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Excerpt
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1 Graphs as Structure in the Ecological Context

Introduction

Ecology is the study of organisms in the context of their environment, including both abiotic effects and interactions among organisms. Ecologists, like other scientists, are looking for patterns in these phenomena that can be used reliably to make predictions, and those predictions can extend the findings to other organisms, to ecological systems not yet studied or merely to similar groups of organisms in different places or at different times. Those predictions may also refer to how a system's form or structure determines its function and dynamics and how function and dynamics constrain or modify structure and form.

A long but not exhaustive list of the kinds of problems ecologists study might include the following:

- the fate of individuals as determined by neighbours and environmental conditions
- the interactions of individuals in a social structure and their effects on population dynamics
- the movement of individuals through their environment and their reactions to it
- the dynamics of populations and communities in fragmented habitats
- the flow of energy and the population and community effects of predation in trophic networks
- the effects of competition, both intra- and inter-specific, on survival, growth and reproduction
- the dynamics of species interactions, such as mutualism, commensalism and parasitism
- the determinants of species composition of multi-species communities in island systems

Almost all of these can be approached in a theoretical or abstracted way, or quite explicitly with locations in time or space, and almost all of these are studied in the context of a system of some sort and usually in the context of that system's structure. In fact, explicit references to "structure" arise in almost every study of ecological systems, from behaviour to trophic networks and from individuals to community interactions. The term "structure" usually refers to how systems are put together or to the relationships among units that determine how they work together. Structure, like pattern, suggests some

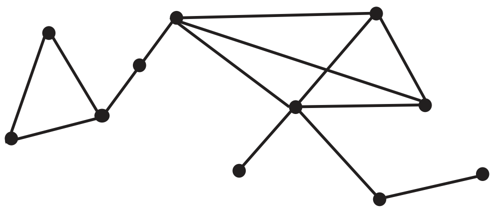

Figure 1.1 A graph. The basic graph consists of nodes (•) and edges (—) joining pairs of nodes. Nodes can have labels, weights or locations. Edges can have directions, signs, weights, functional equations or locations.

predictability in the way a phenomenon is organized, even if the process that gives rise to it has a random origin or stochastic component, such as the fates of individual organisms. Even structures generated by fully random processes may have predictable characteristics, as we will see in Chapter 3. Graph theory is the mathematics of the basics of structure (objects and their connections), providing a rich technical vocabulary and a formal treatment of the concepts and outcomes. Because of the importance of understanding and quantifying structure in all ecological systems, graph theory has important contributions to make to a broad range of ecological studies, including trophic networks (Kondoh et al. 2010), mutualisms (Bascompte & Jordano 2014), epidemiology (Meyers 2007) and conservation ecology (Keitt et al. 1997), where the graphs depict functional connections among organisms or physical connections among spatially structured populations (Grant et al. 2007).

The graphs that are the focus of graph theory are deceptively simple mathematical objects, each consisting of a set of points with a set of lines joining them in pairs. The points are called *nodes*, represented by dots in a diagram (Figure 1.1), and the lines are *edges*, represented by straight or curving lines in a diagram, although a range of terms can be found in the literature (see Harary 1969; West 2001).

Graphs are about connections and the pattern of connections. In a diagram of the most basic graph, the positions of the nodes on the page and the lengths and shapes of the edges joining them have no meaning; they are placed for convenience and clarity. It is the set of connections made by the edges that determines the graph's topology. The nodes usually represent components or units of organization, and the essence of the graph lies in what is connected to what: really very simple! In this way, the graph is an abstract description of *structure* or *topology* because the edges show the relationships among organizational components that the nodes represent.

Graphs and graph theory lend themselves extremely well to applications in many areas of science because there is a wealth of mathematical knowledge that has been developed over the years from studying these simple components. Graph theory investigates all aspects of combinations of nodes with edges joining them; and "all" is no exaggeration. What is continually impressive about graph theory is the way that it can go from what seems simple and intuitive to very sophisticated (and, yes, difficult) results; advances in recent decades have really changed the field, and it has important links (pun intended) to many other branches of mathematics, such as algebra, number theory and topology. An obvious example is the application of graph theory to understanding the properties and vulnerabilities of information networks like the Internet.

A second reason for the great value of graph theory for ecologists is the flexibility of the approach for meaningful applications to a range of ecological phenomena. This is accomplished by including different characteristics in the graphs beyond the simple nodes and edges. These include the following:

- node labels that identify the node as an individual and identifiable component of the system, such as a species name; labels make a difference when counting the number of different structures
- node weights that record qualitative or quantitative characteristics of the components, such as relative abundance
- node locations: the nodes may have spatial or temporal locations, such as the time and place of a single predation event; temporal location allows the possibility of nodes that come into existence or cease to exist

and

- directions for the edges so that A to B is distinct from B to A
- signs for the edges, indicating positive or negative interactions between the nodes
- weights for the edges, or equations describing flow or function
- locations for the edges, spatial or temporal, dependent on the locations of their end-nodes; temporal location allows edges to come into existence or cease to exist

For example, nodes could represent identifiable landscape patches of known locations in a particular year, with their areas as weights; the edges could be movement corridors with weights related to how frequently or how easily the routes can be used for dispersal.

This introductory chapter describes the concepts and terminology that form the foundations of a tour through graph theory and the smart ways to use it for understanding ecological phenomena. This tour illustrates the assertion that these graphs are about structure and the pattern of relationships that are the essence of structure. A subtle distinction here is that despite the fact that "graph" and "network" have come to be almost synonymous, "graph theory" is still more about structure and "network theory" is more about function and flow.

1.1 Graphs as Structure

The branch of mathematics that we know as graph theory has arisen from a number of different sources, developed to solve problems in diverse fields. The most famous of these is Euler's solution in 1736 to the "Königsberg bridge problem," which concerned walking routes around two islands in a river with seven bridges over it. By converting the question into a general problem about graphs, it could be shown that a closed route that crossed each bridge exactly once was impossible (Euler, as cited in Biggs et al. 1976). This solution is usually cited as the beginning of graph theory, although Tutte (1998) has suggested that the discipline might date back to ancient times and the study of

Platonic solids (tetrahedron, octahedron, etc.), which are essentially symmetric graphs on the sphere. Another origin is Kirchhoff's studies of 1847 (Biggs et al. 1976) on the flow of electricity through a network of circuits with different characteristics. A third beginning is Cayley's work on the combinatorics of the chemical structures of organic compounds (e.g. butane and its isomer, isobutene) and the structurally different forms any one chemical might take (Cayley 1857). Other possible sources of the discipline include studies of map colouring problems (any map can be coloured with only four colours), interactions between molecules in statistical mechanics and Markov chains in probability theory (see Harary 1969, Chapter 1). I would, however, add a different, fourth area to the list of inspirations, and that is the study of networks of positive and negative interactions between individuals in a social setting, with developments due to Harary and co-workers from the 1950s.

All these problems are clearly about structure, the structure associated with

1 spatial constraints on physical routes
2 energy flow in a system with alternate pathways and different resistance characteristics
3 physical forms from combinations of component units (atoms)
4 relationships in interaction networks

All these sources of graph theory as a branch of mathematics have close parallels in ecological research, and all require, and take advantage of, different characteristics and results developed in that discipline.

In mathematical terms, a *graph* is an object made up of two sets: *nodes* (also points or vertices) and *edges* (the lines, also called arcs or links) that join pairs of nodes (Harary 1969; West 2001; see Box 1.1). Therefore, graph G can be seen as an ordered pair of sets V and E:

$$G = (V, E) \text{ with E being pairs of the elements of V.}$$

Less formally,

$$\text{graph} = \{\text{nodes}\} \text{ and } \{\text{edge joining pairs of nodes}\}\text{; say } n \text{ nodes and } m \text{ edges.}$$

The density of edges is measured by the *connectance*, which is the proportion of possible edge positions actually occupied; here $2m/n\ (n - 1)$. (This is not the same as a graph being *connected*, with a path between any two nodes, nor is it the same as *connectivity*, which measures how difficult it is to separate a connected graph into pieces.)

In contemporary usage, the terms "graph" and "network" are used interchangeably as equivalents (Estrada 2012), although previous practice was to reserve "network" for graphs or digraphs which had a real number (weight) assigned to each edge (Harary 1969), such as those in trophic networks or transportation systems. Digraph networks, with directed edges, are frequently used to study the flow of material or information, one of the most important applications of graph theory, and for such applications, each edge can have several weights, including capacity, flow and cost (Bang-Jensen & Gutin 2009).

Box 1.1 Graph Theory: Checklist of Objects

Each term has a sketchy phrase to hint at its meaning, rather than a full definition, for which see the text and the Glossary. This is not all the graph theory we need but much of the important material in a concise format. Not everything required will fit into Chapter 1; more will be introduced as needed.

1.1.1 Graphs

Graph (nodes and edges)
Subgraph (subsets of graph's nodes and edges)
Induced Subgraph (subset of nodes, and all edges of the original graph joining those nodes)
Connected Graph (path exists between any two nodes)
Tree (connected with no cycles)
Dendrogram (binary tree, often from cluster analysis)
Complete Graph (all possible edges are included)
Bipartite Graph (nodes in two distinct subsets)
Digraph (directed edges)
Tournament (each pair of nodes has a one-way outcome edge)
Signed Graph and Digraph (edges are positive or negative)
Weighted Graph (nodes or edges have weights)
Weighted Digraph (ditto and edges have directions)
Line Graph (edges become nodes in the derived line graph)
Network (same as graph, or graph with directed weighted edges)
Dynamic Network (changes through time, either edges or their weights)
Spatial Graphs (nodes located in space [vs *aspatial*])
Temporal Graphs [many names] (nodes located in time [vs *atemporal*])
Spatio-temporal Graphs (nodes located in time and space)
Planar Graph (can be drawn flat without edges crossing)
Dendrogram (clustering process and levels of joins)

1.1.2 Parts of Graphs

Subgraph (subsets of nodes and edges)
Cut-point (node removal disconnects)
Cut-edge (edges removal disconnects)
Block (maximal connected subgraph with no cut-points)
Walk (sequence of nodes and their edges; may re-use)
Path (sequence of nodes and edges, no re-use)
Closed Walk (ends at its beginning node)
Cycle (path that ends at its beginning node)
Clique (complete subgraph)
Tree "Leaf Node" (degree = 1; "object" in classification dendrogram)
Tree "Branch Node" (degree > 1; joins objects into groups in dendrogram)
Spanning Tree (connected subgraph with all nodes, but no cycles)
Clusters or Modules (subgraphs well connected within, few connections out)
Components (maximal connected subgraphs)

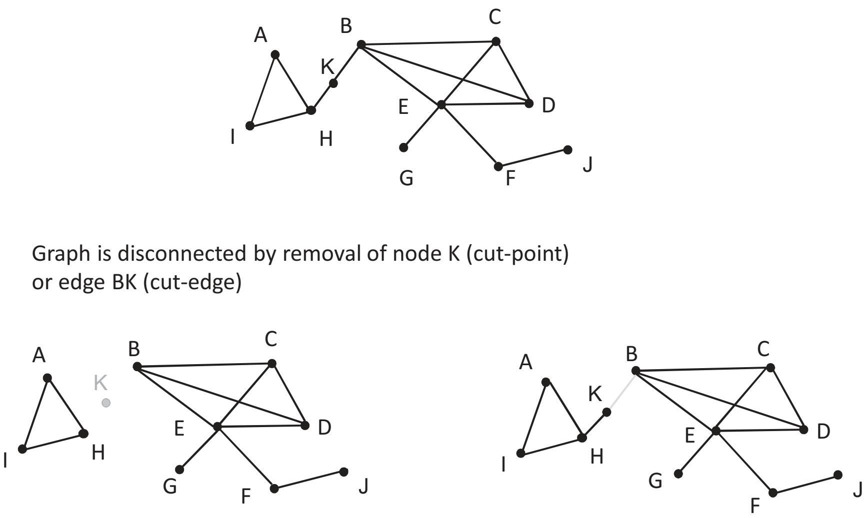

Figure 1.2 Children who play together. The graph is disconnected by removal of node K (a cut-point) or edge BK (a bridge or cut-edge).

Graph theory is usually introduced by formal development, and we cannot avoid that altogether; but we will introduce much of the basic terminology through an example, not trying to cover everything, with more to be introduced in later sections as required. The introductory narrative will be complemented by a checklist table of terms (Box 1.2) as well as the figures that go with them. This book also has a Glossary that collects almost all of the terms introduced throughout the chapters in one place.

To start with an instructive and almost-ecological example, consider children on a playground. Each child is represented by a node of a graph, G, and a simple edge is used to indicate which children are playing together during an observation period (Figure 1.2). There may be large and small groups, or individuals may play mostly alone. We can use graph-theoretical properties to evaluate this social structure for average number of playmates, maximum number of shared-play relationships between any two children and so on, and to determine the most coherent clusters. Each child has a name, and so each node has a natural label. The *degree* of a node is the number of edges attached to it, the number of nodes that are its neighbours. In the playground example, the degree is the number of shared-play interactions, ranging from 1 (nodes G or J) to 5 (node E), averaging around 2.5.

In Figure 1.2, all the children are joined together by at least one sequence of edges through the graph, so that a rumour that is passed only between these pairs of playmates will reach all children. That is, the graph is *connected*, because there is a *path* along nodes and edges between any pair of nodes. It will become disconnected, however, if child K leaves (that node is a *cut-point*) or if B and K become estranged and no longer play together (edge BK is a *cut-edge*) (see Figure 1.2, bottom). There are two obvious *clusters* or *modules*, AIH and BCDE, which are subgraphs of the whole structure. A

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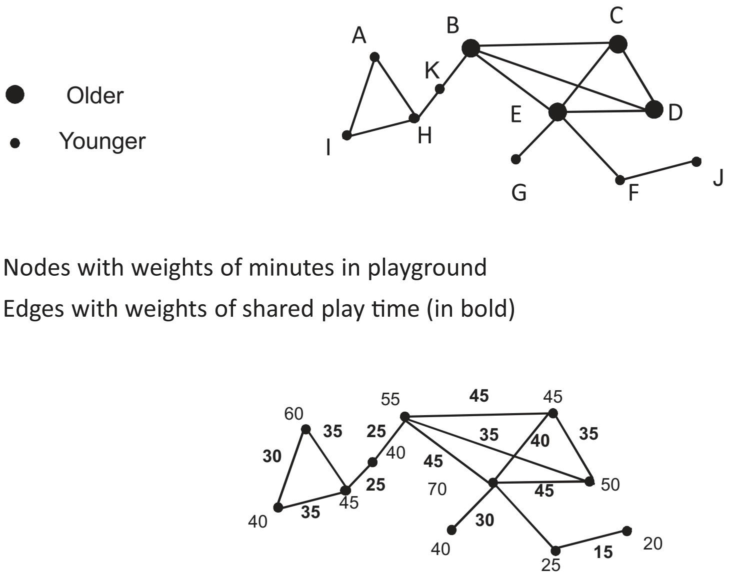

Figure 1.3 Children who play together. (top) Older children indicated by larger nodes. The subgraph of BCDE is a complete graph or clique. (bottom) Nodes with weights of minutes in playground; edges with weights of shared play time (in bold).

subgraph of *G* is itself a graph of which the nodes are a subset of the nodes of *G* and the edges are a subset of the edges of *G*.

Each node can also be categorized by age and gender, and so it can be determined in which categories the graph is *assortative* (most edges between nodes in the same category) or *disassortative* (most edges between nodes in different categories). In our playground example, the graph tends to be associative for age, mainly because of the *clique* (a *complete subgraph*, i.e. with all nodes joined to all nodes) of four older children (B, C, D and E), as shown in Figure 1.3 (top).

Further properties include a weight for each node, such as the total time on the playground, and weights for each edge, such as the total time or proportion of time the two children play together (Figure 1.3, bottom). The simple graph of nodes and edges in the figure is *aspatial*; space is not explicitly included, but the data on which it is based are probably truly spatial, if they were to be thus recorded. For example, some groupings may tend to spend their time by the slides and others by the swings. For some purposes, this spatial information could be included in the graph. Similarly, the graph shown is *atemporal*, but an explicitly temporal graph could be created by recording the different combinations of children at different times of day or by recording the changing links as friendships form and dissolve, evidenced by shared time on the playground. The latter approach gives a dynamic graph or network.

Of course, there are many different ways to define the edges of a graph for the same children in the playground. For example, with children, unlike some of the animals we study, we can complement the observational data by asking them their opinions of the

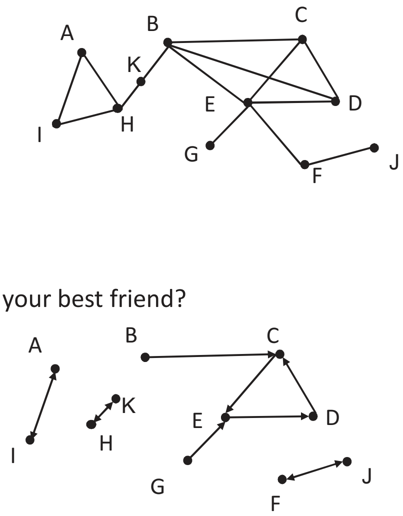

Figure 1.4 Children who play together. Nodes HKBEF with edges between form a path. Nodes AIH with three edges form a cycle. Nodes BCDE with their six edges form a subgraph, a complete graph and a module. The (undirected) graph (top) becomes a digraph (directed graph) (bottom) based on "Who is your best friend?"

others: Who do they like? Who is their best friend? and so on. This gives edges that have direction, because B may consider C to be their best friend, but the "best friend" relationship is not always reciprocated (Figure 1.4). Directional edges allow the inclusion of asymmetric relationships. They also mean that the degree of each node can be divided according to "arrow toward" edges, *in-degree*, and "arrow away" edges, *out-degree*. (In the digraph of Figure 1.4, node E has an in-degree of 2 and an out-degree of 1.)

So far only edges of shared play or liking, which are positive edges, have been included in the graph, but it might also include negative edges indicated pairs that never play together or that actively avoid each other; this gives signs to the edges creating a signed graph (Figure 1.5). By allowing asymmetric "like" and "dislike" for any pair of nodes, the graph then has edges that are signed and directed, allowing A to B to differ from B to A (see nodes K and E in Figure 1.5b). To refine further to include the intensity of "like" and "dislike," the edges may also have quantitative weights. In a real study of social structure, it would be interesting to compare the graph based on observed behaviour and the graph based on stated opinion . . .

A child shows up with a bad cold one day, and the cold spreads among the children from playmate to playmate following the edges of the shared-play graph. How far and fast the cold spreads will depend in part on the position of the initial carrier in the social network, how well connected and how central within the whole population (compare nodes B and J). The spread of the disease will follow a path in that graph consisting of a series of nodes and the edges joining them. In a path, the elements are not re-used, and in this case, the disease does not return to a child who has already had it, and so no *cycles* are formed. (A cycle is a path that ends where it began, such as A – H – I – A

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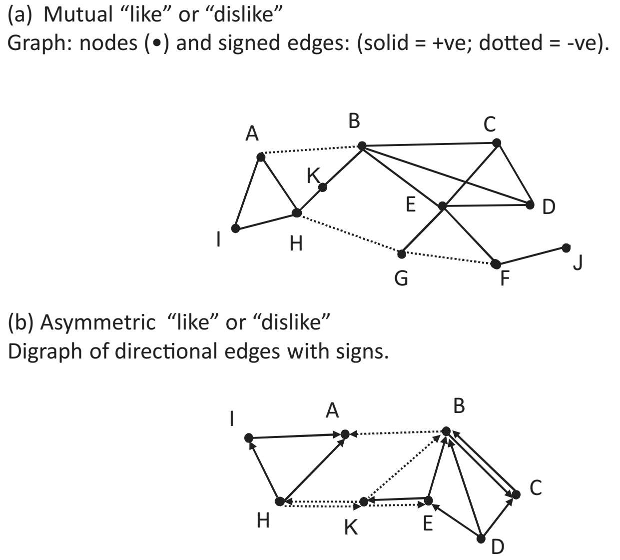

Figure 1.5 Playground children: likes and dislikes. (a) Mutual “like” or “dislike.” Graph: nodes (•) and signed edges: (solid = +ve; dotted = −ve). Two complete subgraph modules: {A,H,I} & {B,C,D,E}.) (b) Asymmetric “like” or “dislike.” Digraph of directional edges with signs. Some relationships are reciprocal: HK, BC. Some are not; the association of K with E is +ve, but the association of E with K is −ve.

in Figure 1.2.) A connected graph without cycles is called a *tree*. The trace of the disease through the shared-play graph is a subgraph that is a tree (Figure 1.6); the nodes are the same as in the original graph, but the edges representing the relationships are different. The edges could be labelled with directions if the actual process of disease spread was known, and they could also be labelled with dates or the order of infection if those data were available. The nodes of a tree are called “leaf” nodes if they have degree 1; “branch” nodes have degree 2 or higher; and the “root” node is a specially designated node that is functionally unique, such as the common ancestor in a phylogeny or the river mouth in a drainage basin, with its meaning depending on the application.

As another example of alternate rules for edges, consider the following. On Saturday morning, each of the four older children is assigned one, two or three of the others to

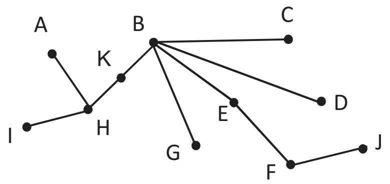

Figure 1.6 A tree made up of shared-play edges showing how a cold may spread. A tree has no cycles. A, I, G, J, D and C are leaf nodes. H, K, B, E and F are branch nodes. No node is identified as the root.

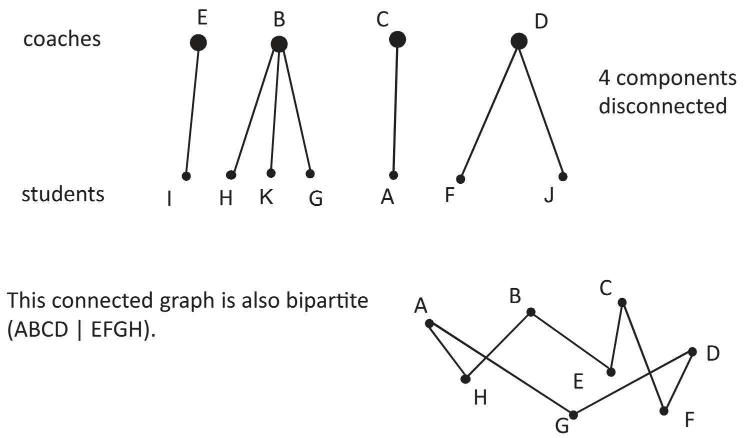

Figure 1.7 Bipartite graph of math coaching in the playground group; this one is disconnected. The lower connected graph is also bipartite (ABCD | EFGH); it is a ring graph and regular because all nodes have the same degree (2).

help coach them in their math skills. This creates a new set of edges that can replace the friendship edges of shared play; with the nodes representing the same individuals and the edges now representing that coaching relationship (Figure 1.7). Here the edges all join older to younger children, with no edges within either age cohort, giving what is called a *bipartite graph* for obvious reasons. In our example, the graph is *disconnected* (some nodes not joined by a path) and consists of four *components* (connected subgraphs).

This narrative has introduced some of the most ecologically important aspects of graphs. These are the basics only and more terms and concepts are introduced throughout the chapters that follow. All are provided in the Glossary at the end of the book.

1.2 Graphs and Ecological Relationships

The objects in ecological studies, which are to be the nodes of a graph, are often individual organisms, populations, communities, or defined spatial areas like habitat patches; and the objects are linked by physiological, behavioural, physical and dispersal processes. The edges between objects vary in weight and in vulnerability versus persistence, according to the nature and intensity of the ecological processes. Research in the related fields of evolutionary biology, population genetics and epidemiology, have as the usual objects individual organisms or other units such as taxa, traits, genes, molecular markers and so on. The edges between these nodes are the relationships of evolutionary history, functional pathways, measured similarity or ecological interactions. Graphs of these systems have the objects as nodes and their relationships as the edges (Harary 1969; West 2001; Bang-Jensen & Gutin 2009; Lesne 2006; Kolaczyk 2009). These graphs of relationships can be thought of as "abstracted" structures, because they