1 Networks and graph properties

Because networks are a way of representing an underlying complex system, there are many variations on the basic idea of a set of V nodes and E pairwise interactions. A given network will thus have a particular set of **graph properties**, which help define the specific aspects of the underlying system that the network captures.

For concreteness, we define a graph or network as G = (V, E), where V is the set of vertices, and E is the set of edges. Each edge is a pair of nodes $i, j \in V$ such that $(i, j) \in E$.

1.1 Simple graphs

The most basic kind of network is called a *simple* graph, which has the following properties:

- 1. edges are **undirected**: a connection $(i, j) \in E$ implies a connection $(j, i) \in E$
- 2. edges are **unweighted**: edges are either present or absent, only (a "binary" relation)
- 3. there are no self-loops: no edge connects a vertex to itself $(i,i) \notin E$
- 4. there are no annotations on the nodes, except that nodes are uniquely indexed.

The following figure shows an example of a simple graph, on the left, and a more exotic (non-simple) graph on the right, which provides some examples of how additional information can be stored in a graph representation.

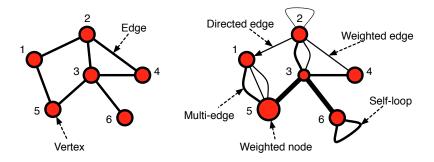


Figure 1: A simple graph (unweighted, undirected, no self-loops), and a more exotic network.

1.2 Non-simple graphs

When we relax one of the graph properties of a simple graph, we get a network representation that can capture additional kinds of information about the underlying system. A simple graph is called "simple" because it is the closest to the basic definition of a set of discrete entities V and their

pairwise interactions.

The table below lists common graph properties, arranged by whether the property is a function of an *edge*, a *node*, or the whole *network*. Properties with a symbol next to them $(\circ, \bullet, \star, \diamond, \dagger)$ represent grouped properties, such that a network will have exactly one property from that group.

	edge	$\mid node$		network
0	unweighted	metadata or attributes	*	sparse
0	weighted	locations or coordinates	*	dense
0	signed	state variables	♦	bipartite
•	undirected		♦	projection
•	directed		†	connected
	multigraph		†	disconnected
	timestamps			acyclic
				temporal
				multiplex
				hypergraph

Networks with edge attributes

Many networks have auxiliary data associated with their edges. For example, an edge can be weighted, meaning that each edge (i,j) has an associated scalar value or edge weight w_{ij} , which might represent the frequency of interaction (as a natural number $w_{ij} \in \mathbb{Z}$) or the interaction's strength (as a real-valued number $w_{ij} \in \mathbb{R}$). Edges may also be signed $w_{ij} \in \{-1, +1\}$, which is a simple way to represent inhibition or activation in a biological system, or distrust and trust in a social system. In fact, edges annotations can be arbitrarily complicated, extending to a whole vector of attributes, a list of "tags," or just a "color" or other kind of categorical variable. When an edge attribute denotes a discrete point in time $t \in \mathbb{N}$ at which that edge exists, we say the network is a temporal network, and each group of co-occurring edges (same t) is a network "snapshot." If, on the other hand, edges are annotated by a starting and stopping time, as in a network of phone calls, or a network of physical proximities, then edges have a continuous duration, and we instead say the network has timestamps. We elaborate on this distinction a little more below.

A multigraph relaxes the prohibition against repeated connections (and generally also the constraint on self-loops), meaning that for at least one pair $i, j \in V$, there exists a multiplicity of edges $(i, j) \in E$. If vertices represent cities, and edges represent driving paths between a pair of cities, then a multigraph will be a reasonable representation because there can be several distinct such paths between a pair of cities. Similarly, in a network of neuron cells, two neurons can have multiple synapses and we might wish to represent each such connection as a distinct edge.

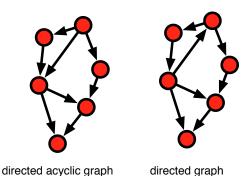
¹Temporal networks and timestamped networks become indistinguishable when each snapshot spans only a small interval of time, e.g., a few seconds. In this limit, most snapshots will be nearly empty graphs. More commonly, a snapshot represents the accumulation of all timestamped interactions over some period, e.g., a day, a week, or a year.

Networks with node attributes

Nodes can also have **attributes** or **metadata** attached to them, denoted as x_i , and these can be categorical variables (sometimes called "labels"), single scalars or vectors representing **state variables**, or even spatial coordinates or **locations** in some metric space.² For example, if nodes are cities, node attributes might include the city's population and GPS coordinates. In a social network, node metadata may include age, sex, and location. In a protein-interaction network, node attributes might include the molecular weight or Gene Ontology functional labels.

Directed networks

If edges can be asymmetric, we call them **directed**, meaning that the edge (i, j) can occur independently of (j, i). Such directed edges are sometimes called arcs, but not always. The World Wide Web is a familiar directed network: webpages are nodes, and hyperlinks are the directed edges. Many biological networks are directed, including gene regulation and neural activation.



We call a directed network **acyclic** if it contains no cycles, i.e., for every possible $i, j \in V$, if there exists a path $i \to \cdots \to j$ then no path exists in the reverse direction $j \to \cdots \to i$. For instance, a citation network is composed of the set of published scientific papers, and an edge $(i, j) \in E$ if paper i cites paper j in its bibliography. Citation networks should be acyclic because of time: a newly published paper can only cite previously published papers, meaning each of its bibliographic links points to older papers. For a cycle to exist, some previously published paper would need to cite a non-yet-published paper, i.e., a paper in the future. (In practice, this kind of oddity does happen, as a result of preprints, and simultaneous publications.) Similarly, in food webs, predation is typically a directed and acyclic activity, with edges pointing "up" from basal species like plants or algae toward, eventually, apex predators like wolves and sharks. However, some food webs are not acyclic because species can predate themselves (cannibalism), and some pairs of species predate

²It has become trendy to refer to such information as "ground truth" when one is trying to predict missing values on the nodes. However, this is wrong—node annotations are just more data, and thus should not be treated as absolute truth under any circumstances. We'll revisit this idea when we talk about community detection.

each other (a 2-cycle).

Bipartite networks and one-mode projections

To be a k-partite graph, where k is an integer, the following must be true. The set of vertices V is composed of k distinct classes of nodes (e.g., producers and consumers) and only nodes of different classes interact (consumers only interact with producers, and vice versa).³ The simplest and most common form of such graph is the **bipartite** network, where k = 2. A popular type of bipartite graph is the actor-film network, in which actors and films represent the two classes, and actors connect to the films in which they play a part.⁴

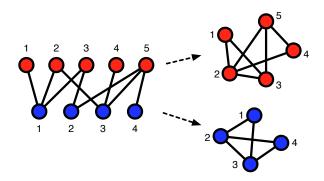


Figure 2: Example of a bipartite graph and its two one-mode projections.

Sometimes, we prefer not to work with a k-partite graph and would instead like to work with a network in which all the nodes are of the same class. This conversion is called a **one-mode projection**. In every k-partite graph, there are k one-mode projections. And, in a one-mode projection, two vertices are connected if and only if they share at least one neighbor in k-partite graph. For instance, to derive the actor-collaboration network from the actor-film network, we add an edge between a pair of actors i, j if they ever appeared in a film together. This procedure is equivalent to saying i, j are connected in the projection if there exists a path of length 2 in the actor-film. Projections can also be weighted, so that (i, j) in the projection is given a weight w_{ij} that corresponds to its multiplicity as a result of the projection procedure, e.g., w_{ij} would count the number of movies in which the actors i, j appeared together.

Warning 1: an important consequence of the one-mode projection procedure is the construction of cliques, i.e., a subgraph of size ℓ in which every pair of nodes is connected. Every node i that

³Mathematically, a bipartite network can be defined in this way: $V = A \cup B$ where $A \cap B = \emptyset$, and $\forall_{(i,j) \in E} ((i \in A) \land (j \in B)) \lor ((i \in B) \land (j \in A))$.

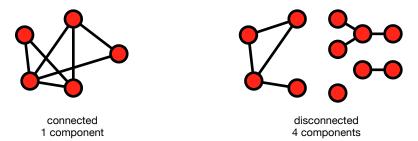
 $^{^4}$ If there are multiple classes of vertices, but edges can exist within each class, then we do not call it a k-partite graph. Instead, it is simply an annotated network with mixed node types.

is being "projected through," meaning i will not be present in the projection, is represented in the projected graph as a clique of size ℓ , because all pairs of its neighbors are exactly distance two away from each other. For instance, all actors in a particular film will be joined in a clique in the one-mode actor projection.

Warning 2: another important consequence of the one-mode projection procedure is that the same one-mode projection may result from multiple different bipartite networks. In this way, the projection operation is not one-to-one i.e., it is not a bijection.⁵ The projection operation is, however, surjective, meaning that any projected network P has at least one bipartite network B such that the projection of B results in P. Can you think of how to prove this statement?

Connected networks and components

A path on a network is a sequence of edges $(i, j), (j, k), \ldots, (y, z)$ in which no vertex is repeated,⁶ and the *length* of the path is the number of edges in the sequence. A simple network is **connected** if for every pair of nodes $i, j \in V$, there exists a path $i \to \cdots \to j$ (which implies the existence of a path in the reverse direction, $j \to \cdots \to i$). In this case, we say that j is *reachable* from i. If there is some set of nodes $T \subset V$ that is not reachable from some node i, then the network is **disconnected**, meaning that it's composed of at least two *components*. The minimum number of edges for a network to be connected is m = n - 1, i.e., a tree.



In a directed network, a set of vertices $T \subseteq V$ that are all pairwise reachable from each other is a strongly connected component, while a set of vertices $S \subseteq V$ in which either i is reachable from j or j is reachable from i (but not necessarily both), is called a weakly connected component. Because of the "or" in the definition, weakly connected components tend to be supersets of strongly connected components.

Temporal, dynamic, and evolving networks

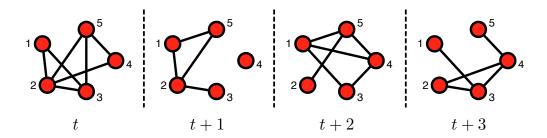
The networks described so far are *static*, meaning that the vertices and edges do not change over time. Graphs that do change over time are an important class of networks. For example, in citation networks, new vertices join the network continuously and each time a new vertex joins, it creates

⁵The namespace here is a little cluttered, but we can, with a grin, say that a bipartite projection is not a bijection.

⁶A trail is a sequence in which vertices may be repeated, but not edges.

new edges representing citations to older papers. If a network varies over time, we call it a *temporal* or *dynamic* or *evolving* network.

A temporal network typically refers to a kind of edge-annotated network in which the annotations represent points in discrete time. We often talk about temporal networks as being a sequence of network "snapshots" $A^{(t_1)}, A^{(t_2)}, \ldots$, where the superscript t_i indexes the passage of discrete time. For instance, all the interactions observed among friends on Monday, and then Tuesday, etc. It may not always be obvious in the data, but a crucial question is whether A^t represents only the interactions present at time t or the aggregation of all interactions between t and t+1. Often, it is the latter.

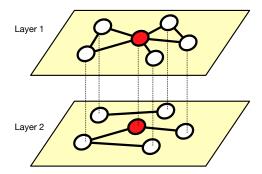


A time-stamped network is one in which edges are annotated with the duration of continuous time in which they existed, e.g., (i, j, t_1, t_2) might represent a phone call or face-to-face interaction that began at time t_1 and ended at time t_2 .

Multiplex networks, spatial networks, and hypergraphs

A network in which edges are marked by which "layer" they exist in is called a **multiplex** or **multipley** network. These networks are used to represent a system in which there are multiple types of interactions, and we store the connectivity of each type in a different "layer" of the multiplex network. A temporal network is a special kind of multiplex network, where these layers form a temporal (ordered) sequence. Crucially, there can dynamics on each vertex that govern which layer some kind of interaction occurs on, so multiplex networks are not merely a special kind of graph in which edges are annotated by different colors or layer numbers.

Spatial networks are a special kind of node-annotated network, in which the annotations represent the node's location in some d-dimensional space. This graph property is most common in transportation networks, e.g., as road and city networks, airport transportation networks, oil and gas distribution networks, shipping networks, etc., but can also appear in social networks. *Planar* graphs are a special case of spatial networks, in which the nodes are embedded on a 2-dimensional surface and edges do not cross.



Hypergraphs are another type of network, in which edges denote the interaction of more than two vertices, e.g, $E \subseteq V \times V \times V$. Scientific collaboration graphs can be represented as a hypergraph, in which each "edge" is the set of coauthors on a scientific article. However, collaboration networks are more commonly represented as bipartite graphs, in which scientists and papers form two sets of vertices, and scientist-nodes are connected to all the paper-nodes on which they are authors.

2 Representing and describing networks

Because networks are a representation of the structure of a complex system, all of network analysis and modeling relies on first specifying what we can represent, and how we represent it mathematically or computationally. In this lecture, we will introduce the three main ways to represent a network, and then explore the standard ways we can use that representation to describe (summarize) a network's structure.

2.1 Representing networks

There are three main ways to represent a network: an adjacency matrix, an adjacency list, or an edge list. As a running example for each representation, consider the following network:

2.1.1 The adjacency matrix

An adjacency matrix is an $n \times n$ matrix, typically denoted A, defined as

$$A_{ij} = \begin{cases} w_{ij} & \text{if nodes } i \text{ and } j \text{ are connected} \\ 0 & \text{otherwise,} \end{cases}$$

where n = |V| is the number of nodes, and $w_{ij} \in \mathbb{R}$ is the weight of the connection between nodes i and j.⁷ If A represents an unweighted network, then edges have "unit" weight, defined as $w_{ij} = 1$.

⁷In some systems, a connection (i, j) may exist but have $w_{ij} = 0$. Such situations require special handling.

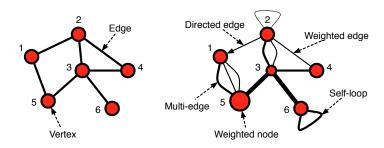


Figure 3: A simple network (left) and a network with more exotic graph properties (right).

In Figure 1, an edge's thickness is proportional to its weight w_{ij} . The corresponding adjacency matrices are

$$A_{\text{simple}} = \begin{pmatrix} 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix} \qquad A_{\text{exotic}} = \begin{pmatrix} 0 & 0 & 0 & 0 & \{1, 1, 2\} & 0 \\ 1 & \frac{1}{2} & \{2, 1\} & 1 & 0 & 0 \\ 0 & \{1, 2\} & 0 & 2 & 3 & 3 \\ 0 & 1 & 2 & 0 & 0 & 0 \\ \{1, 2, 1\} & 0 & 3 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 & 2 \end{pmatrix}.$$

Notice that for the simple graph, (i) the diagonal is all zeros (no self-loops), (ii) all entries are "binary" (0 or 1, and hence unweighted), and (iii) if $A_{ij} = 1$ then also $A_{ji} = 1$ (undirected, implying that A is symmetric across the diagonal). For the non-simple graph, none of these properties holds: it is a directed, weighted, multigraph, with self-loops.

Adjacency matrices are most commonly used in mathematical expressions, e.g., to describe mathematically what a network algorithm or network calculation does.⁸

Sometimes, adjacency matrices are used in network algorithms, because an operation on the matrix A is more efficient (takes less time) than the same operation on another representation, e.g., determining whether some edge exists, $(i,j) \in E$, is fastest in A because it requires only a constant-time O(1) lookup. The tradeoff of fast access to each adjacency A_{ij} , however, is that A takes a quadratic amount $\Theta(n^2)$ of memory to store, because it explicitly stores a value for every pair of nodes $i, j \in V$. As a result, on a modern computer, a simple network with only n = 100,000 nodes

⁸For this reason, many techniques from linear algebra have applications in network analysis and modeling. Here, we will not assume the reader has familiarity with matrix multiplication or spectral techniques, but will try to highlight such connections for those who do.

will take about 8 bytes $\times (10^5)^2/2^{30} = 74.5$ GB of space to store.

When we say an empirical network is **dense**, we mean that most of A's elements are non-zero. In this case, an adjacency matrix is the most space-efficient way to represent the edges. When we define edges using pairwise correlations or similarity scores, we get dense matrices because every pair produces a score. When we say an empirical network is **sparse**, we mean that roughly $c \cdot n$, for a "small" integer c, of A's entries are non-zero. Crucially, most empirical networks are sparse in this sense, which makes an adjacency matrix a very inefficient representation for so small number of non-zero elements.⁹

2.1.2 The adjacency list

An **adjacency list** stores only the non-zero elements of the adjacency matrix, using an array of (unordered) lists, one list for each of the n vertices, and the ith list stores the names of the neighbors of node i. Optionally, edge annotations w_{ij} can be stored together with the neighbor name j in a tuple, e.g., (j, w_{ij}) . Hence, an adjacency list is similar to a hash table of adjacencies. For the two networks in Figure 1, their adjacency list representations are

In the simple case, because the network is undirected, each of the m=7 edges appears twice in the adjacency list, once as j in i's list, and once as i in j's list. The adjacencies for a given vertex are typically stored as a linked list, or in a more efficient data structure, like a self-balancing binary tree (e.g., a red-black or a splay tree). This form of representation is what is meant by a "sparse matrix" data structure, and is used in most mathematical programming languages.

The popular GML file format¹⁰ for storing networks is an adjacency list representation, written out in text. By only storing the non-zero entries of the adjacency matrix, an adjacency list takes space proportional to the number of nodes and edges O(n+m): O(n) space for the array of n nodes and O(m) space to store the m edges. In this representation, checking whether an edge exists,

⁹Mathematical definitions of "sparse" and "dense" networks are asymptotic, e.g., a dense network has $\Omega(n^2)$ connections, which requires assuming a model by which to "grow" the matrix in the limit of large n. However, real-world networks are always finite objects, and we usually do not know the underlying data generating process. Hence, "sparse" and "dense" for empirical networks are only loose descriptive terms, and refer mainly to whether the average degree is closer to 1 or n.

 $^{^{10}\}mathrm{See}\ \mathrm{https://en.wikipedia.org/wiki/Graph_Modelling_Language.}$

 $(i, j) \in E$, is slower than in an adjacency matrix, taking $O(m/n) = O(\langle k \rangle)$ time, where $\langle k \rangle$ is the average number of edges in an adjacency's list.

2.1.3 The edge list

An edge list stores only the edges themselves: (i, j) for unweighted and (i, j, w_{ij}) for weighted edges, without directly listing the nodes. Node indices, the presence of nodes with no edges attached, and whether the network is directed, weighted, bipartite, etc. must all be inferred from the edge list's contents. For the two networks in Figure 1, their edge lists are

$$A_{\text{simple}} = \{(1,2), (1,5), (2,3), (2,4), (3,5), (3,6)\}$$

$$A_{\text{exotic}} = \{(1,5,1), (1,5,1), (1,5,2), (2,1,1), (2,3,2), (2,2,1/2), (2,3,1), (2,4,1), (3,2,1), (3,2,2), (3,4,2), (3,5,3), (3,5,3), (4,2,1), (4,3,2), (5,1,1), (5,1,2), (5,1,1), (5,3,3), (6,3,3), (6,6,2)\}.$$

In a simple network, an edge may appear only as (i, j), implying both that it is unweighted and that its reciprocal edge (j, i) also exists. In a non-simple network, edges can be directed, and hence seeing (i, j) should not imply that (j, i) also exists. This presents an ambiguity that cannot be resolved without external knowledge about whether the edge list represents a directed or undirected network. Furthermore, because only edges are listed, nodes without edges ("singletons") are not listed, which can cause additional ambiguities.

Edge lists may be a convenient and compact way to store a network, but the ambiguity of how to interpret their contents in the absence of additional information make them problematic. In contrast, formats like GML take nearly as little space, but avoid ambiguities.

3 Describing the structure of networks

Regardless of which representation we use, networks are sufficiently complicated objects that we almost always need to use statistical methods in order to gain an intuitive sense of their shape and variations, or to describe their patterns, or test whether these patterns are meaningful. In this section, we will survey some of the most basic of these descriptive statistics. These statistics fall largely into three categories:

- 1. **connectivity** measures are directly or indirectly related to the number of connections a node has, and to the overall degree structure of the network,
- 2. **motif** measures count the frequency of specific subgraphs in a network,
- 3. **positional** measures are related to where in the network a node sits, and to the distances between nodes in the network.

Many of these network measures come in two flavors:

- node-level or "local" measures, which we calculate for an individual node i, and
- network-level or "global" measures, which we calculate across the entire network.

Sometimes, we can obtain the corresponding network-level statistic of a particular quantity by simply computing the average node-level quantity, but not always.

Because network representations can vary, so too do the algorithms for calculating specific network statistics. As a result, before beginning any network analysis, we need to first identify the graph properties of representation being used: Is the network simple? Are edges directed? Are edges weighted? Do nodes have metadata? Does the graph have one or several components? Etc.

3.1 Node degree

The most basic of all network statistics is the **degree** of a node, which counts the number of connections it has in the network. The degree structure of a network is the *first-order* description of a network, and is often sufficient to drive many other statistical patterns in the network's structure. Later, we'll learn how to assess the extent to which degrees alone can explain other structural patterns in networks.

3.1.1 Simple networks

When edges are undirected, an edge (i, j) contributes to the degree of both i and j. By convention, k_i denotes the degree of vertex i. For a simple adjacency matrix A, the degree of node i is

$$k_i = \sum_{i=1}^n A_{ij} = \sum_{i=1}^n A_{ji} . (1)$$

That is, the degree k_i is just the sum of the *i*th column, or *i*th row, of the adjacency matrix A. The row- and column-sum equivalence holds only because edges are undirected. If A represents a weighted network, this sum is called the node **strength**; the term "degree" is reserved for unweighted counts.¹¹

Every edge in an undirected network contributes twice to some degree (once for each endpoint or "stub"), and so the sum of all degrees in a network must be equal to twice the total number of edges in a network m:

$$m = \frac{1}{2} \sum_{i=1}^{n} k_i = \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} = \sum_{i=1}^{n} \sum_{j>i}^{n} A_{ij} .$$
 (2)

¹¹If A is a non-binary adjacency matrix, then a simple row sum will yield the strength s_i of node i; if the summation is modified as a count of non-zero entries, we will get back the correct value of k_i .

Using Eq. (2), we can derive a simple expression for the network's mean degree $\langle k \rangle$:

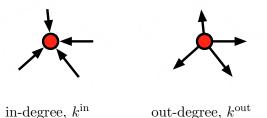
$$\langle k \rangle = \frac{1}{n} \sum_{i=1}^{n} k_i = \frac{2m}{n} . \tag{3}$$

And finally, if we divide the number of edges m by maximum number of possible edges in a simple network, or divide the mean degree by its largest possible value, we obtain a quantity that is sometimes called the network's **connectance** 12 or **density**:

$$\rho = \frac{m}{\binom{n}{2}} = \frac{2m}{n(n-1)} = \frac{\langle k \rangle}{n-1} . \tag{4}$$

3.1.2 Directed networks

In a directed network, a node i has three types of degrees: its **in-degree** k_i^{in} , meaning the number of connections to i; its **out-degree** k_i^{out} , the number of connections from i; and its **total degree** k_i^{tot} , the number of neighbors, ignoring edge directionality. The latter is equivalent to treating directed edges as undirected, and the "collapsing" multi-edges so that only one connection (i, j) exists.



On a binary adjacency matrix A representing a directed network, the in-, out-, and total degrees are defined as

$$k_i^{\text{out}} = \sum_{j=1}^n A_{ij} \tag{5}$$

$$k_i^{\text{in}} = \sum_{j=1}^n A_{ji} \tag{6}$$

$$k_i^{\text{tot}} = \sum_{j=1}^n A_{ji} \vee A_{ij} \quad , \tag{7}$$

¹²Sometimes, connectance is defined as $\langle k \rangle / n$, which is asymptotically equivalent to $\langle k \rangle / (n-1)$.

where \vee is an *or* function. In a directed network, the number of edges m is the sum of the entire adjacency matrix, since each directed edge appears exactly once in A. The fact that each edge contributes exactly once to some in-degree and once to some out-degree also implies that the average in-degree equals the average out-degree:

$$\langle k^{\text{out}} \rangle = \frac{1}{n} \sum_{i=1}^{n} k_i^{\text{out}} = \frac{1}{n} \sum_{i=1}^{n} \left(\sum_{j=1}^{n} A_{ij} \right) = \frac{m}{n} = \sum_{i=1}^{n} \left(\sum_{j=1}^{n} A_{ji} \right) = \frac{1}{n} \sum_{i=1}^{n} k_i^{\text{in}} = \langle k^{\text{out}} \rangle .$$
 (8)

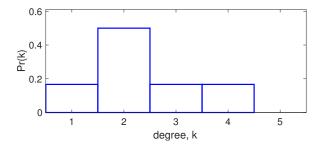
3.2 Degree distributions

If we calculate the degrees of all the vertices in a network, and then write them out, we get something called a **degree sequence**, which enumerates the network's degree structure. For the simple graph in Figure 1, its degree sequence is

$$(1,2,2,2,3,4)$$
.

But a simple sequence doesn't provide much information about the *variability* of node degree across the network. To capture this behavior, we use something called the **degree distribution**, denoted Pr(k), which is simply the probability that a vertex selected uniformly at random will have k neighbors. A degree distribution is a normalized histogram of the degree values. For the simple graph in Figure 1, its degree distribution is

where Pr(k) = 0 for all other values of k. The standard way to present a degree distribution Pr(k) is via a bar plot, like so:



3.2.1 Exploring the degree distribution

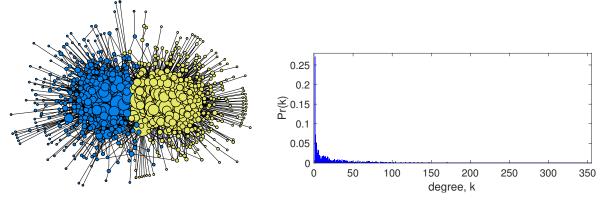
Most real-world networks, biological or otherwise, exhibit a "heavy-tailed" degree distribution, meaning that the variance¹³ of the degree distribution σ^2 is large relative to its mean $\langle k \rangle$. Because

¹³Recall that the sample variance of the degrees would be defined as $\sigma^2 = \frac{1}{n-1} \sum_{i=1}^n (k_i - \langle k \rangle)^2$.

degrees must be non-negative (they are "count" variables), this behavior implies that the degree distribution Pr(k) is "right-skewed," meaning that the largest degree vertices are often several orders of magnitude better connected than the typical node.

This kind of high variance, however, can be difficult to see in a simple distribution plot, and instead, it is conventional to (i) use a log-log plot, which visually compresses the variance in both k and Pr(k), and (ii) plot the complementary cumulative distribution function or CCDF, defined as $Pr(K \ge k)$. In this expression, K is now a random variable, and the CCDF plots the fraction of nodes with degree at least some value k. If the minimum degree of a network is k = 1, then $Pr(K \ge 1) = 1$, because all nodes have degree at least the minimum.¹⁴

To illustrate how the log-plots change the kind of information we can see in a degree distribution, and how plotting the CCDF improves the visual interpretability, we'll use a concrete example. Below is a network of n=1490 weblogs from around the 2004 U.S. Presidential election, along with a standard plot of the degree distribution, which spans m=19090 edges and has a mean degree $\langle k \rangle = 25.6.^{15}$ The details of how these data were collected, or what they mean is not that important, except to note that this is a web graph, and is thus a directed network. Notice that the degree distribution emphasizes the low-degree portion of the distribution, for $k \leq 10$ or so. In fact, the largest degree is $k_{\rm max} = 351$, a value more than 13 times larger than the mean, but you can't tell that from the plot.

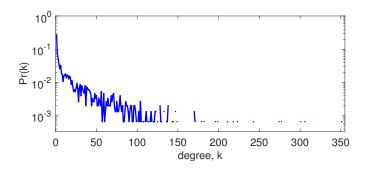


What follows is a sequence of plots, showing the same degree data, as (i) $\log_{10} \Pr(k)$ vs. k (a semilog-y plot), then (ii) $\log_{10} \Pr(k)$ vs. $\log_{10} k$ (a loglog plot), and finally (iii) $\log_{10} \Pr(K \ge k)$ vs.

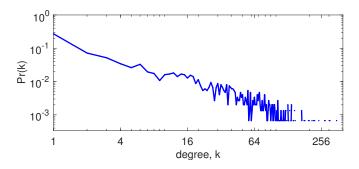
¹⁴Applying a cumsum function to the PDF of a degree distribution almost yields the CDF, which is defined as Pr(K < k). Do you see why? Think about what happens to the first element under cumsum and whether that is correct for $Pr(K < \min(k_i))$. After correcting for this behavior, one can obtain the CCDF by noting that Pr(K > k) = 1 - Pr(K < k).

¹⁵The visualization comes from Karrer & Newman, *Phys. Rev. E* **83**, 016107 (2011), and the network comes from Adamic & Glance, *Proc. WWW-2005 Workshop on the Weblogging Ecosystem* (2005).

 $\log_{10} k$ (a loglog plot of the CCDF).

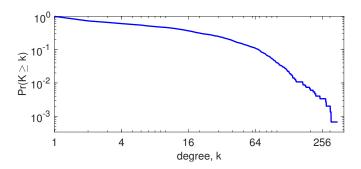


In the semilog-y plot above, we can now see more of the low frequency / high degree events, which we call the "upper tail" of the distribution. The dots represent nodes with unique degree values; hence, $\Pr(k) = 1/n$ for every unique value of k, which is the lowest value possible in $\Pr(k)$. This minimum value is what causes the "flat-bottom" structure of the degree distribution, which starts just over k = 50.



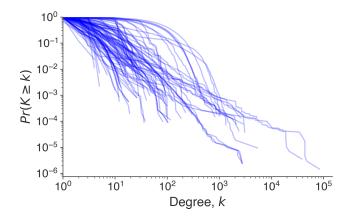
The loglog plot above stretches out the low-degree structure while compressing the range of the high-degree portion of the distribution, allowing us to see both parts together. But, the 1/n artifact is still apparent, and the jagged structure at k > 60 or so is too noisy to see any clear pattern. The solution is the CCDF, which is a monotonically decreasing function that smooths out many of the jaggies in the upper tail.

In the above plot, we can now see clearly that the distribution tends to bend down around k = 64, falling off more quickly than it did below that point. Moreover, we can read off, directly from the plot, the fact that 90% of nodes have degree $k \le 67$ (at what values of x does a horizontal line at $y = 10^{-1}$ intersect the CCDF?), and only 1% of nodes have degree k > 169 (at what value of x does a horizontal line at $y = 10^{-2}$ intersect the CCDF?). Reflecting this extremely uneven distribution



of edges, the bottom 90% of nodes, by degree, touch only 53% of all edges, while those top 1% touch 10% of all edges. This dramatic inequality is ubiquitous in real network degree distributions, and highlights the important role that these "high degree" nodes play in structuring the network. The clarity provided by the CCDF on a loglog plot makes it the most useful way to visualize degree distributions.

How much variability do degree distributions exhibit in reality? The figure below shows the results of applying the above CCDF analysis to 100 networks drawn from biological, social, information, and technological networks. The answer is: they vary enormously in their shape, but are generally high variance, even "heavy tailed." In other words, real-world networks structurally diverse, even in something as simple as their degree structure, and the only commonality across degree distributions is their often enormously high variance.



3.3 Small motifs

A **motif** is a small, connected subgraph $G_{\circ} = (V_{\circ} \subset V, E_{\circ} \subset E)$ with a particular pattern of edges among a small set of nodes, and usually, we want to count how often a motif G_{\circ} occurs within a larger network G. The computational cost of counting motifs scales up quickly with the size of V_{\circ} , and thus most motif-based measures focus on the frequencies of small motifs, e.g., 2, 3, or 4 nodes. ¹⁶

3.3.1 Reciprocity (directed networks)

The smallest non-trivial motif in a directed network is a reciprocated edge, i.e., a 2-cycle or a cycle of length exactly two, and we use a measure called **reciprocity** r to quantify their prevalence. Reciprocity comes in both node-level (local) and network-level (global) versions.



The prevalence of this motif is often interpreted functionally. In some ecological networks, reciprocity can indicate the degree of mutualism present in an ecosystem, while in gene regulatory networks, reciprocated links indicate the presence of self-regulating interactions.

The reciprocity of a network r is given by the fraction of links that are reciprocated, meaning it has a maximum value of r = 1. To compute r, we simply count the number of 2-cycles and divide by the number of edges. When edges have unit weight, a network's reciprocity is defined as

$$r = \frac{1}{m} \sum_{ij} A_{ij} A_{ji} . (9)$$

Note that in a directed network, m counts the number of directed edges, and hence we normalize by $m = \sum_{ij} A_{ij}$ to place r on the unit interval [0,1].

We can also quantify the reciprocity that an individual vertex experiences, which is a node-level measure called *local reciprocity*. Instead of summing over the entire network, in this case, we count

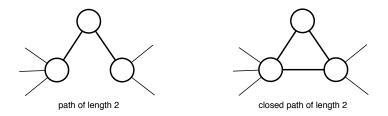
¹⁶Computational complexity and *subgraph isomorphisms* are key problems for motif-counting algorithms. Suppose we are searching for a motif on n_{\circ} nodes. If we blindly check all $f(n_{\circ}) = n^{n_{\circ}}$ groups of nodes, each found motif will occur $|n_{\circ}|!$ times in this search, due to isomorphisms. That is, there are $|n_{\circ}|!$ ways to permute the node labels of any unique motif. Asymptotically, how expensive is such a search for $n_{\circ} = \{2, 3, 4, 5, 6\}$?

the number of 2-cycles attached to vertex i, and divide by its out-degree:

$$r_i = \frac{1}{k_i^{\text{out}}} \sum_j A_{ij} A_{ji} . \tag{10}$$

3.3.2 Clustering coefficient (undirected networks)

In an undirected network, the smallest interesting motif is a triangle, and the **clustering coefficient** C is a network-level measure that captures the relative frequency or the density of triangles in a network. Concretely, C quantifies the fraction of "connected triples," that is, a pair of edges (i, j), (j, k) that are "closed" by an edge (k, i) to form a triangle.



Like reciprocity, C is defined mathematically as a count of the desired motif (a triangle), normalized by a count of the number of possible motifs:

$$C = \frac{\text{(number of triangles)} \times 3}{\text{(number of connected triples)}}$$
(11)

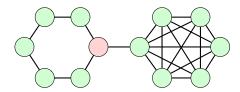
$$= \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{k=1}^{n} A_{ij} A_{jk} A_{ki} / \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{k\neq i}^{n} A_{ij} A_{jk} , \qquad (12)$$

where the factor of 3 in Eq. (11) comes from the symmetry of the triangle (every triangle contains three connected triples), and the $k \neq i$ restriction in the denominator of in Eq. (12) prevents counting (i,j),(j,i) as a triple.¹⁷ Because the numerator can never exceed the denominator, and they are both count variables, $C \in [0,1]$, and we say that it measures the density of triangles in the network.¹⁸ Calculating Eq. (11) directly would take $O(n^3)$ time. How long would it take to calculate C using an adjacency list representation?

A worked example. Consider a simple network composed of cycle and a clique:

¹⁷In linear algebra terms, Eq. (12) is equivalent to $C = \operatorname{trace}(A^3) / \sum_{i \neq j} A^2$. This is because the diagonal of the matrix A^q counts the number of cycles of length q that "originate" at each node.

¹⁸When the network is fully connected, in which every edge exists, C = 1 (do you see why?). Similarly, in any network without triangles, e.g., a tree, a bipartite network, etc., C = 0 (do you see why?).



The clique has 6 vertices, making $\binom{6}{3} = 20$ triangles, and thus also $20 \times 3 = 60$ connected triples. The cycle contains 6 connected triples and no triangles. Finally, there are 2 connected triples starting from the cycle and 5 connected triples starting from the clique that use the edge joining the cycle to the clique. Adding this all up yields a clustering coefficient of C = 60/73 = 0.82.

Local clustering coefficient. The clustering coefficient can also be defined as a node-level measure, which captures the fraction of neighbors j, k of node i that are themselves connected by an edge (j, k):

$$C_i = \frac{\text{(number of pairs of neighbors of } i \text{ that are connected)}}{\text{(number of pairs of neighbors of } i)}$$
(13)

$$= \sum_{i < k} A_{ij} A_{jk} A_{ki} / {k_i \choose 2} . \tag{14}$$

In the cycle-plus-clique example above, the highlighted vertex has a local clustering coefficient of $C_i = 0$ because it participates in no triangles. Its immediate neighbor in the clique is a more interesting case, with $C_i = 10/15 = 0.67$.

3.3.3 Feed-forward and feedback loops (directed networks)

In directed networks, and particularly in biological networks, two slightly larger motifs of special interest are the feed-forward loop and the feedback loop. These motifs are interesting because they represent basic biological circuitry for governing the flow of activation across molecular networks.¹⁹



A feed-forward loop is defined as one that has a two-step path (i, j), (j, k) that is shortcut by an edge (i, k) that "feeds forward" the signal passing along the longer path. In this case, we would

¹⁹For instance, see https://en.wikipedia.org/wiki/Feed_forward_(control).

say that node j is the "feed forward" node. Similarly, a feedback loop is defined the same, except that the third edge is (k, i), which "feeds back" the signal that passed along the longer path.

If a network is directed, then we can count the number of FFL and FBL straightforwardly under an adjacency matrix representation:

$$FFL = \sum_{i=1} \sum_{j} \sum_{k \neq i} A_{ij} A_{jk} A_{ik}$$
 (15)

$$FBL = \sum_{i < j < k} A_{ij} A_{jk} A_{ki} , \qquad (16)$$

These adjacency matrix calculations take $O(n^3)$ time because each has three nested loops over n nodes, and hence don't scale well to large networks.

A more efficient approach, taking $O(n + m\langle k \rangle^2)$ time, would use a simple "path enumeration" algorithm on an adjacency list to find all paths (i,j),(j,k) (where $i \neq k$) and, for each, check whether the edge (i,k) exists, indicating a FFL motif, or (k,i) exists, indicating a FBL motif.

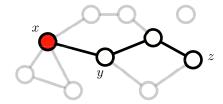
3.3.4 Larger motifs

A motif can be defined on any size subgraph $n_{\circ} < n$, and sometimes "large" motifs, when $n_{\circ} > 3$, are interesting. However, as n_{\circ} increases, it becomes increasingly expensive to both enumerate and count such motifs. For instance, while there are 6 distinct motifs on $n_{\circ} = 4$ nodes, $n_{\circ} = 5$ nodes have 21, $n_{\circ} = 6$ nodes have 112, and $n_{\circ} = 7$ nodes have 853. Even if we successfully count the frequencies of a large motif, its interpretation also requires special care, because there can be many different ways to "normalize" that count relative to an expectation, as we did in Eq. (9) for reciprocated links and Eq. (11) for triangles. We will revisit the idea of assessing the frequency of larger motifs when we discuss random graph models.

3.4 Geodesic paths and network position

Recall that a path in a network is a sequence of distinct vertices $x \to y \to \cdots \to z$ such that for each consecutive pair of vertices $i \to j$, there exists an edge $(i,j) \in E$ in the network, and the length of the path is the number of edges it crosses. A geodesic or shortest path is the shortest of all possible paths between two vertices. These paths serve as the basis for a number of positional measures of network structure.²⁰

²⁰Geodesic paths are fun! The classic Six Degrees of Kevin Bacon game asks plays to enumerate a path on the bipartite network of actors and the movies they appear in from a selected actor to Kevin Bacon. The popular website https://oracleofbacon.org returns answers derived from applying a shortest-path algorithm. If one prefers academics, the website https://www.csauthors.net/distance/ does the same, but for pairs of computer scientists, including yours truly.



To calculate nearly any positional measure, we must first calculate the geodesic distances ℓ_{ij} between all pairs of nodes i, j. Usually, we accomplish this by applying an off-the-shelf algorithm for the All Pairs Shortest Paths (APSP) problem.²¹ The output will be a pairwise distance matrix ℓ , where the entry ℓ_{ij} gives the length of the geodesic path between i and j. Crucially, if no such path exists (because i and j are in different components of the network, e.g., the singleton node vs. any other node in the example above), then $\ell_{ij} = \infty$, and we say that j is not reachable from i.

If G is a weighted network, the pairwise distance matrix ℓ will contain the weight of the lightest path from i to j. In this case, the lightest-weight path may, in fact, have more edges in it than the shortest length path (ignoring edge weights). In an unweighted network, edges have unit weight, and hence ℓ_{ij} is the number of edges in the path.

The path structure of a network also determines whether it is composed of one or multiple *components*, each of which is a set of nodes T such that for any pair of members $i, j \in T$, there exists a path $i \to \cdots \to j$ or vice versa. If all nodes are pairwise reachable from each other, then a network has a single component. Else, the network has multiple components, and there is always a *largest connected component* (LCC), i.e., the component with the largest number of nodes in it.²² In an undirected network, the matrix ℓ is always symmetric, because the shortest path from i to j can be no longer than the shortest path from j to i.

3.4.1 Diameter

The first positional measure is the network's **diameter**, which is the length of the longest of all geodesic paths and is meant to evoke the notion of a volume in a metric space. The diameter of a network is a global measure, and is defined as

$$diameter = \max_{ij} \ell_{ij} . (17)$$

If the network is not connected, i.e., if there is more than one component, then the diameter will trivially be infinite. In these cases, it is customary to drop all $\ell_{ij} = \infty$ elements from the calculation,

²¹Most commonly, the Floyd-Warshall algorithm. Alternatively, applying Dijkstra's algorithm, for solving the single-source shortest path problem, once for each node will build the pairwise distance matrix ℓ one row at a time. If the network is weighted, there are some technical restrictions on the weight values.

²²The number and size of components can be computed straightforwardly, by analyzing the output of an APSP algorithm, or simply a breadth-first or depth-first search algorithm. Do you see how?

and say the diameter is the longest geodesic among all paths that exist.

3.4.2 Eccentricity

While the diameter is a global measure, the **eccentricity** is an equivalent local measure—it measures the length of the longest path originating at some node i, and is defined as

$$\epsilon_i = \max_j \ell_{ij} \ , \tag{18}$$

where again, it is customary to drop all $\ell_{ij} = \infty$ elements from the calculation.

3.4.3 Mean geodesic path length

The **mean geodesic path length** is network-level (global) measure of the average distance between a pair of uniformly random nodes, and is defined as

$$\langle \ell \rangle = \frac{1}{Z} \sum_{ij} \ell_{ij} \quad , \tag{19}$$

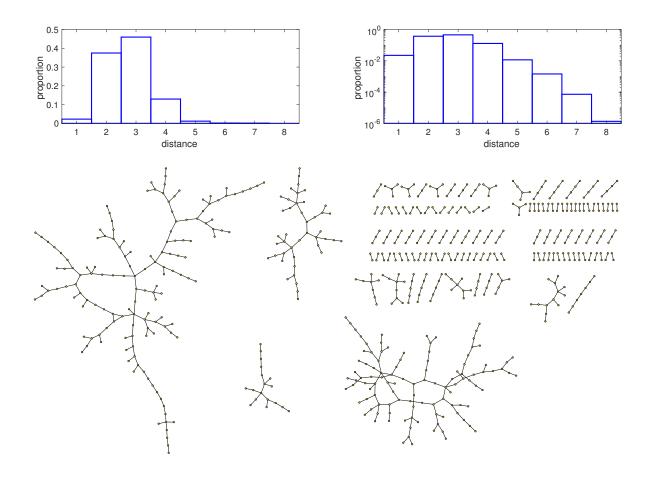
where here it is customary to drop both all $\ell_{ij} = \infty$ elements and $\ell_{ij} = 0$ elements (the diagonal of ℓ) from the calculation, and Z counts the number of the remaining distances.

An example. Consider again the directed network of political blogs from Section 3.2.1, which has n = 1490 nodes. Applying an APSP algorithm to the network yields a 1490×1490 pairwise distance matrix ℓ . This network is not connected: it has 268 components, the largest of which contains 1222 nodes (82%), and the smallest of which contains 1 node.

Taking the set of non-zero and non-infinite geodesic distances, the following two plots show the normalized histograms of those distance, once as a simple bar plot and the other as a semilog-y bar plot. The mean geodesic distance is $\langle \ell \rangle = 2.74$, which we can see reflected in the simple bar plot, where the vast majority of distances are 2 or 3. The diameter, however, is not particularly visible in this version. The longest geodesic distance is $\ell_{\rm max} = 8$, and occurs exactly once, i.e., there is exactly one pair of vertices that are separated by a path of length 8, which is one path out of 1,492,064 pairs of connected nodes. This value is a bit easier to see in the semilog-y plot, which also shows more of a smooth fall-off in the distances above the mean, to the maximum at 8.

3.5 Components

If every pair of vertices is connected by some path, then the network is *connected*. If there is some pair of vertices between which no path exists, the network is said to be *disconnected*, i.e., it is composed of more than one *component*.



In an undirected graph, the set of vertices reachable from one vertex is called a *component* (and, for every vertex j reachable from i, i is also reachable from j). The figure below shows an example of a set of components in an undirected graph.

In a directed graph, reachability in one direction does not imply reachability in the other, and the notion of "connected" becomes more nuanced. A group of nodes that is pairwise reachable only if we ignore the direction of the edges is a weakly connected component, while a group of notes that is pairwise reachable if we obey the directions is a strongly connected component. Similarly, an out component is the set of vertices that can be reached from i, while an in component is the set of vertices that can reach i.

Many empirical networks are composed of multiple components, and among them, there is always a *largest connected component* (the LCC), which is usually the component of greatest interest. You

can spot the LCC in the figure below quite easily. In mathematical models, the *giant component* is also the largest component, but we add an additional property, which is to say that the size of the giant component must be O(n).²³ We will revisit the notion of a giant component later in the semester, when we study models of random graphs.

Counting components.

To count and measure the size of the components within a network, we use any standard SSSP or APSP algorithm. For undirected networks, a breadth-first or depth-first search forest suffices, while for weighed or directed networks, Dijkstra's algorithm works well.

While the algorithm runs, we need only label all vertices that are pairwise reachable with the same vertex label, in an auxiliary array. When the algorithm terminates, we may make a single pass through the array to count the number of unique labels (the number of components) and count the number of times each label occurs (the sizes of each component). In a weighted graph, identifying strongly connected components is most easily done via a depth-first search forest, in O(n + m) time.

3.5.1 Harmonic centrality

[[Add section on harmonic centrality, with figure]]

3.5.2 Eigenvector centrality

[Add section on eigenvector centrality, with figure]

3.6 Other measures of network structure

These measures of network structure cover just the basics. Many other measures exist in the networks literature, and their creation often follows the needs of specific applications. You can think of each such measure as a function f that takes as input a graph G and outputs either a single scalar value or a vector of values. That is, each f(G) projects the space of all possible graphs onto a low-dimensional space. As a result of this projection, information is surely lost and thus each measure f(G) is an incomplete description of the original graph G. A good function f projects graphs in a way that highlights the structural feature of interest by creating good separation among points in the low-dimensional space.

²³The term "giant component" is meaningless in most empirical situations since it is only defined asymptotically. For empirical networks with multiple components, we instead focus on the largest component and reserve the term "giant component" for mathematical models.

By thinking about network measures as functions, it becomes reasonable to want a set of such functions $\{f\}$ that behave like an orthonormal basis set for the space of all graphs, or perhaps all graphs from a particular domain, say, all social networks. That is, are there a set of sufficient statistics to describe all possible structural patterns in a network? Unfortunately, at least at this point in the development of network science, the answer appears to be no, there is no such set.

Instead, what we do know is that many of the canonical network measures (many of which are described above, and summarized in Table 1) are highly correlated with each other. For instance, having a high degree tends to be inversely correlated with having a high local clustering coefficient, but having many high-degree vertices in a network tends to correlate with having a small diameter. Etc. This happens for a simple reason. Networks are not linearly decomposable. Instead, they are complicated, high-dimensional objects, and adding or removing even a single edge can, in some cases, have a dramatic impact on some network measures, but not others. For instance, the average degree is very robust to the addition of a few edges, but the diameter can be exquisitely sensitive (recall the Watts and Strogatz results of Section 3.4).

network measure	scope	graph	definition	explanation
degree	L	U	$k_i = \sum_{j=1}^n A_{ij}$	number of edges attached to vertex i
in-degree	L	D	$k_i^{\text{in}} = \sum_{i=1}^n A_{ji}$	number of arcs ending at vertex i
out-degree	L	D	$k_i^{\text{out}} = \sum_{j=1}^{n} A_{ij}$ $m = \frac{1}{2} \sum_{i,j} A_{ij}$	number of arcs starting from vertex i
edge count	G	U	$m = \frac{1}{2} \sum_{ij} A_{ij}$	number of edges in the network
arc count	G	D	$m = \sum_{ij} \mathring{A}_{ij}$	number of arcs in the network
mean degree	G	U	$\langle k \rangle = 2m / n = \frac{1}{n} \sum_{i=1}^{n} k_i$	average number of edges per vertex
mean in- or out-degree	G	D	$\langle k^{\rm in} \rangle = \langle k^{\rm out} \rangle = 2m/n$	average number of in- or out-edges per
				vertex
reciprocity	G		$r = \frac{1}{m} \sum_{ij} A_{ij} A_{ji}$	fraction of arcs that are reciprocated
reciprocity	L	D	$r_i = \frac{1}{k_i} \sum_{j} A_{ij} A_{ji}$	fraction of arcs from i that are recipro-
				cated
clustering coefficient	G	U	$c = \frac{\sum_{ijk} A_{ij} A_{jk} A_{ki}}{\sum_{ijk} A_{ij} A_{jk}}$	the network's triangle density
clustering coefficient	L	U	$c_i = \sum_{i \leq k} A_{ij} A_{jk} A_{ki} / {k_i \choose 2}$	fraction of pairs of neighbors of i that
				are also connected
diameter	G	U	$d = \max_{ij} \ell_{ij}$	length of longest geodesic path in an
				undirected network
mean geodesic distance	G	UD	$\ell = \frac{1}{Z} \sum_{ij} \ell_{ij}$	average length of a geodesic path
eccentricity	G	UD	$\epsilon_i = \max_j^* \ell_{ij}$	length of longest geodesic path starting
				from i

Table 1: A few standard measures of network structure. The "scope" of a measure indicates whether it describes a vertex-level (local, L) or network-level (global, G) pattern, and the "graph" column indicates whether it is calculated on an undirected (U) or directed (D) graph. In each definition, adjacency matrix notation is used and it is assumed that $A_{ij} = 1$ if the edge (i, j) exists in the network and $A_{ij} = 0$ otherwise. For the geodesic paths, we assume that the graph is connected.

4 At home

- 1. Peruse Chapters 1–5 in Networks (background material)
- 2. Read Chapter 6.1–6.12 in Networks