Multi-* Graphs

Jernej Avsec[a], **Tina Brdnik**[a], **Constance Monluc**[a], **and Anej Umek**[a]

[a]University of Ljubljana, Faculty of Computer and Information Science, Večna pot 113, SI-1000 Ljubljana, Slovenia

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The growing complexity of real-world systems has exposed the limitations of traditional graph models in network analysis. To address this, a range of enhanced graph structures (collectively referred to as multi-* graphs) have emerged. In this handout, we focus on three core types: multilayer, multiplex, and multi-relational graphs. Each provides a distinct framework for representing multiple types of interactions or dimensions within complex networks, making them valuable tools in domains such as social sciences, biology, and transportation. We define each graph type, explore their structural properties, compare their differences, and highlight their applications. To offer a broader perspective, we also briefly introduce other emerging models such as multi-modal, multi-scale and multi-temporal graphs, emphasizing the growing richness and diversity of the field. This handout aims to provide researchers and students with a clear and comparative understanding of the multi-* graph landscape.

Graphs are fundamental structures for representing networks in various domains, including sociology, biology, computer science, and transportation. Traditional graph models, composed of a single set of nodes and edges, are often inadequate for capturing the heterogeneous, dynamic, and multi-dimensional nature of real-world networks. To overcome these limitations, the field has evolved to incorporate a family of enhanced models, commonly referred to as multi-* graphs.

These models allow for more expressive representations by introducing multiple types of edges, layers, or node categories. This handout focuses on three central types: multilayer networks, multiplex networks, and multi-relational networks. Each brings a unique structure and semantics to the analysis of complex systems.

Problem Definition, Motivation and Background

Traditional graph theory assumes that all nodes and edges are homogeneous and that relationships are static and of a single type. However, this assumption fails to capture the complexity of real-world systems, where entities interact in diverse, multi-faceted ways. Consider the following examples:

- In social networks, individuals may interact through friendships, professional ties, and online messaging.
- In transportation systems, cities are connected by various modalities such as road, rail, and air.
- In knowledge graphs, entities like people, locations, and organizations are connected through semantically distinct relationships.

These scenarios highlight the need for more expressive models that can:

- Represent interconnected layers with potentially different node and edge types (*multilayer* graphs),
- Model multiple modes of interaction among the same set of entities (*multiplex* graphs),
- Capture multiple types of relationships within a unified framework (*multi-relational* graphs).

Such models preserve structural and semantic detail that would otherwise be lost or oversimplified, enabling more accurate analysis and better-informed decision-making.

The increasing availability of rich, structured data in various domains further motivates the use of multi-* graphs.

Multilayer Graphs

Introduction. Real-world systems are usually very complex, characterized by dependencies and interactions between a multitude of networks. Multilayer networks provide a flexible framework for modeling such complex systems. They were first introduced in the field of social science which were then adopted in various other domains.

In the most general form multilayer networks consist of many layers, each representing a different type of network which can interact with each other. It consist of two types of links:

1. *intralinks* - links between vertices on the same layers

2. *interlinks* - links between vertices on two different layers

Figure 1 shows an example of a simple multilayer network.*

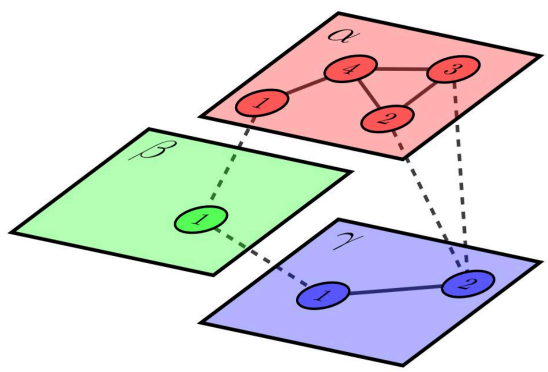

Fig. 1. Example of a simple multilayer network with 3 layers. Solid lines are the intralinks and dashed lines are the interlinks.

*All the material for multilayer network was compiled from [1, 4, 13].

All authors contributed equally to this work.

Definition. An undirected unweighted multilayer network is defined by a tuple of three values

$$\mathcal{M} = (L, G_{intra}, G_{inter}).$$

Here L is a set of numbers from 1 to d (there are d dimentions), indicating different layers of networks

$$L = \{\alpha | \alpha \in \{1, 2, 3, ..., d\}\}.$$

The second argument of the multilayer network $\mathcal{M}$ is a set containing a network from each layer

$$G_{intra} = \{G_1, G_2, ..., G_d\}.$$

There are exactly d elements in G_{intra}, one network for each layer, defined by

$$G_\alpha = (V_\alpha, E_\alpha),$$

where

$$\begin{aligned} n_\alpha &= |V_\alpha|, \\ m_\alpha &= |E_\alpha|, \\ V_\alpha &= \{(i, \alpha) | i \in \{1, 2, ..., n_\alpha\}\}, \\ E_\alpha &= \{\{i, j\} | i, j \in V_\alpha\}. \end{aligned}$$

The last argument of $\mathcal{M}$

$$G_{inter} = \{G_{\alpha,\beta} | \alpha, \beta \in L, \alpha < \beta\},$$

represents a set of bipartite networks between vertices of different layers. Each network

$$G_{\alpha,\beta} = (V_\alpha, V_\beta, E_{\alpha,\beta}),$$

connects vertices of layer α to vertices of layer β, where

$$\begin{aligned} n_{\alpha,\beta} &= |n_\alpha| + |n_\beta|, \\ m_{\alpha,\beta} &= |E_{\alpha,\beta}|, \\ E_{\alpha,\beta} &= \{\{i, j\} | i \in V_\alpha, j \in V_\beta\}. \end{aligned}$$

Note that there are at most $\binom{d}{2}$ elements in G_{inter}.

We can now define the number of vertices (n) and edges (m) of the multilayer network as

$$\begin{aligned} n &= \sum_{\alpha=1}^{d} n_\alpha, \\ m &= \sum_{\alpha=1}^{d} m_\alpha + \sum_{\alpha=1}^{d} \sum_{\beta=\alpha+1}^{d} m_{\alpha,\beta}. \end{aligned}$$

Representation.

Supra-Adjacency Matrix. We can represent a multilayer network as one big matrix ($n \times n$ elements)

$$\mathcal{A} = \begin{pmatrix} \mathbf{a}^{[1,1]} & \mathbf{a}^{[1,2]} & \cdots & \mathbf{a}^{[1,d]} \\ \mathbf{a}^{[2,1]} & \mathbf{a}^{[2,2]} & \cdots & \mathbf{a}^{[2,d]} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{a}^{[d,1]} & \mathbf{a}^{[d,2]} & \cdots & \mathbf{a}^{[d,d]} \end{pmatrix},$$

called *supra-adjacency matrix* that consist of $d \times d$ smaller matrices, each matrix $\mathbf{a}^{[\alpha,\beta]}$ of size $n_\alpha \times n_\beta$, containing connected vertices between layer α and β. To check if the vertex i on layer α is connected to vertex j on layer β, we check i-th row and j-th column on the submatrix $\mathbf{a}^{[\alpha,\beta]}$:

$$\mathcal{A}_{i\alpha,j\beta} = \mathbf{a}_{ij}^{[\alpha,\beta]}.$$

Note that the matrices on the diagonal are just regular adjacency matrices containing the intralinks, and off diagonal matrices contain the interlinks between different layers.

Adjacency list. Multilayer graph can also be represented as an adjacency list. Each vertex hold a list of tuples

$$(\alpha, i),$$

where the first argument tells you the layer of the connected node and the second argument tells you the node in that layer to which it is connected.

Edge list. Another way to represent a multilayer networks in an edge list format. Each element is a 4-tuple:

$$(\alpha, i, \beta, j),$$

which states that the vertex i on layer α is conncted to vertex j in layer β. If both vertices of an edge are on the same layer ($\alpha = \beta$) it is an intralink, else it is an interlink ($\alpha \neq \beta$).

Examples. Multilayer networks are a powerful tool for analyzing and modeling real-world data, which is usually complex and multidimentional. Here are some examples of those networks.

Transportation. Transportation systems are a crucial aspects of our daily lives. Studying and analyzing different means of transport on a multilayer network can help us make better decisions in the future (optimizing connectivity or improving efficiency). One such example of a network can be seen on Figure 2.

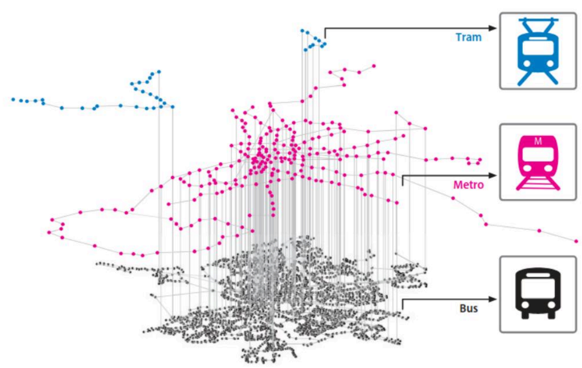

Fig. 2. Madrid transportation system multilayer network. Each layer represents a different mode of transport. Two vertices (stops) on different layers are connected if they are within 150 meter range of each other [1].

Interconnected infrastructures. Different types of infrasrurctures (like power grid, transporation system, internet, water, emergency services, etc.) all depend on each other (example in Figure 3). By modeling and analyzing this as a multilayer network we can determine the resilience and robustness (if one infrastructure is down, how it will affect the other) of the network and try to remove bottleneck that could potentially lead to a cascade of failures in the future.

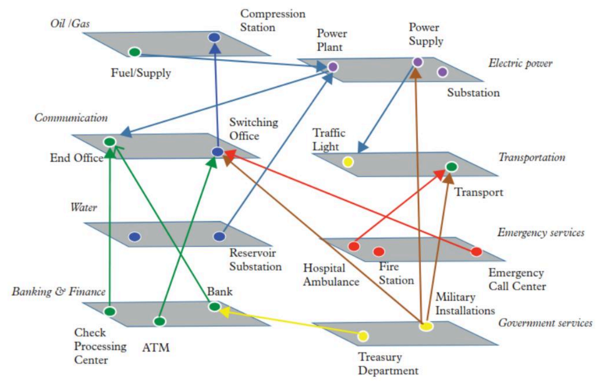

Fig. 3. An example of interconnected infrastructure multilayer network. Each layer represents a different infrastructure while the links represent the dependencies [4].

Other examples. Some other popular fields, where multilayer networks are especially applicable:

- *social networks* - people with different social ties,
- *economical and financial networks* - import / export relations between different countries,
- *molecular networks* - different types of molecular interactions interacting with each other,
- *brain networks* - more realistic representation of the connected neuron structure than single networks,
- *ecological networks* - interactions between ecological communities,

and many more.

Tools. There are a number of software libraries for multilayer network analysis. Most notable are

- *Multinet* - a C++ library that supports manipulation, visualisation and mining of multilayer networks (also includes methods for community detection, evaluation and comparison),
- *MuxViz* - R library for multilayer network analysis, manipulation, visualization, centrality measures, structural analysis, community detection and more,
- *Pymnet* - a Python library which offers functionalities such as manipulation, visualization and computing different clustering coefficient metrics,
- *Py3plex* - a Python library that provides analysis, visualization, manipulation of multilayer networks as well as node classification and network embedding methods.

Multiplex Graphs

Multiplex graphs are a specific type of multilayer network. While multilayer graphs allow each layer to have different node sets and interconnections, a multiplex graph imposes a constraint: all layers must share the same set of nodes, and each layer represents a different kind of interaction among them.

Definition. A **multiplex graph** is a multilayer network with N nodes and d layers, where each layer represents a different type of interaction among the same set of nodes. It is formally described by a vector of adjacency matrices:

$$A = \{A^{[1]}, A^{[2]}, \ldots, A^{[d]}\}$$

where $A^{[\alpha]}$ is the adjacency matrix of layer α, and $a_{ij}^{[\alpha]} = 1$ indicates that nodes i and j are connected in that layer [3].

This framework captures multiple types of relationships, such as friendship, communication, or collaboration, without aggregating them into a single network.

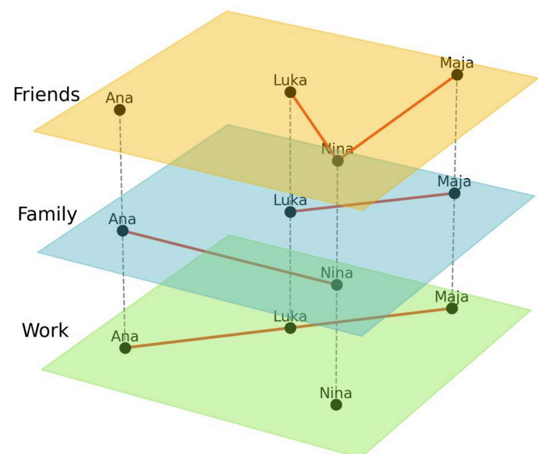

Fig. 4. A multiplex network with three layers: work, family, and friendship. Each layer represents a different type of interaction among the same set of nodes (Ana, Luka, Nina, Maja). Dotted vertical lines show that each node appears across all layers.

Structural Properties. Multiplex graphs can be analyzed using extended structural measures:

- **Degree vector**: The degree vector of a node describes how connected it is across each distinct layer of the multiplex graph. Formally, for node i, the degree at each individual layer α is defined as [3] :

$$k_i^{[\alpha]} = \sum_j a_{ij}^{[\alpha]}$$

from which it follows that $0 \leq k_i^{[\alpha]} \leq N-1$ for all nodes i and layers α. The complete degree vector of node i across all layers is then given by:

$$\mathbf{k}_i = (k_i^{[1]}, k_i^{[2]}, \ldots, k_i^{[d]})$$

- **Edge overlap**: This measure counts how many layers include a connection between two nodes. The edge overlap of edge $i - j$ is:

$$o_{ij} = \sum_\alpha a_{ij}^{[\alpha]}$$

A higher overlap means the connection is stronger or more important because it exists in multiple types of relationships or settings [3, 5]

- **Overlapping Degree of a Node** i: The overlapping degree o_i is the total number of connections node i has across all layers. It is the sum of its degrees in each layer:

$$o_i = \sum_{\alpha=1}^{d} k_i^{[\alpha]} = \sum_j o_{ij}$$

where o_{ij} is the number of layers connecting nodes i and j.

This measures how connected node i is throughout the multiplex.

- **Multiplex Clustering Coefficients**: These coefficients extend the traditional clustering concept to multiplex networks by considering triangles (or triads) formed by edges that can span multiple layers. Instead of limiting to a fixed number of layers, clustering is measured based on the number m of distinct layers involved in the triangle.

Formally, a multiplex triangle involving node i is said to be an m-triangle if its three edges belong to exactly m different layers, with $1 \leq m \leq 3$. For example:

  - $m = 1$ corresponds to traditional single-layer triangles.
  - $m = 2$ corresponds to triangles where edges span exactly two distinct layers.
  - $m = 3$ corresponds to triangles where each edge is on a different layer.

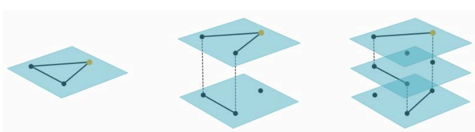

Fig. 5. Examples of multiplex triangles involving one layer (left), two layers (middle), and three layers (right). These illustrate the concept of triadic relations spanning different numbers of layers in multiplex networks.

The multiplex clustering coefficient $C_i^{(m)}$ measures the fraction of m-layer triangles a node has out of all possible. It shows how connected a node's neighbors are across layers.

These coefficients reveal tightly connected groups that single-layer clustering misses, helping to understand social support, network stability and information spread [3, 7].

- **Participation Coefficient** P_i: The participation coefficient measures how evenly a node's connections are spread across layers:

$$P_i = \frac{d}{d-1}\left(1 - \sum_{\alpha=1}^{d}\left(\frac{k_i^{[\alpha]}}{o_i}\right)^2\right)$$

where d is the number of layers, $k_i^{[\alpha]}$ is the degree in layer α, and o_i is the total degree across layers.

Values close to 1 mean connections are well distributed across layers; values near 0 mean connections are focused in one layer. This helps identify nodes that link different types of relationships [3].

- **Interdependence** λ_i: This measures how much a node relies on using multiple layers to reach other nodes efficiently. It looks at the shortest paths from node i to others and counts how many of those paths go through more than one layer:

$$\lambda_i = \sum_{j \neq i} \frac{\psi_{ij}}{\sigma_{ij}}$$

Here, σ_{ij} is the total number of shortest paths from i to j, and ψ_{ij} is how many of those paths use edges in different layers. A high λ_i means the node plays an important role in connecting across layers and helping information flow [3].

Feature	Multiplex Graphs	General Multilayer Graphs
Node Set	Identical across all layers	May differ between layers
Interlayer Edges	Only identity edges or none	Arbitrary interlayer edges allowed, connecting different nodes
Layer Purpose	Different types of interactions among the same nodes	Can represent time, scale, hierarchy, or different contexts
Simpler Model	Yes, more constrained and easier to analyze	No, more general and complex model

Table 1. Differences between multiplex graphs and general multilayer graphs.

Differences from General Multilayer Graphs. Multiplex graphs are simpler to model and analyze, making them useful when nodes interact in consistent, clearly separated contexts (e.g., work vs. friendship).

Applications. Multiplex networks are especially valuable in analyzing social systems where individuals interact through multiple types of ties. For example:

- **Social behavior**: understanding how people communicate, collaborate, and trust each other across different contexts.
- **Infrastructure**: modeling overlapping transportation systems like metro, buses, and bike-sharing.
- **Biological systems**: capturing different forms of interaction such as gene co-expression and physical binding.

A study of Indonesian terrorists revealed that **trust ties** were often predictive of future **operational or communication ties**, demonstrating how one layer can influence others [11].

Multi-relational Graphs

Introduction. Multi-relational graphs are a type of multi-* network that incorporate a heterogeneous set of edge labels, enabling the representation of multiple types of relationships within a single data structure. In contrast, traditional single-relational networks typically represent only one type of relationship such as friendship, kinship, or collaboration but not all simultaneously [14]. Multi-relational graphs, however, can model all these relationship types together, providing a richer and more flexible framework for network analysis. These networks have been applied across various disciplines, including cognitive science, artificial intelligence, and social or scholarly modeling [15]. Each edge set in E has a specific nominal, or categorical, interpretation, allowing the semantics of each relationship type to be preserved as can be seen in Figure 6.

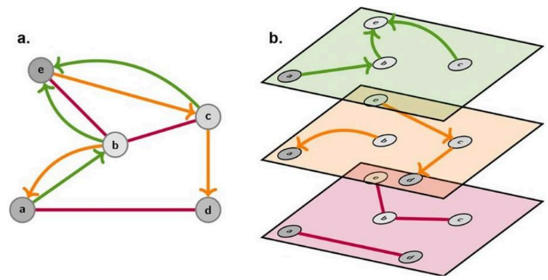

Fig. 6. A multi-relational network with three edge types (left) shown as a single graph; equivalent multiplex representation (right) separates edges by relation type.[8]

Definition. The multi-relational graph G contains a node set V, a relation set R, and an edge set E. The edge set in the multi-relational graph can be represented as:

$$E \subseteq V \times R \times V$$

The relation set R denotes the types of links between nodes, where $|R| > 2$ [12].

Representation.

Three-way Tensor Representation. Multi-relational graph can be represented using a *three-way tensor*. Where

$$M = (V, E = \{E_1, E_2, \ldots, E_m \subseteq (V \times V)\})$$

is a multi-relational network, where each E_k represents a distinct type of relation. The network can then be encoded as a tensor $A \in \{0,1\}^{n \times n \times m}$, where $n = |V|$ is the number of nodes and $m = |E|$ is the number of distinct edge types. The tensor entries are defined as:

$$A^k_{i,j} = \begin{cases} 1 & \text{if } (i,j) \in E_k \text{ for } 1 \leq k \leq m \\ 0 & \text{otherwise} \end{cases}$$

In this representation, the first two dimensions correspond to node indices, while the third dimension indexes the relation types. Each matrix slice $A^k \in \{0,1\}^{n \times n}$ represents the adjacency matrix for the k-th relation [14].

Path Matrices. In a multi-relational network, edges belong to different relation types, each conveying distinct semantics. Such a network can be represented as a three-way tensor as mentioned above.

The *path algebra* operates on these adjacency matrices $A^k_{i,j}$ to construct semantically meaningful paths between nodes [14]. A simple path of length 1 using a single relation is directly represented by A^k. However, more complex paths, formed by combining multiple relations, are computed through matrix operations such as multiplication and scalar weighting:

$$Z = \sum_{k_1, k_2, \ldots, k_l} \lambda_{k_1, k_2, \ldots, k_l} \cdot A^{k_1} A^{k_2} \cdots A^{k_l},$$

where $\lambda_{k_1, \ldots, k_l} \in \mathbb{R}^+$ are scalar weights determining the contribution of each path pattern.

The resulting matrix $Z \in \mathbb{R}^{n \times n}_+$ is referred to as a *path matrix*. Each entry $Z_{i,j}$ reflects the strength or frequency of connection from node i to node j via composite paths. Importantly, values in Z may exceed 1 and are not restricted to binary values, allowing a richer encoding of indirect and semantically complex relationships.

The matrix Z can be interpreted as a positively weighted, single-relational network:

$$G = (V, E, w), \quad \text{where } w : E \to \mathbb{R}^+.$$

This transformation facilitates the application of classical graph algorithms such as clustering, ranking, or embedding—that assume a single edge type. So, path matrices serve as a powerful abstraction that compress multi-relational information into a unified, analyzable format without losing semantic richness. Additionally, filter matrices can be applied to selectively mask edges or paths, allowing for focused analysis on specific nodes, directions, or substructures within the graph.

Examples.

Knowledge Graphs for Question Answering and Semantic Search. Here we represents human knowledge as a large-scale, directed multi-relational graph, where each edge in the graph has a specific relation type (e.g., "bornIn", "worksAt", "locatedIn"), making it a canonical multi-relational structure [6].

Biomedical Knowledge Graphs. In biomedical research, understanding complex relationships among biological entities is crucial for tasks like drug discovery, re-purposing, and disease pathway analysis. Multi-relational graphs allow researchers to integrate heterogeneous biomedical data—such as drugs, genes, diseases, pathways, and side effects—into a unified structure [9] (as show in Figure 7).

Differences to other Multi-* Graphs. It is important to distinguish multi-relational graphs from multiplex and multilayer graphs, which are related but structurally different. Multiplex graphs represent different relationship types as separate layers over the same set of nodes, while multi-relational graphs encode these types as edge labels within a single graph. Multilayer graphs generalize both by allowing variations in both node and edge types across layers. Though all three capture relational heterogeneity, they differ in structure and application focus.

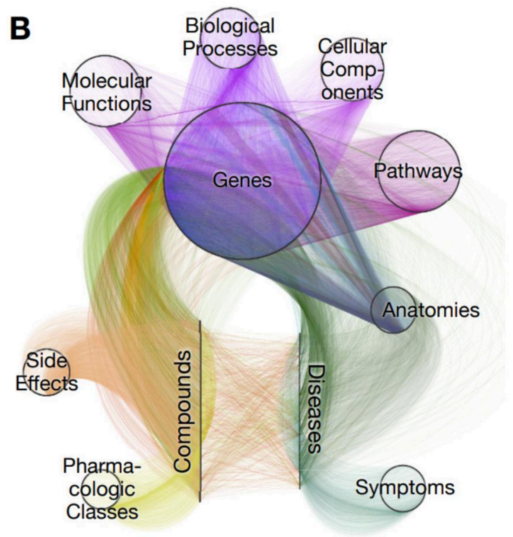

Fig. 7. Schema of Biomedical Knowledge Graph. Nodes are drawn as dots and laid out orbitally, thus forming circles. Edges are colored by type [9]

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Multi-modal, Multi-scale and Multi-temporal Graphs

Beyond the commonly studied multilayer, multiplex, and multi-relational graphs, other multi-* graph models address different aspects of real-world complexity. Multi-modal graphs model networks with heterogeneous node types—such as users, items, and tags in recommendation systems—enabling rich interactions across entity types [16]. Multi-scale graphs capture hierarchical or nested structures, useful in representing systems across different resolutions or abstraction levels, as seen in applications like brain connectivity or climate systems [2]. Multi-temporal graphs, on the other hand, model how networks evolve over time by incorporating temporal dimensions into layers or edges, enabling the analysis of dynamic phenomena [10]. These extended models further enhance the expressiveness of network representations and are increasingly relevant in domains with complex, evolving, or structured data.

Conclusion

The exploration of multi-* graphs highlights the limitations of traditional models in capturing real-world complexity. Enhanced structures like multilayer, multiplex, and multi-relational graphs offer robust frameworks for modeling diverse interactions and dimensions. Each brings unique strengths: multilayer graphs represent multiple layers and link types, multiplex graphs handle varied interactions among the same nodes, and multi-relational graphs capture different relationships within a single structure. These models are vital in domains such as social sciences, biology, and transportation. Emerging models—multi-modal, multi-scale, and multi-temporal graphs—further enrich the field by addressing heterogeneity, hierarchy, and temporal dynamics. Together, multi-* graphs greatly enhance our ability to analyze complex networks.

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