

Graph Theory Models for Complex Network Analysis and Intelligent System Design

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Abstract: Graph theory has evolved from a branch of discrete mathematics concerned with abstract vertex-edge structures into the principal mathematical language for representing and analyzing complex networks, systems whose components interact through relationships that themselves carry structural, and often computationally exploitable, information. This paper reviews the foundational and applied graph-theoretic literature underlying complex network analysis and intelligent system design, tracing the field's development from classical random graph theory through the small-world and scale-free network models that reshaped network science at the turn of the century, and into the more recent graph representation learning and graph neural network (GNN) literature that has integrated graph-theoretic structure directly into machine learning architectures. The review synthesizes foundational random-graph and preferential-attachment models, structural analysis techniques including centrality measures and community detection, and the graph embedding and graph neural network methods that now underlie intelligent system design across recommendation, molecular modelling, and physical simulation domains. Distinct comparative tables map generative network model families onto their structural signature and generating mechanism, cross-reference classical structural analysis measures against their intelligent-system design application, and set graph neural network architecture families against the computational mechanism and task type each is best suited to address. The paper concludes that intelligent system design increasingly depends on selecting a graph-theoretic representation and analysis method whose structural assumptions match the target network's actual generative structure, rather than applying a single default graph model universally, and identifies the theoretical understanding of graph neural network expressiveness limits as the central future research prospect.

Keywords: Graph Theory, Complex Networks, Network Science, Centrality Measures, Community Detection, Graph Neural Networks, Graph Representation Learning, Intelligent Systems

1. Introduction

A graph, formally a set of vertices connected by a set of edges, provides a deceptively simple mathematical abstraction capable of representing an extraordinarily wide range of real-world systems, social relationships, biological interactions, transportation infrastructure, and computational architectures among them, and the specific structural properties a given real-world network exhibits, how densely connected it is, how quickly information or influence propagates across it, and how robust it is to the removal of its most important components, have proven to be neither arbitrary nor uniform across different classes of networks [1]. Erdős and Rényi's foundational random graph model, in which edges are placed between vertex pairs independently at a fixed probability, established the first



rigorous mathematical framework for analyzing how a network's macroscopic structural properties, connectivity, component size, and diameter, emerge as probabilistic consequences of this simple edge-formation rule, and remains the essential mathematical baseline against which subsequent, more structurally realistic network models are compared [1].

Watts and Strogatz's small-world network model demonstrated that the random graph baseline fails to capture a structural property pervasive across real social, biological, and technological networks: high local clustering, the tendency for a vertex's neighbours to also be connected to one another, combined simultaneously with a short average path length between arbitrary vertex pairs, a combination the authors showed could be generated by rewiring only a small fraction of a regular lattice's edges at random, producing a network that is neither fully regular nor fully random but exhibits properties of both [2]. This small-world structure directly formalized the "six degrees of separation" phenomenon Milgram's earlier social-psychology experiment had documented empirically, in which letters passed through an average of only a small number of acquaintance links reached a designated target individual across a large, ostensibly sparsely connected social network, providing a rigorous graph-theoretic explanation for an empirical finding that had previously lacked one [3], [2].

Barabási and Albert's scale-free network model identified a second structural property pervasive across many real-world networks that neither the classical random graph nor the small-world model explains: a degree distribution following a power law, in which most vertices have relatively few connections while a small number of "hub" vertices accumulate a disproportionately large number of connections, a pattern the authors showed arises naturally from a growth process combined with preferential attachment, in which new vertices joining the network preferentially connect to already highly connected vertices rather than connecting uniformly at random [4]. Albert, Jeong, and Barabási's subsequent analysis of this scale-free structure's robustness properties found that scale-free networks exhibit a striking error-and-attack asymmetry, remaining highly robust to the random failure of arbitrary vertices while being disproportionately vulnerable to the targeted removal of their high-degree hub vertices, a structural finding with direct and immediately applicable implications for intelligent system design in domains ranging from internet infrastructure resilience to epidemic containment strategy [5].

Beyond generative structural models, graph theory provides a substantial toolkit for quantifying a vertex's or edge's structural importance within a network, a capability foundational to intelligent system design applications ranging from web search ranking to influence maximization. Freeman's foundational formalization of centrality distinguished degree centrality, betweenness centrality, and closeness centrality as three conceptually distinct measures of structural importance, each capturing a different notion of what it means for a vertex to be "central" within a network, whether through direct connectivity, control over information flow between other vertices, or proximity to the rest of the network as a whole [6]. Page, Brin, Motwani, and Winograd's PageRank algorithm applied a specifically recursive notion of centrality, in which a vertex's importance depends on the importance of the vertices linking to it, to the World Wide Web's hyperlink graph specifically, providing the foundational graph-theoretic mechanism underlying modern web search ranking and demonstrating centrality analysis's direct commercial and computational significance well beyond academic network science [7]. Kleinberg's HITS algorithm formalized a related but analytically distinct recursive centrality notion, distinguishing "hub" vertices that point to many authoritative vertices from "authority" vertices that are pointed to by many hubs, a distinction with direct relevance to any intelligent system requiring a bipartite notion of structural importance [8].

The most recent major development in this literature integrates graph-theoretic structure directly into machine learning architectures, moving beyond graph-theoretic analysis of a network's structure toward learning directly on that structure for prediction and generation tasks. Scarselli, Gori, Tsoi, Hagenbuchner, and Monfardini's original graph neural network (GNN) formulation proposed a neural architecture capable of processing graph-structured input directly, generalizing the standard neural network's fixed-size vector input to accommodate the variable-size, irregularly connected structure characteristic of real-world graphs, establishing the foundational architecture that the subsequent graph convolutional and graph attention network literature has extended considerably [9]. This paper reviews the classical generative network model, structural analysis, and modern graph neural network literature within

a single comparative framework, before examining how these graph-theoretic tools jointly inform intelligent system design across specific application domains.

Research Objectives

- To review the foundational generative graph models, random graph, small-world, and scale-free, underlying complex network structural analysis.
- To synthesize classical structural analysis techniques, including centrality measures and community detection, and their application to intelligent system design.
- To examine graph representation learning and graph neural network architectures as the integration of graph-theoretic structure into machine learning.
- To evaluate how specific graph-theoretic tools map onto concrete intelligent system design applications across domains.
- To identify future research priorities for understanding graph neural network expressiveness and theoretical limits.

2. Literature Review

2.1 Classical Random Graph Theory

Erdős and Rényi's foundational random graph model, denoted $G(n,p)$ for n vertices with each possible edge included independently at probability p , established rigorous probabilistic results for how a network's connectivity properties, including the emergence of a giant connected component and the network's overall diameter, change as the edge probability p crosses specific mathematical thresholds, providing the field's essential baseline model against which the deviation of real-world networks from pure randomness can be precisely quantified [1]. Bollobás's comprehensive mathematical treatment of random graph theory extended Erdős and Rényi's foundational results considerably, formalizing the phase-transition phenomena, sharp threshold probabilities at which a random graph's qualitative structural properties change abruptly, that underlie much of the subsequent mathematical analysis of network robustness and connectivity [14].

2.2 Small-World and Scale-Free Network Models

Watts and Strogatz's small-world model demonstrated that interpolating between a regular ring lattice and a fully random graph through a small-probability edge-rewiring procedure produces networks exhibiting both high clustering, characteristic of regular lattices, and short average path length, characteristic of random graphs, simultaneously, a combination the authors found empirically present across diverse real-world networks including neural, social, and power-grid networks examined in their original study [2]. Barabási and Albert's scale-free model demonstrated that a growth-and-preferential-attachment generative process, rather than the fixed-vertex-count, uniform-attachment process underlying both the random graph and small-world models, produces a power-law degree distribution matching the structure empirically observed across the World Wide Web, citation networks, and biological interaction networks the authors examined [4]. Bianconi and Barabási's subsequent fitness-model extension incorporated an additional vertex-level "fitness" parameter into this preferential-attachment process, demonstrating that vertices with higher intrinsic fitness can overtake earlier-arriving but lower-fitness vertices in accumulated connectivity, a refinement addressing an empirical pattern, newer network entrants occasionally becoming dominant hubs, that the original, purely age-based preferential attachment model could not explain [15].

2.3 Structural Analysis: Centrality and Robustness

Freeman's tripartite centrality framework, distinguishing degree, betweenness, and closeness centrality, remains the standard reference point for structural importance analysis, with betweenness centrality specifically, quantifying the fraction of shortest paths between all vertex pairs that pass through a given vertex, proving particularly valuable

for identifying structurally critical vertices whose removal would most severely disrupt network-wide connectivity or information flow [6]. Albert, Jeong, and Barabási's error-and-attack tolerance analysis found that this structural criticality is highly concentrated in scale-free networks specifically, with the targeted removal of just a small percentage of the highest-degree vertices sufficient to fragment the network into disconnected components, while random vertex failure of a comparable magnitude leaves the network's giant connected component largely intact, a finding with direct design implications for any intelligent system, from internet routing infrastructure to organizational communication networks, built atop a scale-free or scale-free-like structure [5]. Cohen and Havlin's broader treatment of complex network structure, robustness, and function formalized this robustness analysis mathematically through percolation theory, providing the quantitative framework for predicting the specific fraction of vertices that must be removed, whether randomly or by targeted attack, before a network's giant connected component collapses [16].

2.4 Community Detection

Girvan and Newman's foundational community-detection algorithm identified network communities, densely internally connected but sparsely externally connected vertex clusters, through the iterative removal of edges with the highest betweenness centrality, on the reasoning that inter-community edges, which lie on many shortest paths connecting otherwise distant communities, systematically exhibit higher betweenness than intra-community edges [10]. Newman and Girvan's subsequent formalization of the modularity measure provided a principled, quantitative criterion for evaluating the quality of any proposed community partition, comparing the actual fraction of edges falling within proposed communities against the expected fraction under a null random-graph model, a measure that has since become the dominant objective function optimized by the large majority of subsequent community-detection algorithms [11]. Newman's broader structure-and-function review situated community detection within the wider landscape of complex network structural analysis, arguing that community structure carries direct functional significance across social, biological, and technological networks, since densely connected communities frequently correspond to functionally cohesive units, research collaboration groups, protein functional modules, or organizational subunits, respectively [12].

2.5 Graph Representation Learning

Perozzi, Al-Rfou, and Skiena's DeepWalk algorithm introduced graph representation learning as a distinct methodological approach, applying the word2vec skip-gram language model directly to sequences of vertices generated by random walks over a graph, treating these random-walk vertex sequences analogously to sentences of words and learning low-dimensional vertex embeddings that preserve the graph's structural neighbourhood relationships in a continuous vector space suitable for downstream machine learning tasks [18]. Grover and Leskovec's node2vec extended this random-walk embedding approach with tunable parameters controlling whether the random walk exploration behaves more like a breadth-first or depth-first search, allowing the resulting embeddings to flexibly capture either homophily, structural similarity between closely connected vertices, or structural equivalence, similarity between vertices occupying analogous structural roles even when not directly connected, a flexibility the original DeepWalk formulation did not provide [19].

2.6 Graph Neural Networks

Scarselli, Gori, Tsoi, Hagenbuchner, and Monfardini's original GNN formulation proposed an iterative message-passing mechanism in which each vertex's representation is updated based on the representations of its neighbouring vertices, repeated until the representations converge to a fixed point, establishing the foundational computational pattern, neighbourhood aggregation, that essentially all subsequent graph neural network architectures continue to employ in some form [9]. Kipf and Welling's graph convolutional network (GCN) reformulated this neighbourhood-aggregation idea as a spectral graph convolution operation with an efficient, localized first-order approximation, producing an architecture that scales considerably more efficiently to large graphs than the original GNN's iterative fixed-point formulation while achieving strong empirical performance on semi-supervised node classification benchmarks [20]. Veličković et al.'s graph attention network (GAT) further refined this neighbourhood-

aggregation mechanism by learning attention weights that determine how much each neighbouring vertex should contribute to a given vertex's updated representation, rather than aggregating neighbour information with fixed, structurally determined weights as the GCN does, allowing the model to learn which specific neighbourhood relationships carry the most task-relevant information [21]. Hamilton, Ying, and Leskovec's GraphSAGE addressed a distinct limitation of both the GCN and the original GNN formulation, their reliance on the entire graph being available during training, by introducing an inductive framework that learns a general neighbourhood-aggregation function capable of generating embeddings for previously unseen vertices or entirely new graphs at inference time, a capability essential for the many intelligent-system applications, recommendation systems and evolving social networks among them, where the graph continuously grows after model training [22]. Wu, Pan, Chen, Long, Zhang, and Yu's comprehensive survey of graph neural networks synthesized this architectural progression, spectral and spatial convolutional networks, attention-based networks, and graph autoencoders, into a unified taxonomy, and found consistent evidence across the reviewed applications that GNN architectures incorporating explicit graph structure outperformed structure-agnostic neural architectures applied to the same underlying data whenever genuine relational structure, rather than merely tabular or sequential structure, was present in the task [23].

2.7 Graph Neural Networks for Intelligent Physical System Design

Pfaff, Fortunato, Sanchez-Gonzalez, and Battaglia's MeshGraphNets extended the graph neural network message-passing paradigm specifically to physical simulation, representing a simulation mesh directly as a graph and learning to predict per-vertex physical state updates via message passing across mesh edges, and demonstrated that this graph-native representation generalizes to mesh resolutions and geometries unseen during training, a generalization property that architectures designed for fixed, regular-grid data structures do not straightforwardly provide [17]. This physical-simulation application illustrates a broader pattern evident across the reviewed graph neural network literature: whenever an intelligent system's underlying data possesses a natural graph structure, whether a molecular bond graph, a physical simulation mesh, or a social interaction network, incorporating that structure directly into the model architecture, rather than flattening it into a fixed-size vector representation, consistently improves both predictive performance and generalization to previously unseen graph instances [9], [17], [23].

2.8 Research Gap

While the classical generative network model literature reviewed in Sections 2.1 and 2.2 and the structural analysis literature reviewed in Sections 2.3 and 2.4 have each established mature, mathematically rigorous frameworks, and the graph neural network literature reviewed in Sections 2.6 and 2.7 has established strong empirical performance across diverse intelligent-system applications, comparatively few studies directly connect a given intelligent system's underlying graph neural network architecture choice to a rigorous, prior structural characterization of the target network's actual generative model, meaning that GNN architecture selection in applied practice frequently proceeds without the kind of structural diagnostic analysis the classical network science literature reviewed in Sections 2.1 through 2.4 was specifically designed to provide [4], [20], [23]. This review addresses this gap by organizing the reviewed evidence within a comparative framework spanning generative model family, structural analysis measure, and graph neural network architecture.

3. Methodology

This study adopts a qualitative, descriptive, and comparative research design synthesizing foundational and applied graph theory, network science, and machine learning literature addressing complex network analysis and intelligent system design. Reviewed works were compared along four axes: theoretical lineage (classical random graph theory, small-world/scale-free network models, structural analysis, or graph representation learning/graph neural networks); primary structural property addressed (connectivity, clustering, degree distribution, community structure, or learned vertex representation); computational mechanism (probabilistic generative process, iterative graph algorithm, or neural message passing); and applicability to specific intelligent-system design domains.

4. Results and Discussion

4.1 Generative Network Model Families and Their Structural Signatures

Table 1 maps the classical generative graph model families reviewed in Section 2 onto their structural signature and generating mechanism, providing a diagnostic reference for matching a real-world network's observed properties to the model family that best explains its structure.

Table 1. Generative Network Model Families and Structural Signatures

Model Family	Generating Mechanism	Structural Signature	Key Reference
Erdős-Rényi random graph	Independent edge inclusion at fixed probability	Poisson degree distribution; low clustering	Erdős & Rényi [1]; Bollobás [14]
Watts-Strogatz small-world	Regular lattice with small-probability random rewiring	High clustering + short average path length	Watts & Strogatz [2]
Barabási-Albert scale-free	Growth + preferential attachment	Power-law degree distribution; hub vertices	Barabási & Albert [4]
Fitness/Bose-Einstein model	Preferential attachment weighted by vertex fitness	Power-law with possible "winner-take-all" hub reordering	Bianconi & Barabási [15]
Percolation-theoretic robustness models	Random or targeted vertex/edge removal	Predicts giant-component collapse threshold	Cohen & Havlin [16]; Albert, Jeong & Barabási [5]

4.2 Structural Analysis Measures and Intelligent System Design Applications

Table 2 cross-references the classical structural analysis measures reviewed against their concrete application within intelligent system design, a structure emphasizing measure-to-application translation rather than the generative-model comparison in Table 1.

Table 2. Structural Analysis Measures and Intelligent System Design Applications

Structural Measure	Conceptual Definition	Intelligent System Application	Key Reference
Degree centrality	Number of direct connections a vertex holds	Identifying highly connected nodes for targeted intervention (e.g., influence, failure risk)	Freeman [6]
Betweenness centrality	Fraction of shortest paths passing through a vertex	Identifying structurally critical bridge nodes; community-detection edge removal	Freeman [6]; Girvan & Newman [10]
Recursive/eigenvector-based centrality (PageRank)	Importance derived from importance of connected vertices	Web search ranking; influence and recommendation ranking	Page, Brin, Motwani & Winograd [7]
Hub/authority centrality (HITS)	Bipartite distinction between referring and referenced importance	Information retrieval; identifying authoritative vs. aggregating sources	Kleinberg [8]

Modularity-based community detection	Comparison of intra-cluster density against random-graph null model	Detecting functional modules (social groups, protein complexes, organizational units)	Newman & Girvan [11]; Newman [12]
Percolation/robustness threshold	Critical removal fraction before giant-component collapse	Network resilience design; targeted-attack vulnerability assessment	Albert, Jeong & Barabási [5]; Cohen & Havlin [16]

4.3 Graph Neural Network Architectures Mapped to Mechanism and Task Type

Table 3 organizes the graph neural network architectures reviewed in Section 2.6 by their core computational mechanism and the task type each is best suited to address, a structure distinct from Tables 1 and 2 in that it addresses learned, rather than purely structural or algorithmic, graph analysis.

Table 3. Graph Neural Network Architectures by Computational Mechanism and Task Type

Architecture	Core Computational Mechanism	Best-Suited Task Type	Key Limitation	Reference
Original GNN (Scarselli et al.)	Iterative message passing to a fixed point	Static graph node/graph-level prediction	Computationally expensive iterative convergence	Scarselli et al. [9]
DeepWalk / node2vec	Random-walk-based embedding (skip-gram analogy)	Vertex similarity and downstream classification via embeddings	Transductive; does not generalize to unseen vertices	Perozzi, Al-Rfou & Skiena [18]; Grover & Leskovec [19]
Graph Convolutional Network (GCN)	Localized spectral convolution (first-order approximation)	Semi-supervised node classification on large graphs	Fixed, structurally determined neighbor weighting	Kipf & Welling [20]
Graph Attention Network (GAT)	Learned attention weighting over neighbors	Tasks where neighbor importance varies and must be learned	Higher computational cost than uniform aggregation	Veličković et al. [21]
GraphSAGE	Inductive neighborhood-sampling and aggregation function	Evolving graphs; unseen-vertex inference (e.g., recommendation)	Sampling introduces variance in aggregated neighborhood	Hamilton, Ying & Leskovec [22]
MeshGraphNets	Message passing over physical simulation mesh graphs	Physical simulation; generalization across mesh geometry/resolution	Computational cost of high-resolution mesh graphs	Pfaff et al. [17]

4.4 Discussion

Read together, Tables 1 through 3 support the paper's central claim that intelligent system design benefits from an explicit, sequential graph-theoretic diagnostic process rather than defaulting immediately to a graph neural network architecture without first characterizing the target network's underlying structure. Table 1 establishes that real-world networks exhibit qualitatively distinct generative signatures, and Albert, Jeong, and Barabási's robustness finding demonstrates that this distinction carries direct, practically consequential design implications, since a system built atop a scale-free network requires fundamentally different resilience engineering than one built atop an Erdős-Rényi-like

random structure [1], [4], [5]. Table 2 indicates that the classical structural analysis toolkit, centrality and community detection specifically, remains directly applicable to intelligent system design even in an era dominated by learned graph representations, since PageRank's continued centrality to web search ranking and modularity-based community detection's continued relevance to organizational and biological network analysis demonstrate that these algorithmic, non-learned measures retain practical value precisely where interpretability and mathematical guarantees matter more than the flexible pattern-fitting graph neural networks provide [7], [11]. Table 3's architecture-to-mechanism mapping indicates that no single graph neural network architecture dominates across all task types, with GCNs favoured for large-scale transductive node classification, GraphSAGE favored for inductive, evolving-graph settings, and MeshGraphNets-style architectures favored specifically for physical simulation tasks where the graph itself represents a spatial mesh rather than a social or informational network, a heterogeneity directly paralleling the generative-model heterogeneity Table 1 documents at the classical, non-learned level [9], [17], [20], [22]. This parallel structure across Tables 1 and 3 suggests that graph neural network architecture selection should ideally be informed by the same structural diagnostic considerations, degree distribution, clustering, and community structure, that the classical network science literature developed specifically to characterize a network's generative structure, rather than treating architecture selection as a purely empirical, benchmark-driven exercise disconnected from the network's actual underlying structural properties [4], [12], [23].

5. Conclusion

This paper has reviewed the foundational and applied graph-theoretic literature underlying complex network analysis and intelligent system design, synthesizing classical random graph, small-world, and scale-free generative models, structural analysis techniques including centrality and community detection, and the graph representation learning and graph neural network literature that has integrated graph structure directly into machine learning architectures. The evidence indicates that real-world complex networks exhibit structurally distinct generative signatures with direct, practically consequential implications for intelligent system design, particularly regarding network robustness and resilience, and that the classical structural analysis toolkit developed to characterize these signatures remains directly relevant to contemporary intelligent system design even as graph neural network architectures have come to dominate applied practice. Graph neural network architecture selection itself exhibits a parallel heterogeneity, with different architectures suited to transductive, inductive, and physical-simulation task types respectively, suggesting that effective intelligent system design depends on matching both classical structural analysis method and graph neural network architecture to a network's actual, empirically characterized generative structure rather than applying either a single default graph model or a single default learning architecture universally.

6. Future Work

Future research should prioritize developing a more rigorous theoretical understanding of graph neural network expressiveness limits, building on formal analyses showing that standard message-passing architectures cannot distinguish certain non-isomorphic graph structures, to establish clearer guidance for when a GNN architecture's representational capacity is genuinely sufficient for a given intelligent-system task rather than relying solely on empirical benchmark performance. Further work is needed to develop principled, automated diagnostic tools that characterize a target network's generative structure, degree distribution, clustering, and community structure, as a standard preprocessing step informing graph neural network architecture selection, directly operationalizing the structural-diagnostic-to-architecture-selection connection this review identifies as currently underdeveloped in applied practice. Continued research should also extend the physical-simulation graph neural network literature, exemplified by MeshGraphNets, toward a broader class of engineering and scientific simulation domains beyond the fluid and structural mechanics applications that have dominated the literature to date. Finally, future work should examine how classical robustness and percolation theory, developed for the generative network models reviewed in Section 2.2, can be formally extended to characterize the robustness properties of learned graph neural network representations themselves, since a GNN's predictive robustness to targeted adversarial perturbation of high-centrality vertices

remains considerably less theoretically understood than the classical robustness properties Albert, Jeong, and Barabási established for the underlying network structures such models are trained on.

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