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Chapter 1

Understanding Graphs and Graph Data Science

Graph approaches to data are exploding in the commercial world to better reveal meaning in data as well as forecast behavior of complex systems. This burst is due to the increasing connectedness of data, breakthroughs in scaling graph technology to enterprise-sized problems, excellent results when integrated with machine learning (ML) and artificial intelligence (AI) solutions, and more accessible tools for general analytics and data science teams.

In this chapter, you discover how we define a graph and the relationship of graphs to analytics and data science. You also get a foundation in how graphs are used to answer tough questions about complex systems.

Explaining What a Graph Is

Networks are a representation, a tool to understand complex systems and the complex connections inherent in today's data. For example, you can represent how a social system works by thinking about interactions between pairs of people. By analyzing the

structure of this representation, you can answer questions and make predictions about how the system works or how individuals behave within it. In this sense, network science is a set of technical tools applicable to nearly any domain, and graphs are the mathematical models used to perform analysis. Simply put, graphs are a mathematical representation of complex systems.

Graphs have a history dating back to 1736. The origins of graph theory hail from the city of Königsberg, which included two large islands connected to each other and the two mainland portions of the city by seven bridges. The puzzle was to create a walk through the city, crossing each bridge once and only once. Leonhard Euler solved that puzzle by asking whether it was possible to visit all four areas of a city connected by seven bridges, while only crossing each bridge once. It wasn't.

With the insight that only the connections themselves were relevant to solving this kind of problem, Euler established the groundwork for graph theory and its mathematics. As one of Euler's original sketches, Figure 1-1 depicts Euler's progression:

- » **Walking the bridges of Königsberg:** Four main areas of Königsberg with seven bridges. Can you cross each bridge only once and return to your starting point?
- » **Euler's insight:** The only relevant data is the main areas and the bridges *connecting* them.
- » **Origins of graph theory:** Euler abstracted the problem and created generalized rules based on nodes and relationships that apply to any connected system.

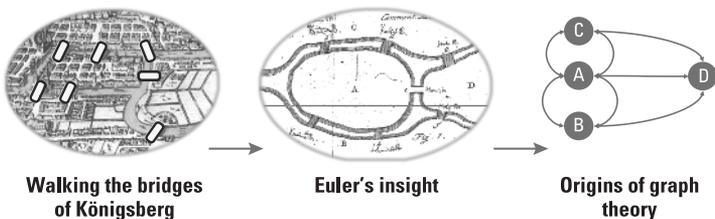


FIGURE 1-1: The origins of graph theory.



While graphs originated in mathematics, they are also a pragmatic and faithful representation of data for modeling and analysis. A graph is a representation of a network, often illustrated with circles to represent entities, also called *nodes* or *vertices*, and lines between them. Those lines are known as *relationships*, *links*, or *edges*. Think of nodes as the nouns in sentences, and relationships as verbs that give context to the nodes. To avoid any confusion, the graphs we talk about in this book have nothing to do with graphing equations or charts. Take a look at the differences in Figure 1-2.

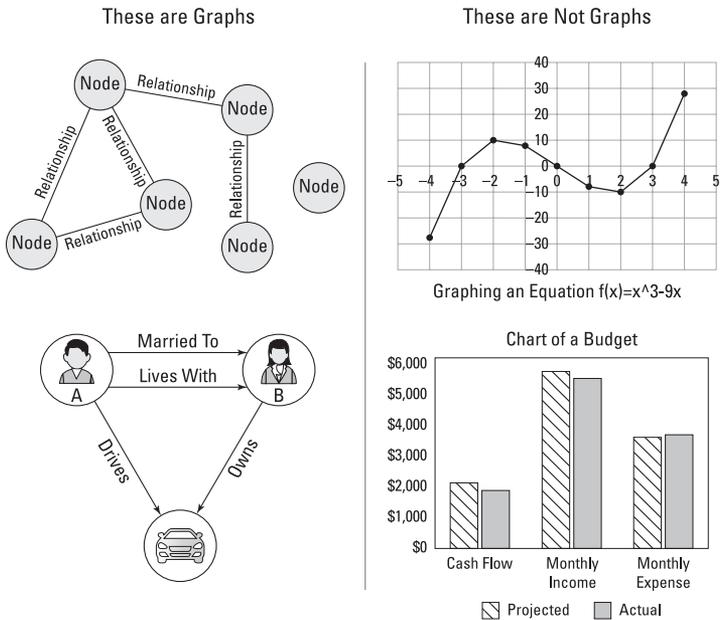


FIGURE 1-2: A graph is a representation of a network.

The bottom graph on the left in Figure 1-2 is a person graph. When looking at that graph, you can construct several sentences to describe it. For example, person A lives with person B who owns a car, and person A drives a car that person B owns. This modeling approach maps easily to the real world and is whiteboard-friendly, which helps align data modeling and analysis.



We often use the phrase “whiteboard-friendly” for anything that’s easy to describe with simple drawings that you could illustrate on a whiteboard.

Defining Graph Analytics and Graph Data Science

Modeling graphs is only half of the story. You may also want to analyze them to reveal insight that isn't immediately obvious. So in this section, we explain the domain of graph data science (GDS) and graph analytics.

GDS is a science-driven approach to gain knowledge from the relationships and structures in data, typically to power predictions. It uses multi-disciplinary workflows that may include queries, statistics, algorithms, and ML.

GDS can typically be broken down into three areas:

- » **Graph statistics** provides basic measures about a graph, such as the number of nodes and distribution of relationships. These insights may influence how you configure and execute more complex analysis as well as interpret results.
- » **Graph analytics** builds on graph statistics by answering specific questions and gaining insights from connections in existing or historical data. Graph queries and algorithms are typically applied together in “recipes” during graph analytics, and the results are used directly for analysis.
- » **Graph-enhanced ML and AI** is the application of graph data and analytics results to train ML models or support probabilistic decisions within an AI system.

Graph statistics and analytics are often used in conjunction to answer certain types of questions about complex systems and the subsequent insights, applied to improve ML.

Looking at the Types of Questions for GDS



REMEMBER

Data scientists try to tackle many types of questions when using GDS to evaluate interdependencies, infer meaning, and predict behavior. At the most abstract level, these questions fall into a few broad areas: movement, influence, groups and interactions, and patterns, as shown in Figure 1-3.

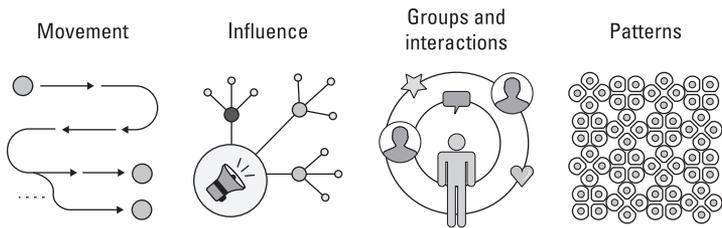


FIGURE 1-3: GDS questions fall into four different areas.

The areas in Figure 1-3 answer the following questions:

»» **How do things travel (move) through a network?**

Understanding how things move through a network involves deep path analysis to find propagation pathways, such as the route of diseases or network failures. It can also be used to optimize for the best possible route or for flow constraints. We cover these classic uses for pathing algorithms more in Chapter 3.

»» **What are the most influential points?** Identifying influencers involves uncovering the structurally well-placed nodes that represent the control points in a network. These influencers can act as fast dissemination points, bridges between less connected groups, or bottlenecks. Influencers can accelerate or slow the flow of items through networks from finances to opinions. The concept of highly connected and influential nodes in a graph is referred to as *centrality*. Centrality algorithms are essential for understanding influence in a network.

»» **What are the groups and interactions?** Detecting communities requires grouping and partitioning nodes based on the number and strength of interactions. This method is the primary way to presume group affinity, although neighbor likeness can also be a factor. Link prediction is about inferring future (or unseen) connections based on network structure. Heuristic Link Prediction algorithms are often used to predict behavior. In addition to community detection algorithms, similarity algorithms are also used to understand groupings.

»» **What patterns are significant?** Uncovering network patterns reveals similarities and can also be used for general exploration.

For example, you may look for a known relationship pattern between a few nodes or compare attributes of all your nodes to find similarities. Or perhaps you want to evaluate the entire structure of a network, with its intricate hierarchies, to correlate patterns to certain social behavior to investigate. Aggregating related but ambiguous information in large datasets is a common activity that relies on finding similar and related information. Finding patterns may employ simple queries or various types of algorithms found in Chapter 3.

Multiple types of graphs queries and algorithms are usually applied in a recipe fashion as part of a GDS workflow. For example, a query to understand the density of relationships in a graph may help determine the appropriate community detection algorithm for the most relevant results. Tactically, graph queries and algorithms are the tools for understanding the overall nature of a connected system and for using relationships in various data science pipelines.

THE RISE OF GRAPH DATA SCIENCE

The rise of graph data science (GDS) is the result of more accessible technologies, increased ability to compute over massive graph datasets, and an awareness of the power of graphs to infer meaning and improve forecasts. Researchers play an essential role in developing awareness and advocating for the best techniques. As data scientists see the potency of structural information, they're increasingly incorporating graphs into their statistics, analytics, and ML practices. In fact, according to the Dimensions Knowledge system for research publications, the use of graph technology in AI research is accelerating. In the last ten years, the number of AI research papers that feature graph technology has increased over 700 percent.