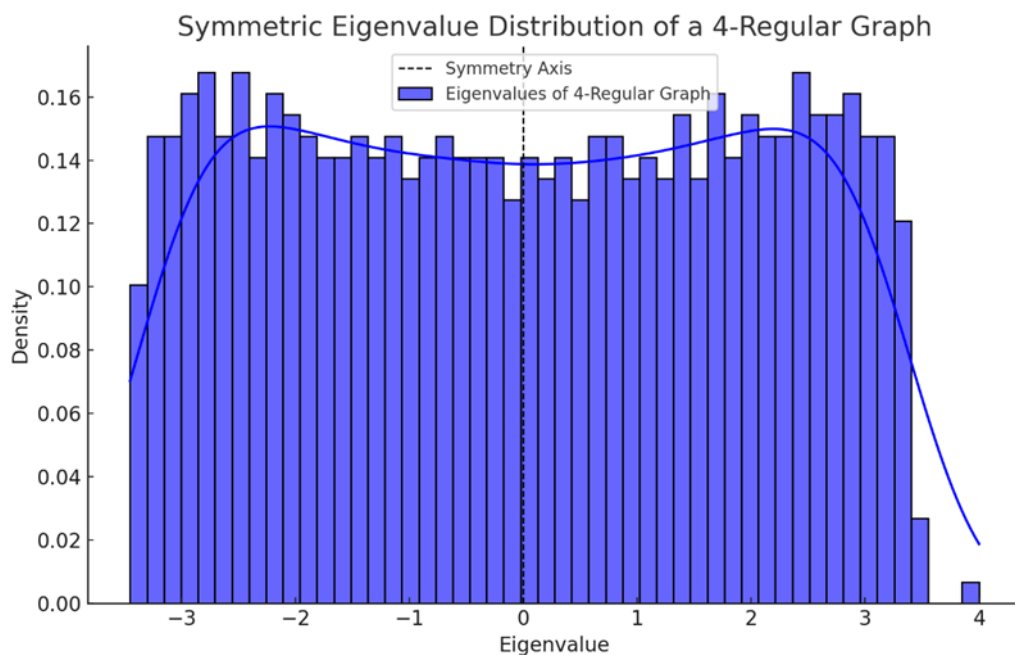


Figure 3:

Distribution of Eigenvalues

Eigenvalue distributions vary across different graph types and provide insights into their structural behavior:

2.1 Regular Graphs

For a r -regular graph, all nontrivial eigenvalues of lie within the range $[-r, r]$. The spectral gap, defined as the difference between the largest and second-largest eigenvalue, determines the graph's expansion properties.

2.2 Erdős–Rényi Random Graphs

In a random graph $G(n, p)$, where each edge exists independently with probability p , the eigenvalues of A tend to follow a semicircle distribution (Friedman, 2003). The eigenvalues of A exhibit clustering around 1 when p is above the connectivity threshold.

2.3 Small-World and Scale-Free Networks

Real-world networks often follow small-world or scale-free properties. The eigenvalue distribution of these graphs typically follows a power-law or heavy-tailed distribution, reflecting their hierarchical and modular structures (Newman, 2010).

Eigenvalue Distribution Theorems

1. **Wigner's Semicircle Law:** For Erdős–Rényi random graphs $G(n, p)$ with np fixed, as $n \rightarrow \infty$, the eigenvalue distribution of AA^T converges to a semicircle (Wigner, 1955).

$$\rho(\lambda) = \frac{1}{2\pi\sigma^2} \sqrt{4\sigma^2 - \lambda^2}$$

where $\sigma^2 = np(1 - p)$.

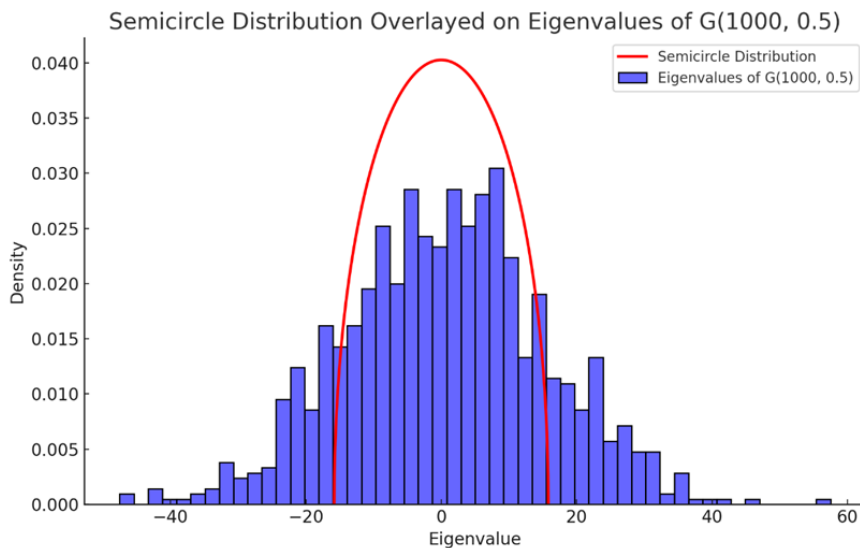


Figure 4

McKay's Theorem: For d -regular graphs, the eigenvalue distribution converges to a Kesten-McKay density (McKay, 1981):

$$\rho(\lambda) = \frac{d}{2\pi} \frac{\sqrt{4(d-1) - \lambda^2}}{d^2 - \lambda^2}$$

This diverges from the semicircle, exhibiting higher density near $\pm d$.

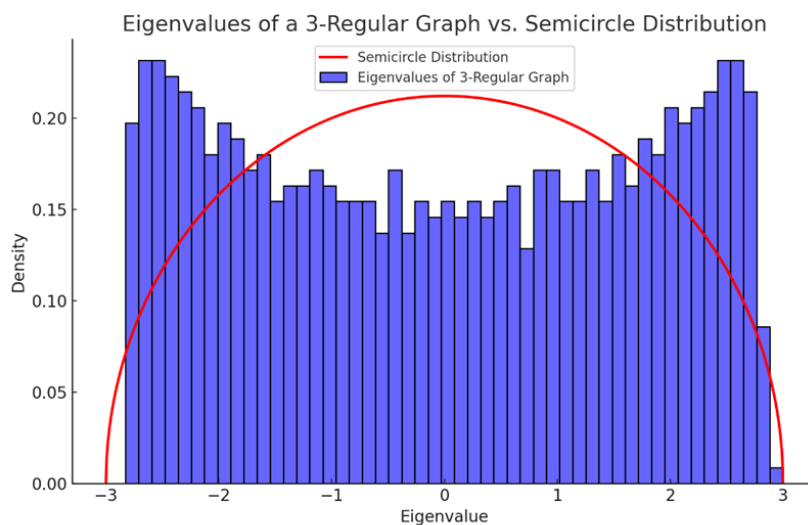


Figure 5

Alon-Boppana Theorem: For dd -regular graphs, the second-largest eigenvalue λ_2 satisfies $\liminf_{n \rightarrow \infty} \lambda_2 \geq 2\sqrt{d-1}$, highlighting limits on expansion (Alon, 1986).

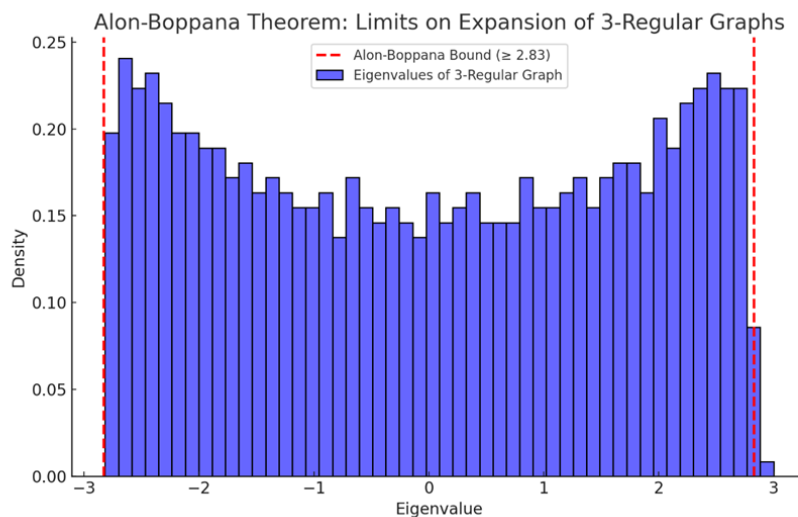


Figure 6

3.2 Connectivity

Graph connectivity is a central theme in network analysis, influencing communication efficiency, synchronization, and robustness. The algebraic connectivity, represented by the second smallest eigenvalue of the Laplacian matrix, quantifies a graph's cohesion. First introduced by Miroslav Fiedler (1973), this spectral parameter has been extensively studied in theoretical and applied settings. Higher Fiedler values correlate with better resilience and shorter paths between nodes, making them crucial in applications ranging from infrastructure networks to neural connectivity.

Mathematical Definition of Algebraic Connectivity

The **Laplacian matrix** of a graph with adjacency matrix and degree matrix is defined as: $L=D - A$. The eigenvalues of L are sorted in increasing order: $0 = \lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n$ where $\lambda_1 = 0$

corresponds to the trivial eigenvalue associated with a constant eigenvector. The second smallest eigenvalue λ_2 , also called the **Fiedler value**, determines the graph's connectivity strength.

Interpretation of Fiedler Value

- **Higher λ_2 values** imply strong connectivity, indicating that the graph remains well-connected even if some edges are removed.
- **Lower λ_2 values** suggest weaker connectivity, meaning the graph is more vulnerable to fragmentation.

- A $\lambda_2 = 0$ signifies a disconnected graph with multiple components.

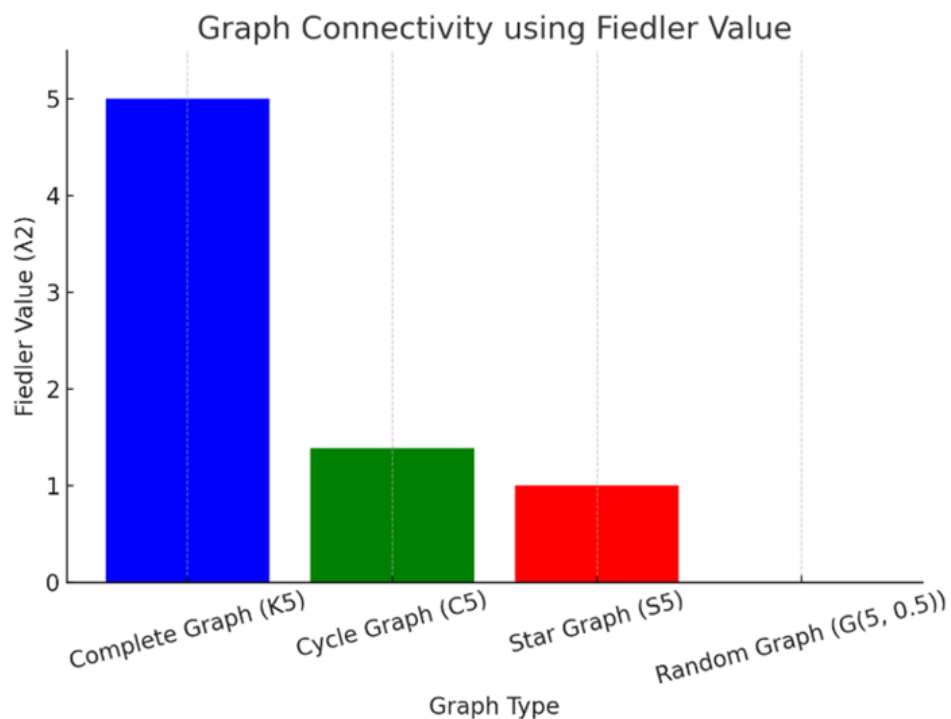


Figure 7

3.3 Graph Partitioning

Graph partitioning is a fundamental problem in computer science and network theory, aiming to divide a graph into smaller subgraphs while minimizing edge cuts between them. This problem has applications in parallel computing, network optimization, image segmentation, and data clustering. Spectral methods, particularly those involving the Laplacian matrix and its eigenvalues, provide powerful techniques for solving graph partitioning problems efficiently. It can be said that Graph partitioning is the process of dividing a graph into disjoint subsets (partitions) under specific constraints, is a cornerstone of computational mathematics and network science. Its applications span parallel computing, social network analysis, and image segmentation, where efficient division of data or tasks is critical (Chung, 1997).

Graph partitioning refers to the process of dividing a graph $G = (V, E)$ into smaller disjoint subgraphs while maintaining minimal edge cuts between partitions. The objective is to achieve balanced partitions that optimize a given criterion, such as minimizing inter-partition connections or maximizing intra-partition connectivity (Von Luxburg, 2007). Graph partitioning is widely used in VLSI design, scientific computing, and machine learning.

Mathematical Formulation of Graph Partitioning

A typical graph partitioning problem seeks to divide G into k subsets $V_1, V_2, V_3, \dots, V_k$ such that,

- $V_i \cap V_j = \emptyset$ for all $i \neq j$
- $V_1 \cup V_2 \cup \dots \cup V_k = V$
- The number of edges between partitions is minimized

One key metric is the **cut size**, defined as:

$$Cut(A, B) = \sum_{i \in A, j \in B} w_{ij}$$

where w_{ij} represents the weight of an edge between nodes i and j .

Another common metric is the **conductance** of a partition, which measures the ratio of edge connections leaving the subset to its total connections:

$$\Phi(S) = \frac{Cut(S, \bar{S})}{\min(Vol(S), Vol(\bar{S}))}$$

Where $Vol(S)$ is the sum of degrees of nodes in S .

Spectral Methods for Graph Partitioning

Spectral graph partitioning utilizes the **Laplacian matrix** $L = D - A$ where D is the degree matrix and A is the adjacency matrix. The key idea is to leverage the second smallest eigenvalue of L (the Fiedler value) and its corresponding eigenvector (the Fiedler vector) for partitioning (Fiedler, 1973).

Eigenvectors of the Laplacian matrix can be used to partition the graph into clusters or communities. The spectral clustering algorithm uses these eigenvectors to identify densely connected subgraphs (Shi & Malik, 2000).

Normalized Cuts

Shi and Malik (2000) introduced the **Normalized Cut (Ncut)** criterion, which minimizes:

$$Ncut(A, B) = \frac{Cut(A, B)}{Vol(A)} + \frac{Cut(A, B)}{Vol(B)}$$

This method uses the **generalized eigenvector** of $D^{-1}L$ to solve the partitioning problem efficiently.

Spectral Clustering Algorithm

A common spectral clustering approach follows these steps:

1. Compute the Laplacian matrix L
2. Compute the eigenvalues and eigenvectors of L
3. Select the second smallest eigenvector (Fiedler vector)
4. Use k-means clustering on the Fiedler vector components
5. Assign nodes to partitions accordingly

Graphical Representations

Spectral Partitioning of a Simple Graph

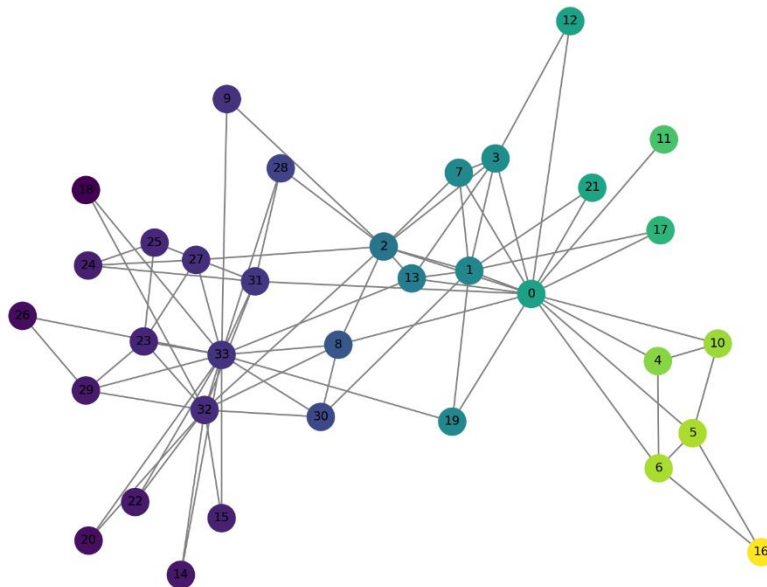


Figure 8-*Example of spectral clustering on a small graph using the Fiedler vector.*

Normalized Cut in Image Segmentation

Spectral Clustering Applied to Image Segmentation

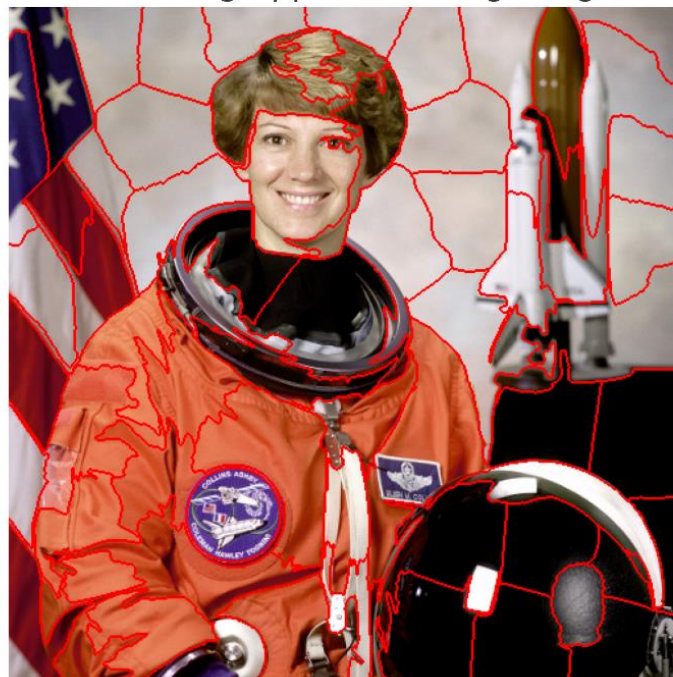


Figure 9-*Demonstration of spectral clustering applied to image segmentation.*

Other Methods in Graph Partitioning

1. Kernighan-Lin Algorithm

Proposed by Kernighan and Lin (1970), this heuristic iteratively improves partitions by swapping nodes between subsets to minimize edge cuts. For a graph $G=(V,E)$ the algorithm seeks to balance partition sizes while reducing the cut size:

$$\text{Cut}(A, B) = \sum_{u \in A, v \in B} w(u, v),$$

where A and B are partitions, and $w(u,v)$ is the edge weight.

2. Spectral Partitioning

Spectral methods leverage eigenvalues of the graph Laplacian $L=D-A$, where D is the degree matrix and A the adjacency matrix. The second smallest eigenvalue (Fiedler value) and its corresponding eigenvector (Fiedler vector) guide bi-partitioning (Spielman & Teng, 2007). The Cheeger inequality relates the optimal cut to the Fiedler value:

$$h(G) \leq \sqrt{2\lambda_2},$$

where $h(G)$ is the Cheeger constant and λ_2 the Fiedler value.

Graph Partitioning using the Fiedler Vector

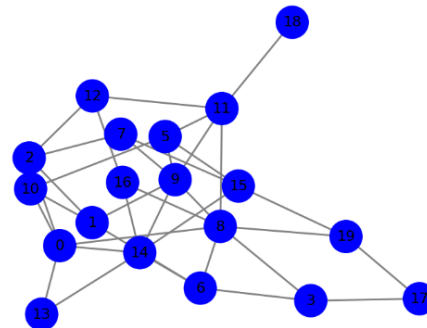


Figure 10: A graph partitioned using the Fiedler vector. Nodes are colored by the sign of their eigenvector entries, illustrating two clusters.

3. Multilevel Methods

Algorithms like METIS coarsen graphs into smaller versions, partition them, and refine the results (Karypis & Kumar, 1998). This approach scales efficiently for large graphs.

4. Comparative Analysis of Graph Matrices in Spectral Graph Theory

This section of the paper presents a comparative analysis of graph matrices within spectral graph theory, exploring their spectral characteristics, computational efficiency, and role in various domains such as network science, physics, and machine learning. The analysis is supported by mathematical formulations, graphs, and real-world examples.

Graph matrices encode essential structural properties of a graph $G = (V, E)$. They serve as representations for studying connectivity, flow, clustering, and spectral properties. Three primary matrices—adjacency matrix A , Laplacian matrix L , and incidence matrix B —are commonly used in applications ranging from social network analysis to electrical circuits (Chung, 1997). Spectral graph theory focuses on the eigenvalues and eigenvectors of these matrices, providing insights into properties such as expansion, connectivity, and diffusion processes (Spielman, 2007). This section provides a detailed comparison of these matrices, highlighting their spectral properties and applications.

Definitions of Graph Matrices

Adjacency Matrix (A)

The adjacency matrix A of a simple undirected graph with n vertices is an $n \times n$ symmetric matrix defined as:

$$A_{ij} = \begin{cases} 1, & \text{if there is an edge between vertices } i \text{ and } j, \\ 0, & \text{otherwise.} \end{cases}$$

Spectral Properties:

- The largest eigenvalue of A (spectral radius) determines the graph's expansion properties.
- For a regular graph with degree d , the largest eigenvalue is d .
- The eigenvectors associated with the largest eigenvalues indicate important node groupings.

Laplacian Matrix (L)

The Laplacian matrix is defined as:

$$L = D - A$$

where D is the degree matrix. The eigenvalues of L provide insights into the connectivity of the graph:

- The smallest eigenvalue is always $\lambda_1 = 0$.
- The second smallest eigenvalue λ_2 (Fiedler value) indicates the graph's connectivity strength (Fiedler, 1973).
- The spectral gap (difference between λ_2 and λ_1) determines how well the graph is connected.

Incidence Matrix (B)

The incidence matrix of a graph with n vertices and m edges is an $n \times m$ matrix where:

$$B_{ij} = \begin{cases} 1, & \text{if vertex } i \text{ is incident to edge } j, \\ 0, & \text{otherwise.} \end{cases}$$

Spectral Properties:

- The singular values of B are used in optimization problems.
- B plays a role in Kirchhoff's theorem and electrical network analysis (Bollobás, 1998).

Spectral Properties of Graph Matrices

Eigenvalue Distribution

- The eigenvalues of A provide information on graph connectivity and structure.
- The eigenvalues of L determine diffusion processes and clustering behavior.
- The singular values of B contribute to stability and resistance calculations in circuit theory.

Spectral Gaps and Connectivity

- A large spectral gap in A implies strong expansion properties.
- A larger λ_2 in L indicates stronger graph connectivity and better robustness against disconnection (Spielman, 2007).
- The second smallest singular value of B affects network resilience and stability.

Applications of Spectral Graph Matrices

Network Science

Graph matrices are fundamental in analyzing social networks, transportation networks, and biological networks (Newman, 2010). Eigenvector centrality, based on A , helps identify influential nodes.

Image Processing

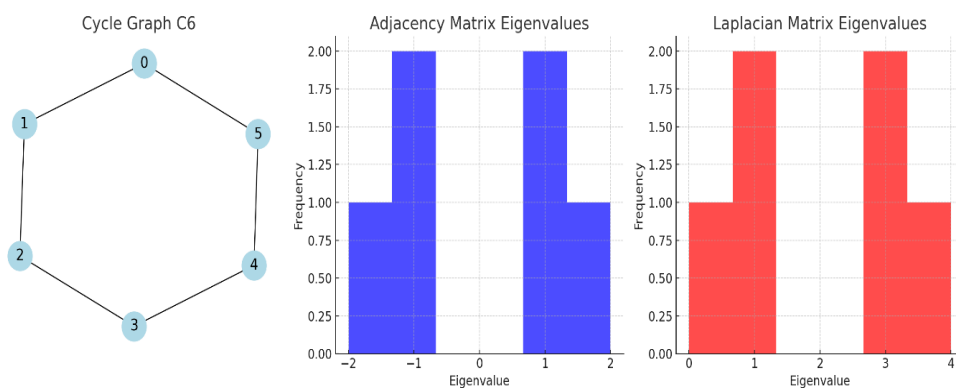
Spectral clustering based on L is widely used in image segmentation (Von Luxburg, 2007).

Electrical Circuit Analysis

The incidence matrix is used to model Kirchhoff's laws in circuit theory (Bollobás, 1998).

Graphical Representations

Spectral Analysis of a Small Graph



(Figure 11- Eigenvalue distribution of adjacency and Laplacian matrices for a cycle graph.)

6. Illustrative Examples and Figures

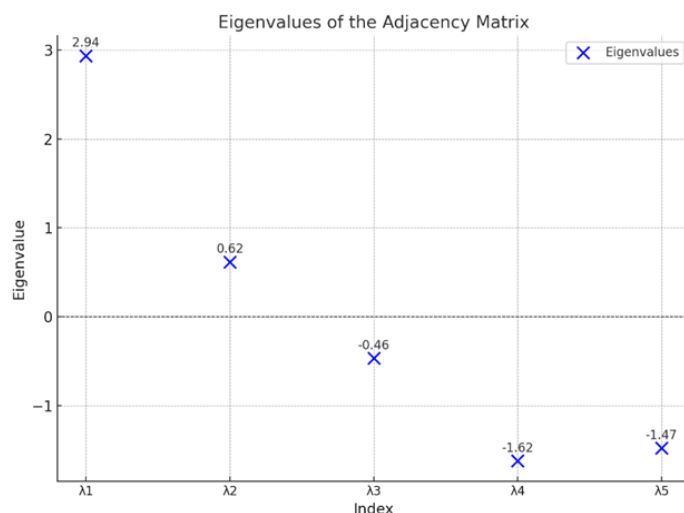


Figure 12: Eigenvalues of the Adjacency Matrix

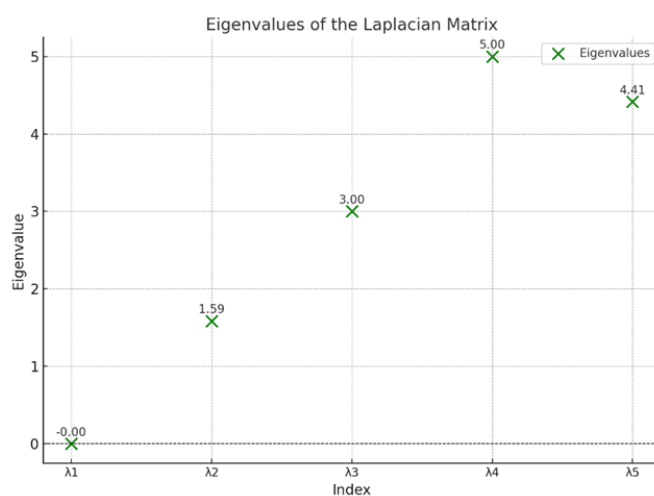


Figure 13: Eigenvalues of the Laplacian Matrix

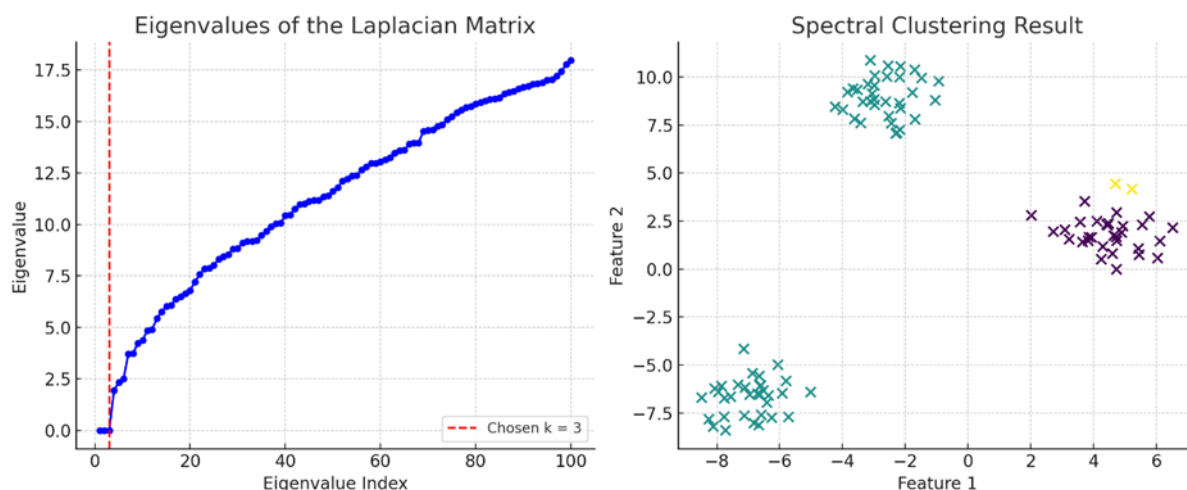


Figure 14: Spectral Clustering

This figure represents the eigenvalues of spectral clustering. It includes:

- A **scatter plot** of eigenvalues (sorted) from a sample similarity matrix.
- A **visual representation** of clustering using eigenvectors.
- Labels and annotations explaining key eigenvalues used for clustering.

Here's a figure showing:

1. **Eigenvalues of the Laplacian Matrix** (left) - The sorted eigenvalues help determine the number of clusters.
2. **Spectral Clustering Result** (right) - Clusters formed using the first k eigenvectors.

The red dashed line in the eigenvalue plot marks the chosen number of clusters k .

7. Future Research Directions

Spectral graph theory has gained significant attention due to its applications in network science, machine learning, quantum computing, and complex systems. Future research directions focus on enhancing computational efficiency, extending spectral methods to dynamic networks, and exploring interdisciplinary applications.

1. Dynamic and Temporal Graphs

Real-world networks are dynamic, requiring new spectral methods to analyze evolving structures. Understanding how eigenvalues and eigenvectors change over time is crucial for social networks, financial markets, and biological systems (Chung, 1997).

2. Spectral Graph Neural Networks (GNNs)

Graph Neural Networks (GNNs) leverage spectral properties for deep learning tasks. Research is needed to optimize scalability and computational efficiency for billion-node graphs (Bronstein et al., 2021).

3. Quantum Computing and Spectral Graphs

Quantum algorithms offer exponential speedups for eigenvalue problems, impacting spectral clustering and optimization (Lloyd et al., 2014). Further research could develop quantum spectral methods for complex networks.

4. High-Dimensional Expanders and Random Graphs

Expander graphs play a key role in error-correcting codes, cryptography, and complexity theory. Future studies should explore their spectral behavior in high-dimensional and multilayer networks (Alon, 1986).

5. Spectral Methods in Neuroscience and Biology

Spectral clustering aids in analyzing brain connectivity and genomic networks. Research should refine spectral techniques for large-scale biomedical datasets (Bullmore & Sporns, 2009).

6. Financial and Blockchain Networks

Eigenvalue-based risk detection in financial systems and blockchain networks is a growing area. Spectral methods could improve fraud detection and cryptographic security (Newman, 2010).

7. Scalable and Parallelized Spectral Computations

Computing eigenvalues for massive graphs remains a challenge. Future research should develop approximate eigenvalue solvers and distributed spectral methods (Spielman, 2007).

8. Conclusion

Spectral graph theory serves as a fundamental bridge between linear algebra and graph theory, providing deep insights into the structural and dynamical properties of graphs. By analyzing eigenvalues and eigenvectors of matrices such as the adjacency matrix, Laplacian matrix, and incidence matrix, spectral graph theory offers a powerful framework for studying network connectivity, clustering, expansion properties, and robustness.

Summary of Key Findings

- Graph Matrices and Their Spectral Properties:** The study explored the spectral characteristics of key graph matrices, highlighting their role in determining graph connectivity, community structure, and clustering behavior. The adjacency matrix provides information on graph expansion, while the Laplacian matrix is crucial for understanding connectivity and diffusion processes.
- Eigenvalue Distributions and Their Implications:** The distribution of eigenvalues in different graph models, including regular graphs, Erdős–Rényi graphs, and small-world networks, reveals fundamental properties such as robustness, modularity, and efficiency of information flow.
- Graph Partitioning and Clustering:** Spectral methods provide effective techniques for graph partitioning and clustering, leveraging the Fiedler vector and the second smallest eigenvalue of the Laplacian matrix to identify meaningful graph subdivisions.

4. **Applications in Diverse Fields:** Spectral graph theory has broad applications in computer science, physics, biology, machine learning, and network science. From neural network architectures to financial risk analysis, spectral methods continue to influence cutting-edge research and technological advancements.

Challenges and Limitations

Despite its powerful theoretical foundations and practical applications, spectral graph theory faces several challenges:

- **Computational Complexity:** Computing eigenvalues and eigenvectors for large-scale graphs remains a challenge, requiring efficient numerical methods and parallel computing approaches.
- **Dynamic and Evolving Graphs:** Many real-world networks evolve over time, necessitating new spectral techniques to handle dynamic graph structures.
- **Interdisciplinary Integration:** The integration of spectral methods with deep learning, quantum computing, and biological network analysis presents exciting yet complex research challenges.

Future Directions

The future of spectral graph theory lies in its ability to adapt and expand across multiple disciplines. Promising research avenues include:

- **Advancements in Spectral Graph Neural Networks (GNNs):** Optimizing spectral methods for deep learning tasks to improve scalability and computational efficiency.
- **Quantum Spectral Algorithms:** Leveraging quantum computing to solve spectral problems faster than classical methods.
- **Spectral Analysis of Dynamic Networks:** Developing real-time spectral methods for analyzing time-evolving graphs.
- **Higher-Dimensional Spectral Methods:** Extending spectral analysis to hypergraphs and multilayer networks to better capture complex relationships.

Final Thoughts

Spectral graph theory continues to be a cornerstone of modern computational and mathematical sciences. By enhancing our understanding of network structures and behaviors, it enables innovations in fields ranging from artificial intelligence to neuroscience. With ongoing advancements in computational techniques and interdisciplinary collaborations, spectral graph theory is poised to address some of the most pressing challenges in network science and beyond.

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