1 Representations and statistics of 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.

1.1 Representing networks

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

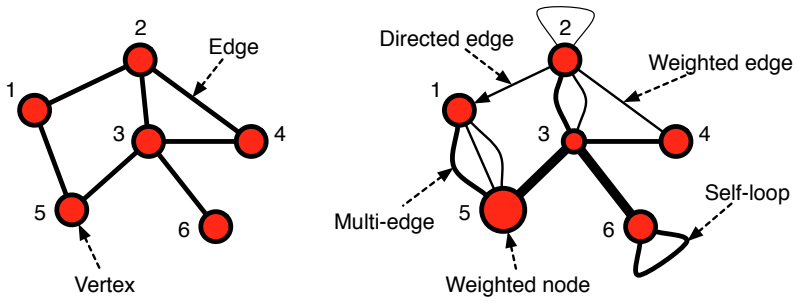


Figure 1: A simple network (left) and a network with more exotic graph properties (right).

1.1.1 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.[1] If A represents an *unweighted network*, then edges have "unit" weight, defined as $w_{ij} = 1$.

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

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

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.[2]

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 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.[3]

[2]For 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.

[3]Mathematical 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.

1.1.2 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

$A_{\text{simple}} =$

[1]	→	(2, 5)
[2]	→	(3, 1, 4)
[3]	→	(2, 5, 4, 6)
[4]	→	(2, 3)
[5]	→	(1, 3)
[6]	→	(3)

$A_{\text{exotic}} =$

[1]	→	((5,1),(5,1),(5,2))
[2]	→	((1,1),(2,$\frac{1}{2}$),(3,2),(3,1),(4,1))
[3]	→	((2,1),(2,2),(4,2),(5,3),(5,3))
[4]	→	((2,1),(3,2))
[5]	→	((1,1),(1,2),(1,1),(3,3))
[6]	→	((3,3),(6,2))

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 format[4] 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, $(i, j) \in E$, 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.

1.1.3 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

$$
\begin{aligned}
A_{\text{simple}} &= \{(1,2),(1,5),(2,3),(2,4),(3,5),(3,6)\} \\
A_{\text{exotic}} &= \{(1,5,1),(1,5,1),(1,5,2),(2,1,1),(2,3,2),(2,2,1/2),(2,3,1), \\
&\qquad (2,4,1),(3,2,1),(3,2,2),(3,4,2),(3,5,3),(3,5,3),(4,2,1), \\
&\qquad (4,3,2),(5,1,1),(5,1,2),(5,1,1),(5,3,3),(6,3,3),(6,6,2)\} \ .
\end{aligned}
$$

[4] See `https://en.wikipedia.org/wiki/Graph_Modelling_Language`.

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.

2 Summarizing networks using statistics

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.

2.1 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.

2.1.1 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

$$k_i = \sum_{j=1}^{n} A_{ij} = \sum_{j=1}^{n} A_{ji} \ . \tag{1}$$

That is, the degree k_i is just the sum of the ith column, or ith 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.[5]

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:

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

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** [6] or **density**:

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

[5] If 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.

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

2.1.2 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.

in-degree, k^{in} out-degree, k^{out}

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

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

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

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

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:

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

2.2 Degree distributions

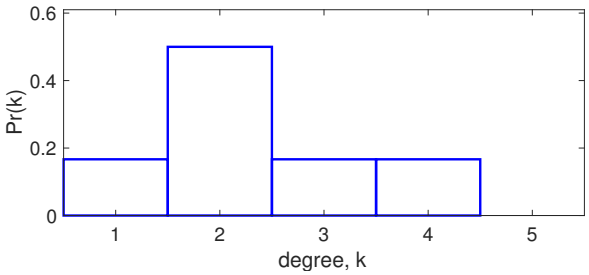
If we calculate the degrees of all the vertices in a network, and then write them out, we get something called a **degree sequence**, which enumerates the network's degree structure. For the simple graph in Figure 1, its degree sequence is

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

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

k	1	2	3	4
$\Pr(k)$	1/6	3/6	1/6	1/6

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:



2.2.1 Exploring the degree distribution

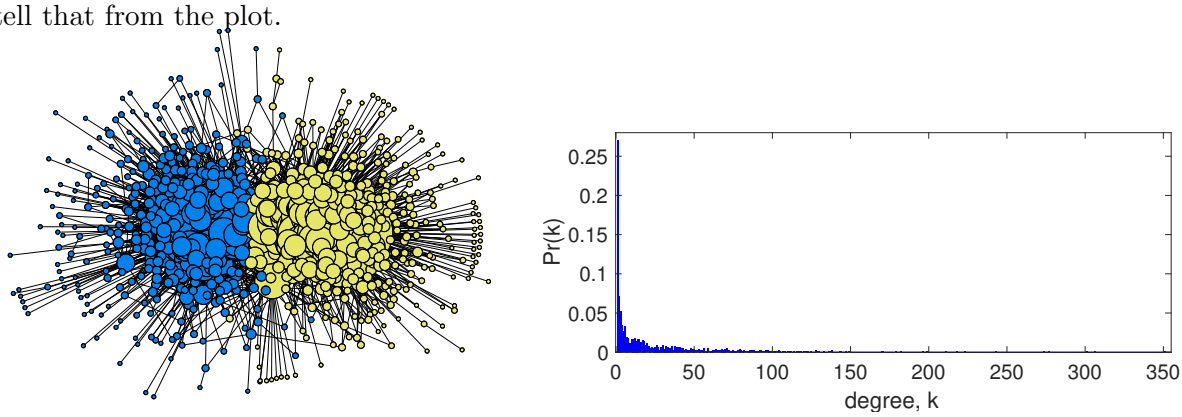
Most real-world networks, biological or otherwise, exhibit a "heavy-tailed" degree distribution, meaning that the variance[7] of the degree distribution σ^2 is large relative to its mean $\langle k \rangle$. Because degrees must be non-negative (they are "count" variables), this behavior implies that 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 $\Pr(K \geq k)$. 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 $\Pr(K \geq 1) = 1$, because all nodes have degree at least the minimum.[8]

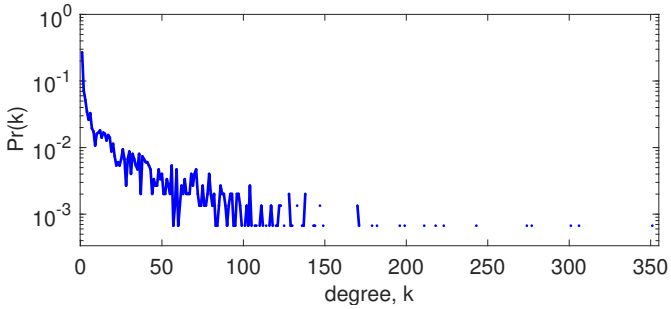
[7] Recall that the sample variance of the degrees would be defined as $\sigma^2 = \frac{1}{n-1} \sum_{i=1}^{n} (k_i - \langle k \rangle)^2$.

[8] Applying 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 $\Pr(K \geq k) = 1 - \Pr(K < k)$.

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 $\langle k \rangle = 25.6$.[9] 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 $k_{\max} = 351$, a value more than 13 times larger than the mean, but you can't tell that from the plot.



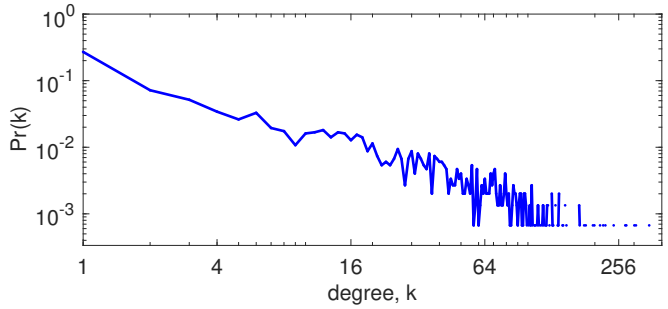
What follows is a sequence of plots, showing the same degree data, as (i) $\log_{10} \Pr(k)$ vs. k (a semilog-y plot), then (ii) $\log_{10} \Pr(k)$ vs. $\log_{10} k$ (a loglog plot), and finally (iii) $\log_{10} \Pr(K \geq k)$ vs. $\log_{10} k$ (a loglog plot of the CCDF).



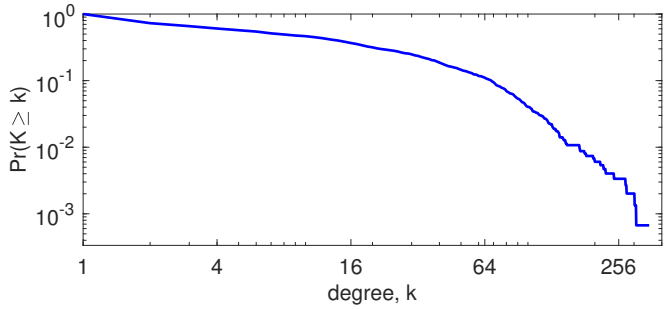
In the semilog-y plot above, we can now see more of the low frequency / high degree events, which we call the "upper tail" of the distribution. The dots represent nodes with unique degree values; hence, $\Pr(k) = 1/n$ for every unique value of k, which is the lowest value possible in $\Pr(k)$. This

[9] The 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).

minimum value is what causes the "flat-bottom" structure of the degree distribution, which starts just over $k = 50$.

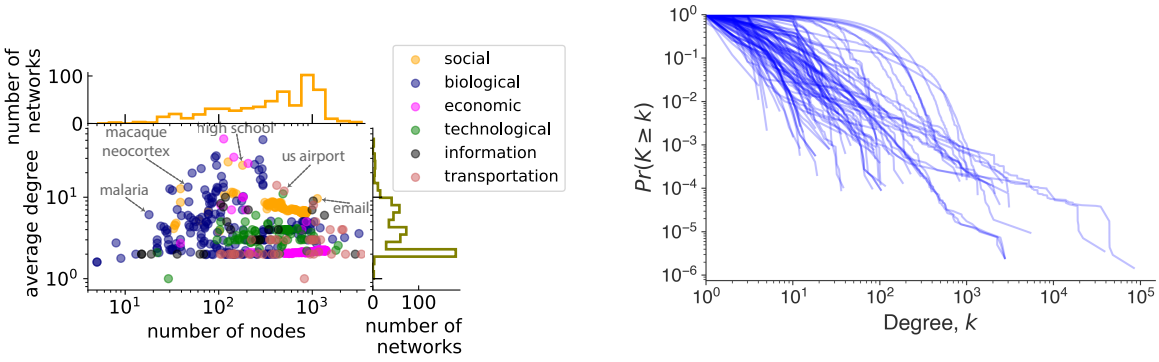


The loglog plot above stretches out the low-degree structure while compressing the range of the high-degree portion of the distribution, allowing us to see both parts together. But, the $1/n$ artifact is still apparent, and the jagged structure at $k > 60$ or so is too noisy to see any clear pattern. 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 $k \leq 67$ (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, and how much similarity do real degree distributions exhibit? Below, the left-hand panel shows the average degree $\langle k \rangle$ of about 500 real-world networks from six different domains, as a function of network size. Although there's ample variability, note the small range of $\langle k \rangle$ relative to the enormous range of n. That is, real-world networks are generally very *sparse*, with each node connecting to only a small number of others. But, the right-hand panel, which shows the CCDFs for 100 of these networks, illustrates that the variance around that pattern is enormous. Real degree distributions vary enormously in their shape, but are generally high variance, or *heavy tailed*, in which a relatively small fraction of nodes participate in a very large fraction of all of the connections in the entire network.



2.3 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.[10]

2.3.1 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.

[10]Computational 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 $n_\circ = \{2, 3, 4, 5, 6\}$?

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

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

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 $[0, 1]$.

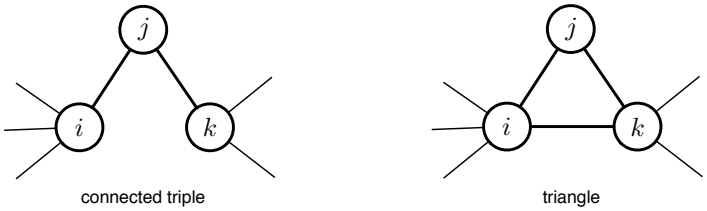
We can also quantify the reciprocity that an individual vertex experiences, which is a node-level measure called *local reciprocity*. Instead of summing over the entire network, in this case, we count the number of 2-cycles attached to vertex i, and divide by its out-degree:

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

2.3.2 Clustering coefficient (undirected networks)

In an undirected network, the smallest interesting motif is a triangle, and the **clustering coefficient** C (sometimes called "transitivity") 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



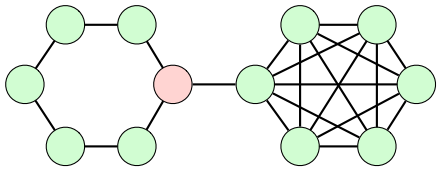
by a count of the number of possible motifs:

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

$$= \sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{n} A_{ij}A_{jk}A_{ki} \Bigg/ \sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k\neq i}^{n} A_{ij}A_{jk} \quad , \tag{12}$$

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.[11] 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.[12] [13] 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:



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 $C = 60/73 = 0.82$.

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

[12] When 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?).

[13] Although Eq. (11) suffices for most networks, it breaks whenever the number of connected triples is 0. (What kind of networks have that property?) In that case, strictly speaking, C is undefined, although for simplicity, we might just define it to be $C = 0$.

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):

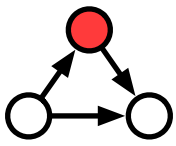
$$C_i = \frac{\text{(number of pairs of neighbors of } i \text{ that are connected)}}{\text{(number of pairs of neighbors of } i\text{)}} \tag{13}$$

$$= \sum_{j<k} A_{ij}A_{jk}A_{ki} \Big/ \binom{k_i}{2} \quad . \tag{14}$$

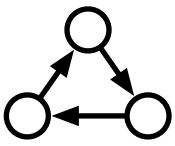
In the cycle-plus-clique example above, the highlighted vertex has a local clustering coefficient of $C_i = 0$ because it participates in no triangles. Its immediate neighbor in the clique is a more interesting case, with $C_i = 10/15 = 0.67$.

2.3.3 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.[14]



feed-forward loop (FFL)



feedback loop (FBL)

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 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:

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

$$\text{FBL} = \sum_{i<j<k} A_{ij}A_{jk}A_{ki} \quad , \tag{16}$$

[14] For instance, see `https://en.wikipedia.org/wiki/Feed_forward_(control)`.

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.

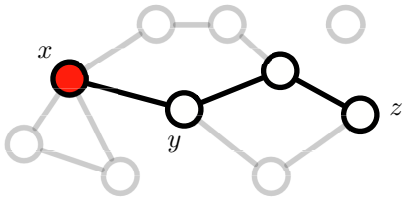
A more efficient approach, taking $O(n + m\langle k\rangle^2)$ time, would use a simple "path enumeration" algorithm on an adjacency list to find all paths $(i,j),(j,k)$ (where $i \neq k$) and, for each, check whether the edge (i,k) exists, indicating a FFL motif, or (k,i) exists, indicating a FBL motif.

2.3.4 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.

2.4 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.



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.[15] 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

[15]Most 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.

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.[16] 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.

2.4.1 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

$$\text{diameter} = \max_{ij} \ell_{ij} \ . \tag{17}$$

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

2.4.2 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.

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

2.4.3 Mean geodesic path length

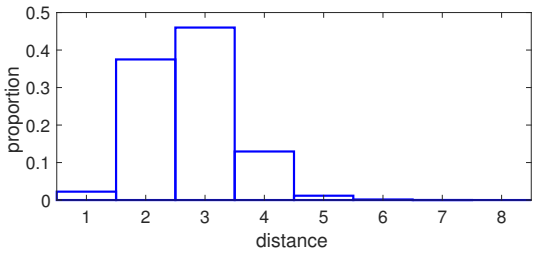
The **mean geodesic path length** is network-level (global) measure of the average distance between a pair of uniformly random nodes, and is defined as

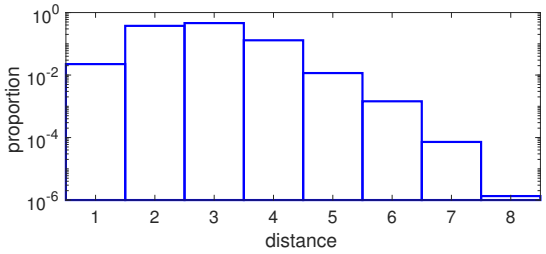
$$\langle \ell \rangle = \frac{1}{Z} \sum_{ij} \ell_{ij} \ , \tag{19}$$

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 2.2.1, 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 $\ell_{\max} = 8$, 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.





Small worlds and network diameter.
In mathematical models of networks, the diameter can often be shown analytically to grow very slowly with a network's size n, e.g., $\ell_{\max}(n) = O(\log n)$. In network data, we often cannot estimate how the diameter is changing because we don't have snapshots of a growing network, e.g., we have one human metabolic network. Nevertheless, empirical diameters still tend to be very small compared to the size of the network, e.g., $\ell_{\max} \approx 6$ or something. Hence, *all* nodes are "close" to each other, and information only has to transit through a small number of intermediaries to get from

one side of the network to the other. That is, real networks tend to be very compact![17]

A small diameter is a pretty weak constraint on the overall architecture of the network, which means that networks can be "compact" and yet still have many other interesting structural characteristics. This fact is well-illustrated by the so-called "small world" network model.[18] In this model, we arrange n nodes into a 1-dimensional circular lattice (a "ring" network) and connected with their k nearest neighbors. We then "rewire" each edge with probability p, meaning, we delete that edge (i, j) and connect a uniformly random pair of vertices $x, y \in V$. At $p = 0$, the network is fully ordered, where the density of local connections is largest and the diameter is $O(n)$—a "big world." At $p = 1$, the network is fully disordered, local connections are absent and the diameter is $O(\log n)$—a "small world." See Figure 2 below.

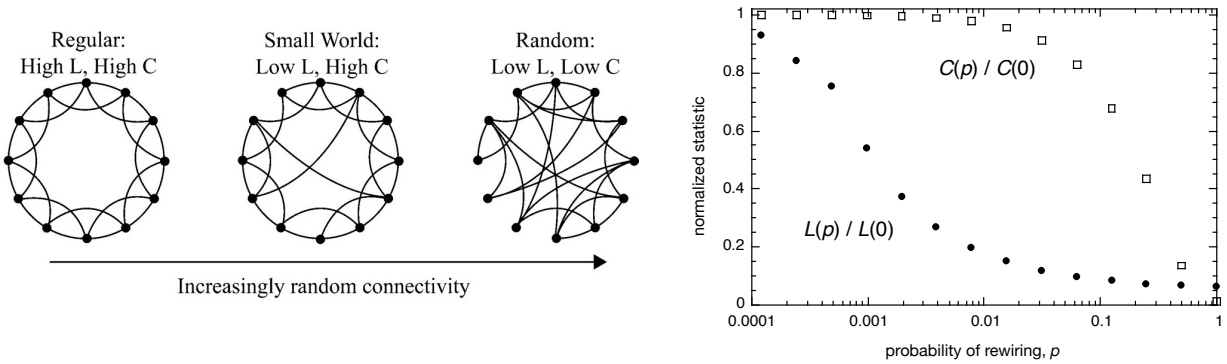


Figure 2: (A) Watts and Strogatz's schematic illustrating the small worlds model. (B) The small-world phenomenon, in which at even modest levels of randomization, the network exhibits both small mean geodesic path lengths *and* a high clustering coefficient.

Something interesting happens as we vary p between these two extremes: when only a small number of edges have been rewired (small p), the diameter of the network collapses from $O(n)$ (big world) to $O(\log n)$ (small world) even as the local structure is still largely preserved. That is, a highly-ordered "big world" can be transformed, by rewiring only a small number of connections, into a still mostly ordered small world, in which geodesic paths are short, most nodes are "close" to each other, and the network overall is very compact. As a result of this compactness, one issue that many network systems have to deal with is how to prevent information from being everywhere, all at once. We'll revisit this puzzle later in class.

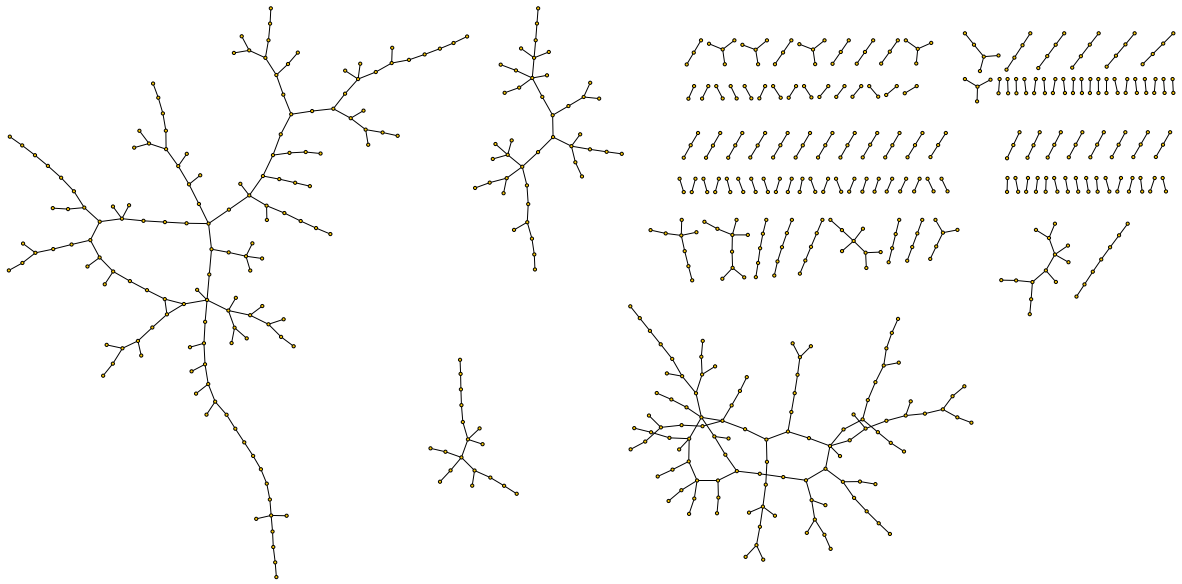
[17] This is a key fact about networks, that allows us to *reason* about networks, their structure and dynamics.
[18] Watts and Strogatz, "Collective dynamics of small-world networks." *Nature* **393**, 440–442 (1998).

2.5 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 $O(n)$.[19] 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 sizes of a network's components, we use any standard `single-source shortest path` (SSSP) or `all-pairs shortest path` (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.

2.6 Other measures of network structure

These measures of network structure cover just the basics. For convenience, most of the measures above are summarized in Table 1 below. There are, of course, many other measures of network structure—in fact, there are an infinite number of them. You can think of each 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.

Because they are all measuring different aspects of the same network, most network measures 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.

3 Supplemental readings

1. Read Chapter 6.1–6.4, and 6.6–6.12, and 7.3–7.4 in *Networks*

[19] The 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.

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	$k_i^{\text{in}} = \sum_{j=1}^{n} A_{ji}$	number of arcs ending at vertex i
out-degree	L	D	$k_i^{\text{out}} = \sum_{j=1}^{n} A_{ij}$	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	$m = \sum_{ij} A_{ij}$	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	$\langle k^{\text{in}} \rangle = \langle k^{\text{out}} \rangle = 2m/n$	average number of in- or out-edges per vertex
reciprocity	G	D	$r = \frac{1}{m}\sum_{ij} A_{ij}A_{ji}$	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 reciprocated
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	$c_i = \sum_{j<k} A_{ij}A_{jk}A_{ki} \big/ \binom{k_i}{2}$	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	U D	$\ell = \frac{1}{Z}\sum_{ij} \ell_{ij}$	average length of a geodesic path
eccentricity	G	U D	$\epsilon_i = \max_j \ell_{ij}$	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.