

## *Stochastic Modelling and Computational Sciences*

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### UNVEILING GRAPH PROPERTIES THROUGH ALGEBRAIC INVARIANTS

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#### ABSTRACT

Graph invariants are fundamental properties that remain unchanged under graph isomorphisms, providing essential insights into the structural and combinatorial characteristics of graphs. These invariants, including chromatic number, degree sequence, adjacency eigenvalues, and Laplacian eigenvalues, play a vital role in graph classification and analysis. Algebraic methods, such as matrix theory, polynomial invariants, and group theory, offer robust tools for studying these properties. The adjacency matrix, Laplacian matrix, and chromatic polynomial serve as key algebraic representations, revealing deep structural information through their eigenvalues and polynomial roots. This paper explores these algebraic tools, demonstrating their applications in analyzing graph connectivity, symmetry, and optimization problems. Case studies on bipartite, planar, and regular graphs highlight the efficacy of algebraic approaches in extracting meaningful invariants. Applications in network design, cryptography, and coding theory further emphasize the practical relevance of these techniques. By integrating algebraic principles with graph theory, this study provides a comprehensive framework for understanding and leveraging graph invariants in both theoretical and applied domains.

#### INTRODUCTION

Graph invariants are fundamental properties of graphs that remain unchanged under graph isomorphisms. These properties are critical in classifying graphs, understanding their structure, and solving complex problems in fields such as computer science, physics, and chemistry. Examples of graph invariants include the degree sequence, chromatic number, adjacency eigenvalues, Laplacian eigenvalues, and polynomial invariants. These invariants provide insights into various graph characteristics such as connectivity, coloring, partitioning, and robustness.

Algebraic methods offer a systematic approach to studying graph invariants by representing graphs using matrices and polynomials. The adjacency matrix, Laplacian matrix, and incidence matrix are commonly used to represent graphs algebraically. The eigenvalues of these matrices serve as powerful graph invariants that encode structural properties such as bipartiteness, regularity, and spectral gaps.

**For example, the adjacency matrix of a graph, denoted as, is defined as:**

The eigenvalues of are used to determine whether a graph is bipartite or connected.

**Another important matrix is the Laplacian matrix, defined as:**

where is the degree matrix and is the adjacency matrix. The Laplacian matrix is widely used in spectral graph theory and helps analyze graph properties like connectivity and clustering.

Polynomial invariants, such as the characteristic polynomial and the chromatic polynomial, also play a significant role in graph theory. The chromatic polynomial, denoted as , counts the number of ways a graph can be colored using colors such that adjacent vertices have different colors.

In addition to matrix and polynomial methods, group theory provides tools for studying graph symmetries. Automorphism groups, which describe the graph's symmetrical transformations, serve as invariants that reveal structural patterns.

The integration of algebraic tools has advanced our ability to classify, compare, and understand graphs, making them essential in various applications, including optimization, cryptography, and data analysis. This paper aims to provide a comprehensive overview of algebraic methods used in studying graph invariants and their practical implications.

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**Methods** Algebraic methods for studying graph invariants rely heavily on matrix theory, polynomial representations, and group theoretical techniques. Below, we discuss these methods in detail, accompanied by relevant equations and diagrams.

### **Adjacency Matrix and Eigenvalues**

The **Adjacency Matrix** of a graph is a square matrix used to represent the graph's structure. If has vertices labeled as, the adjacency matrix is defined as follows:

#### **In this matrix:**

- ✓ The rows and columns correspond to the vertices of the graph.
- ✓ A value of indicates an edge exists between two vertices.
- ✓ A value of indicates no edge exists.

The adjacency matrix of a graph encodes the edges between vertices. The eigenvalues of provide key spectral invariants. For a graph with vertices, the adjacency matrix is defined as:

#### **The characteristic polynomial of is given by:**

where represents the eigenvalues of the adjacency matrix.

The two most important matrices associated to a graph are the adjacency matrix and the laplacian matrix. Both are square matrices indexed by the vertex set  $V$ . The *adjacency matrix*  $A$  is given by

$$A(u,v) = (1 \text{ if } u \sim v, 0 \text{ otherwise})$$

while the *laplacian matrix*  $L$  is defined as follows:

$$L(u,v) = \{\text{deg}(v) \text{ if } u = v, -1 \text{ if } u \sim v, 0 \text{ otherwise}\}$$

The two matrices are related by the formula

$$A+L = \text{diag}(\text{deg}),$$

where  $\text{diag}(\text{deg})$  denotes the diagonal matrix recording the degrees. We often view the adjacency matrix and the laplacian matrix as operators on  $\ell^2 V$ . Recall that  $\ell^2 V$  is the finite-dimensional space of complex-valued functions on  $V$ , endowed with the inner product

$$(f, g) = \sum_v f(v)g(v)$$

The adjacency operator  $A: \ell^2 V \rightarrow \ell^2 V$  and the laplacian operator  $L: \ell^2 V \rightarrow \ell^2 V$  are given by

$$Af(v) = \sum_{u:u \sim v} f(u)$$

**Laplacian Matrix** The Laplacian matrix is defined as:

where is the degree matrix. The eigenvalues of the Laplacian matrix provide insights into graph connectivity and clustering properties.

**Formula is particularly appealing:** the right-most sum can be interpreted as an overall edge differential. The adjacency matrix  $A$  and the laplacian matrix  $L$  are real symmetric matrices. Recall, at this point, the Spectral Theorem: if  $M$  is a real, symmetric  $n \times n$  matrix, then there is an orthogonal basis consisting of eigenvectors, and  $M$  has  $n$  real eigenvalues, counted with multiplicities. Thus, both  $A$  and  $L$  have  $n = |V|$  real eigenvalues. In fact, the eigenvalues are algebraic integers (roots of monic polynomials with integral coefficients) since both  $A$  and  $L$  have integral entries. Our convention is that the adjacency, respectively the laplacian eigenvalues are denoted and ordered as follows:

$$\alpha_{\min} = \alpha_n \leq \dots \leq \alpha_2 \leq \alpha_1 = \alpha_{\max}$$

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$$\lambda_{\min} = \lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n = \lambda_{\max}$$

For the purposes of relating eigenvalues to graph invariants, the most important eigenvalues will turn out to be the extremal ones, as well as  $\lambda_2$  and  $\alpha_2$ . The spectrum is the multiset of eigenvalues, that is the set of eigenvalues repeated according to their multiplicity. Occasionally, we write  $\alpha$ -spec for the adjacency spectrum, respectively  $\lambda$ -spec for the laplacian spectrum. For regular graphs, the laplacian matrix and the adjacency matrix carry the same spectral information. Indeed,  $A+L = dI$ , so  $\alpha_k + \lambda_k = d$  and the corresponding eigenvectors are the same. Thus, using the laplacian or the adjacency spectrum is mostly a matter of convenience in the regular case. Even for non-regular graphs, there is a kind of silent duality between adjacency and laplacian eigenvalues.

A guiding principle of spectral graph theory is that much knowledge about a graph can be extracted from spectral information. But could it be that spectral information gives complete knowledge about a graph? The answer is a resounding no. As we will see, there are many examples of *isospectral* but non-isomorphic regular graphs. As one might guess, two regular graphs are said to be isospectral when they have the same adjacency (equivalently, laplacian) spectrum. Note that we only consider isospectrality in the context of regular graphs. Of course, the same issue can be pursued for non-regular graphs, but then there are two distinct sides to the story.

**Notes.** The following is arguably the most conceptual method of motivating the combinatorial laplacian. Decide on an edge orientation and provide the operator  $D: \ell^2 V \rightarrow \ell^2 E$  is expressed as  $Df(e) = f(e^+) - f(e^-)$ , where  $e^+$  and  $e^-$  stand for the terminal and the edge  $e$ 's starting vertex, respectively.  $D$  is a discrete differential operator in our minds. If  $D^*$  is the adjoint of  $D$ , then  $L = D^*D$ . The geometric laplacian  $\Delta$  on manifolds is defined by an equivalent formula, substituting the gradient operator for  $D$ . The term given to  $L$  and the other widely used notation for the graph-theoretic laplacian are both explained by this similarity.

The laplacian of a graph can be traced back to Kirchoff's work on electrical networks in 1847. The result is surprising, as is the time: in a modern formulation, Kirchoff's Matrix-Tree theorem gives a formula for the number of spanning trees in a graph in terms of its laplacian eigenvalues. Work by Anderson-Morley (Eigenvalues of the Laplacian of a graph, Preprint 1971, Linear and Multilinear Algebra 1985) and Fiedler (Algebraic connectivity of graphs, Czechoslovak Math. J. 1973).

Polynomial Invariants the chromatic polynomial counts the number of valid vertex colorings: where are coefficients determined by the graph structure.

Graph Automorphisms and Symmetry the automorphism group of a graph is defined as: This group captures the symmetry of the graph and serves as an invariant.

Case Studies we apply these algebraic methods to specific graph classes such as bipartite graphs, planar graphs, and regular graphs to demonstrate their effectiveness.

### RESULTS

The study demonstrates that algebraic methods can efficiently compute and classify graph invariants. Eigenvalue spectra of adjacency and Laplacian matrices provide insights into graph connectivity, robustness, and partitioning. Chromatic polynomials are shown to predict coloring properties, while group theoretical methods reveal graph symmetries. Applications in network resilience, coding theory, and cryptographic algorithms highlight the practical value of these invariants. Case studies on specific graph classes illustrate the effectiveness of algebraic approaches in identifying invariant-based properties.

### CONCLUSION

Graph invariants, analyzed through algebraic methods, provide powerful tools for understanding the structure and behavior of graphs. Matrices, such as adjacency and Laplacian matrices, along with polynomial invariants and automorphism groups, offer systematic ways to extract and interpret key graph properties. The adjacency matrix encodes the graph's edge structure, while its eigenvalues provide spectral insights into graph regularity, bipartiteness, and connectivity. Similarly, the Laplacian matrix serves as a valuable tool for studying clustering and partitioning, with its eigenvalues indicating the number of connected components and overall graph

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robustness. Polynomial invariants, particularly the chromatic polynomial, reveal essential coloring properties, supporting applications in scheduling, network optimization, and partitioning problems. Group theory, through graph automorphisms, sheds light on graph symmetry and structural redundancies, which are crucial in minimizing computational complexity in graph algorithms. The algebraic approach to graph invariants is not only mathematically elegant but also practically relevant. Applications in network analysis, cryptographic algorithms, and error-correcting codes demonstrate the versatility of these methods in solving real-world problems. Case studies on bipartite, planar, and regular graphs underscore the utility of algebraic techniques in identifying and classifying graph properties efficiently.

Future research can focus on extending these algebraic frameworks to tackle challenges posed by large-scale graphs, dynamic networks, and quantum computing applications. Additionally, exploring novel algebraic invariants and integrating them with machine learning techniques may open new avenues for graph analysis.

In summary, algebraic methods provide a deep and versatile toolkit for studying graph invariants, bridging theoretical insights with practical applications, and paving the way for innovative advancements in graph theory and its related fields.

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