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Computer–Assisted Graph Theory and Interdisciplinary Applications

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Abstract
Graph theory has become a central tool for modelling and analyzing complex systems in computer science, biology, neuroscience, social sciences, engineering, and geosciences. Recent advances in algorithms, high-performance computing, and machine learning have led to a new paradigm of computer-assisted graph theory, where exhaustive graph generation, optimization methods, and learning-based techniques are used to attack both classical and modern problems. This paper surveys key ideas in computer-assisted graph theory and highlights selected interdisciplinary applications, including network optimization, molecular modelling, brain connectivity, and graph neural networks. We outline a unifying framework for integrating mathematical graph theory, algorithmic techniques, and domain-specific modelling.

Keywords: Computer-assisted graph theory, Graph algorithms and optimization, Graph neural networks (GNNs), Complex network modelling, Interdisciplinary applications of graphs

1. Introduction

Graph theory is a cornerstone of discrete mathematics and provides a natural framework for representing entities as vertices and relationships as edges. Classical topics such as graph coloring, extremal graph theory, and spectral graph theory have evolved into powerful tools for modelling real-world networks in communication, biology, and social systems. At the same time, computers and algorithms now play an ever-increasing role in obtaining new results in graph theory itself. Computer-assisted graph theory uses algorithmic and computational methods to generate, test, and optimize graphs under structural and combinatorial constraints. Techniques include exhaustive generation of non-isomorphic graphs, mixed integer linear programming (MILP), semidefinite programming (SDP), SAT solving, dynamic programming, metaheuristics, and machine learning methods tailored to graph problems. These ideas have been fruitfully applied to extremal problems, coloring, structural graph theory, and chemical graph theory, among other areas.

Parallel to this methodological development, interdisciplinary applications of graph theory have expanded drastically. Graph-based models support network optimization and routing, clustering in data science, molecular connectivity in chemistry, functional and structural brain networks in neuroscience, and social

network analysis in the social sciences. Modern applications increasingly combine graph theory with probabilistic models and graph neural networks (GNNs), forming an essential framework for understanding and optimizing complex networks.

The objective of this paper is twofold:

- To provide a concise survey of core techniques in computer-assisted graph theory.
- To present a structured view of interdisciplinary applications where these techniques play a central role.

2. Preliminaries on Graph Theory

We first recall basic notions that will be used throughout the paper. A (simple) graph $G = (V, E)$ consists of a finite vertex set V and an edge set $E \subseteq \{\{u, v\}: u, v \in V, u \neq v\}$. A graph is called directed (or a digraph) if edges are ordered pairs. Fundamental concepts include:

- Degree of a vertex, paths, cycles, connectivity, and components.
- Special classes: trees, bipartite graphs, planar graphs, regular graphs.
- Graph invariants: chromatic number, clique number, independence number, diameter, eigenvalues of the adjacency or Laplacian matrix.

Figure 1 demonstrates the fundamental concepts of graph theory.

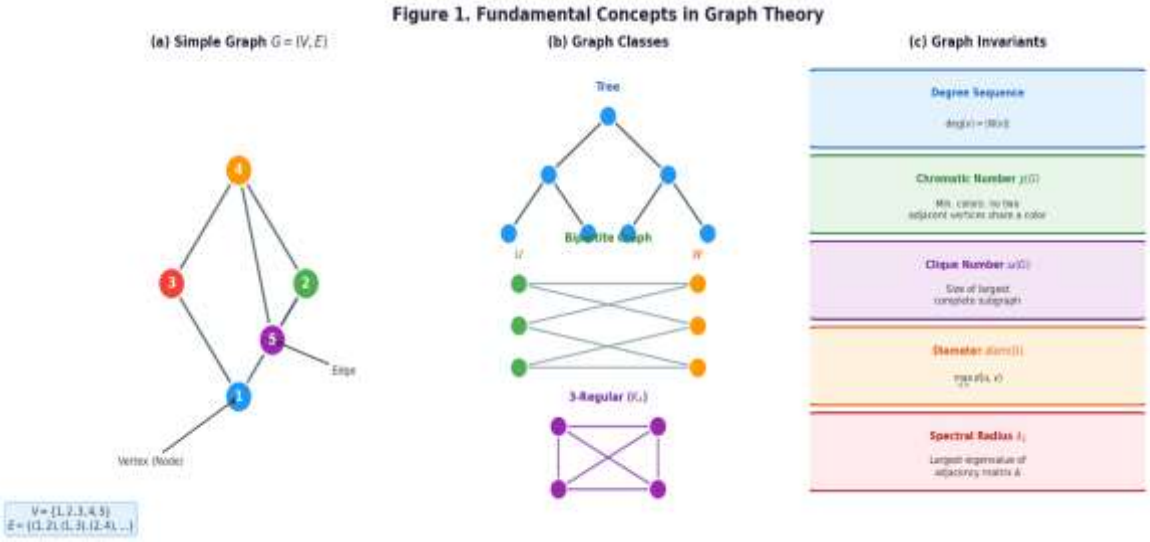


Figure 1. Fundamental Concepts in Graph Theory: (a) a simple graph G=(V,E) with labelled vertices and edges, (b) key graph classes (tree, bipartite graph, K_4-regular), and (c) principal graph invariants with formal definitions.

Subfields relevant to this paper include (Figure 2):

- Extremal graph theory: bounds on numbers of edges avoiding certain subgraphs.
- Graph coloring: proper colorings, chromatic number, list coloring.
- Structural graph theory: decomposition theorems, minor-closed families.
- Spectral graph theory: eigenvalues and eigenvectors as encodings of structure.
- Chemical graph theory: graphs representing molecules and their properties.

Many long-standing open problems in graph theory have inspired the development of computational techniques in this area.

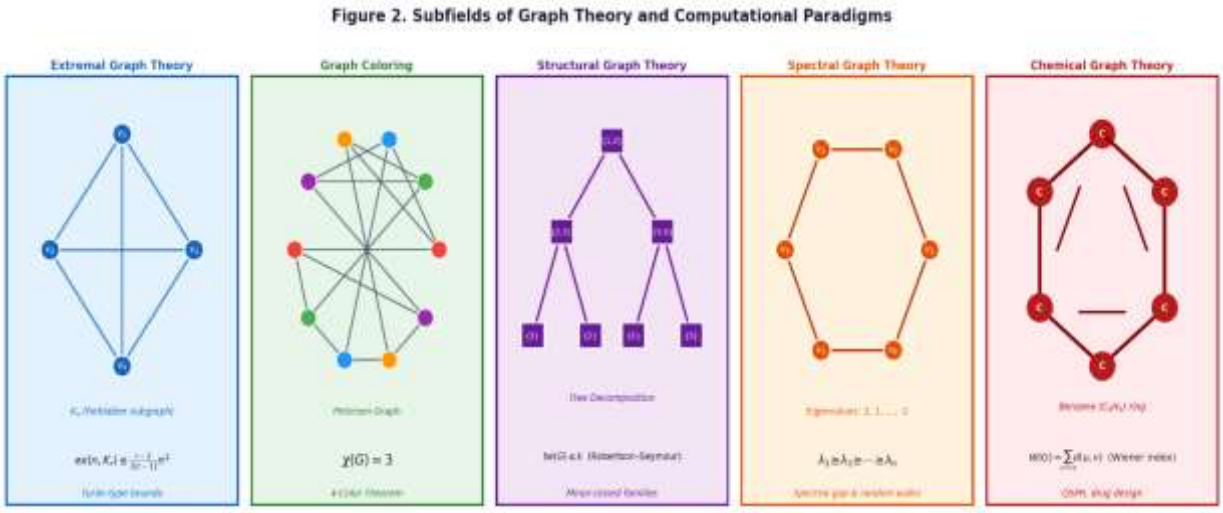


Figure 2. Subfields of Graph Theory and Computational Paradigms: Extremal Graph Theory (Turán-type bounds), Graph Coloring (Petersen graph, $\chi(G) = 3$), Structural Graph Theory (tree decomposition), Spectral Graph Theory (eigenvalue ordering), and Chemical Graph Theory (benzene/Wiener index).

3. Computer–Assisted Graph Theory

3.1. Exhaustive Graph Generation and Databases

A central approach in computer-assisted graph theory is the exhaustive generation of all pairwise non-isomorphic graphs within a given class, subject to constraints such as order, degree sequence, or forbidden subgraphs. Canonical labeling and isomorphism testing algorithms allow one to avoid duplications and to systematically explore the space of graphs. Such exhaustive catalogues enable:

- Experimental exploration of conjectures by checking small cases.
- Discovery of extremal examples and counterexamples.
- Construction of searchable databases of graphs and associated invariants.

These databases can store structural parameters, spectral data, labelings, and other invariants, providing a resource for both pure and applied investigations.

3.2. Optimization Paradigms: MILP, SDP, and SAT

Many graph-theoretic problems can be formulated as optimization problems with combinatorial constraints. Computer-assisted graph theory leverages:

- Mixed Integer Linear Programming (MILP), where binary variables encode adjacency, cuts, color classes, or other structural features.
- Semidefinite Programming (SDP), particularly for problems involving eigenvalues and quadratic forms, relevant to spectral bounds and coloring.
- SAT and Max-SAT solving, where graph properties are encoded as propositional formulas whose satisfiability corresponds to existence or non-existence of certain graphs.
- These methods have been applied to extremal problems, graph coloring, and the search for highly regular or symmetric graphs.

3.3. Dynamic Programming and Metaheuristics

Dynamic programming on tree decompositions and related structures is effective for graph problems with bounded tree width. Metaheuristics such as evolutionary algorithms, tabu search, and simulated annealing

can search through large graph spaces to approximate solutions when exact algorithms are infeasible. Such approaches are especially useful in network design and layout optimization.

3.4. Machine Learning and Graph Neural Networks

Machine learning increasingly supports graph-theoretic research in two ways:

1. Predictive modelling on graphs: supervised and unsupervised learning for node classification, link prediction, and graph classification using graph neural networks (GNNs).
2. Assisting mathematical discovery: learning to predict extremal constructions, approximate invariants, or suggest promising candidates for counterexamples.
3. GNNs provide a neural architecture that exploits neighborhood aggregation and message passing, making them well-suited for complex, high-dimensional graph data.

4. Interdisciplinary Applications of Graph Theory

4.1. Computer Science and Communication Networks

Graph theory is fundamental in modelling communication and information networks, including the structure of the World Wide Web, routing in communication networks, and ranking of web pages via hyperlink graphs. Graph-based algorithms support:

Shortest-path and routing protocols in communication and transportation networks.

- Network optimization (flow, cut, reliability).
- Data structures such as trees, heaps, and search structures, which can be viewed as special graphs.

Graph-driven methods are also central to modern areas such as graph neural networks, graph-based clustering, and anomaly detection in cybersecurity.

4.2. Biology, Chemistry, and Neuroscience

In biology and systems biology, graphs model gene regulatory networks, protein–protein interaction networks, metabolic pathways, and epidemic spread. Dynamic graph models help analyze cell differentiation, immune responses, and host–pathogen interactions. In chemistry, chemical graph theory represents atoms as vertices and bonds as edges, enabling graph-based approaches to isomer enumeration, structure–property prediction, and computer-aided drug design. Neuroscience uses graphs to model brain connectivity, both structural (anatomical connections) and functional (statistical dependencies between brain regions). Graph-theoretic measures such as degree distribution, clustering coefficient, and modularity have been applied to understand brain disorders and network reorganization.

Figure 3 demonstrates the graph-theoretical models in interdisciplinary applications.

Figure 3. Graph-Theoretic Models in Interdisciplinary Applications

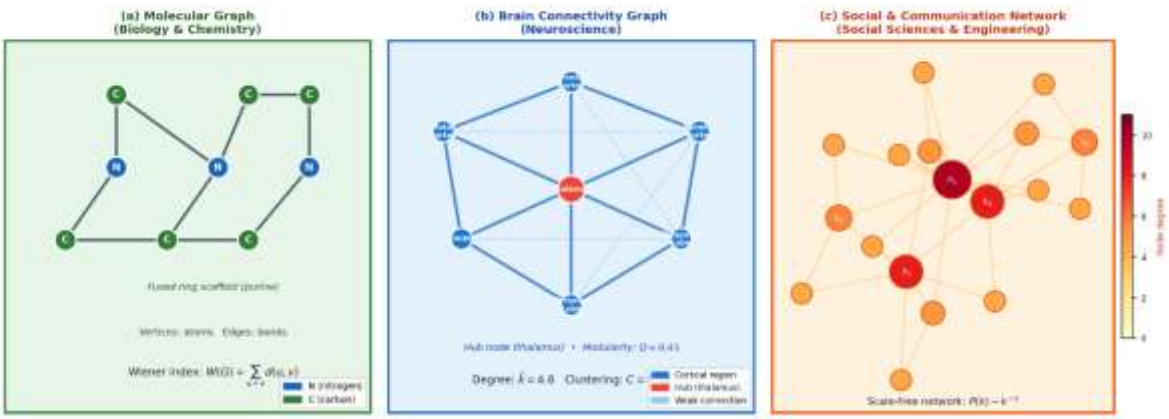


Figure 3. Graph-Theoretic Models in Interdisciplinary Applications: (a) fused-ring molecular scaffold (biology & chemistry), (b) brain connectivity graph with hub detection and modularity (neuroscience), and (c) scale-free social/communication network with degree-based centrality (social sciences & engineering).

4.3. Social Sciences and Economics

Graph theory underpins social network analysis by modelling individuals as vertices and social relationships as edges. Graph measures help characterize central actors, community structures, and patterns of influence in social and organizational networks. Applications extend to committee decision-making, political lobbying, peer influence in education, criminology, and security studies. In economics and finance, graphs represent trading networks, ownership structures, and interbank exposures, allowing systemic risk and contagion to be studied using network models.

4.4. Engineering, Geosciences, and Environmental Systems

Engineering systems—including power grids, transportation systems, and sensor networks are naturally modelled as graphs. Graph theory supports reliability analysis, fault detection, and optimal design in these networks. In geosciences and environmental studies, graphs are used to model ecological networks, spatial connectivity, and resource distribution, providing insights into spatial patterns and resilience. Recent interdisciplinary reviews emphasize that spectral methods, probabilistic models, and GNNs enhance graph-based analysis in these domains, yielding more accurate models and better optimization strategies.

4.5. Summary of Application Domains:

Table 1 summarizes how graph-theoretic models are applied across diverse domains, with each field characterized by specific graph objects such as networks, molecular structures, or connectivity graphs. These representations enable a wide range of applications including optimization, pattern discovery, prediction, and system analysis.

Overall, graphs serve as a unifying framework to model complex relationships, supporting tasks like routing, drug discovery, community detection, and reliability analysis across science, engineering, and social systems.

Table 1: Summary of application domains

Domain	Typical Graph Objects	Representative Uses
Computer science	Communication networks, data structures, web graphs	Routing, search, GNNs, clustering, anomaly detection
Biology & chemistry	Molecular graphs, gene and protein networks	Drug design, metabolic networks, epidemic modelling
Neuroscience	Brain connectivity graphs	Network biomarkers, disease characterization
Social sciences	Social and institutional networks	Influence, community detection, decision-making
Engineering & geoscience	Power grids, transport, ecological networks	Reliability, spatial patterns, environmental modelling

5. A Unifying Framework

Integrating mathematical graph theory, computational methods, and domain knowledge suggests a three-layer framework for computer-assisted, interdisciplinary graph research:

1. **Mathematical layer**: Precise graph-theoretic models, definitions, and conjectures drawn from classical and modern graph theory.
2. **Algorithmic/computational layer**: Exhaustive enumeration, MILP/SDP formulations, SAT encodings, dynamic programming, and heuristic search to explore the space of graphs and validate or refute conjectures.
3. **Domain-specific layer**: Mapping real-world entities and interactions to graph models, incorporating noise and uncertainty, and validating models against empirical data; here, machine learning and GNNs provide flexible tools for high-dimensional data.
4. This architecture enables a bidirectional flow: mathematical insights inform better algorithms and models, while computational experiments and domain applications suggest new structures and problems for theoretical investigation.

6. Conclusion

Graph theory has evolved from an abstract mathematical discipline into a central framework for representing and analyzing complex systems across disciplines. The rise of computer-assisted graph theory, combining exhaustive search, optimization, and machine learning, has significantly expanded our ability to tackle both pure and applied problems. By unifying mathematical foundations, algorithmic techniques, and domain-specific models, this area offers a rich landscape for future research and international collaboration.

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