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Network Properties Revealed through Matrix Functions*

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Abstract. The emerging field of network science deals with the tasks of modeling, comparing, and summarizing large data sets that describe complex interactions. Because pairwise affinity data can be stored in a two-dimensional array, graph theory and applied linear algebra provide extremely useful tools. Here, we focus on the general concepts of *centrality*, *communicability*, and *betweenness*, each of which quantifies important features in a network. Some recent work in the mathematical physics literature has shown that the exponential of a network's adjacency matrix can be used as the basis for defining and computing specific versions of these measures. We introduce here a general class of measures based on matrix functions, and show that a particular case involving a matrix resolvent arises naturally from graph-theoretic arguments. We also point out connections between these measures and the quantities typically computed when spectral methods are used for data mining tasks such as clustering and ordering. We finish with computational examples showing the new matrix resolvent version applied to real networks.

Key words. centrality measures, clustering methods, communicability, Estrada index, Fiedler vector, graph Laplacian, graph spectrum, power series, resolvent

AMS subject classifications. 05C50, 05C82, 91D30

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1. Motivation.

1.1. Introduction.

Connections are important. Across the natural, technological, and social sciences it often makes sense to focus on the pattern of interactions between individual components in a system [1, 8, 61]. Large networks arise, for example,

- in the cell, connecting genes [59], proteins [25, 60], or other genomic quantities [2, 37],
- in the brain, connecting neurological regions [16, 47, 65],
- in epidemiology, connecting individuals who come into contact [14],
- in zoology, connecting animals that interact socially [15],
- in energy, connecting power suppliers or users [45],
- in telecommunications, connecting mobile phone users [63],
- in the World Wide Web, connecting web pages [53, 64], and
- in the Internet Movie Database, connecting costarring actors [41].

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By focusing on the underlying connectivity, it becomes apparent that common questions are being asked across these disparate areas of study, and hence a universal set of tools could be developed for modeling, analyzing, and summarizing complex networks [18, 67]. Our aim here is to unify and extend some recently developed concepts that are designed to pick out important topological features by assigning quantitative values to nodes, or pairs of nodes, in a network. More precisely, we concentrate on specific instances of centrality and communicability. We will begin by briefly describing some of the historical developments in the areas that are most relevant to our work, while noting that there is a well-established literature in which many variants have been proposed. We refer the reader to [11, 62, 70] for further details and references.

In this work the term *network* refers to an undirected, unweighted graph with N nodes. This can be represented through a symmetric adjacency matrix $A \in \mathbb{R}^{N\times N}$ which has $a_{ij} = 1$, if nodes i and j are connected, and $a_{ij} = 0$ otherwise. We assume that $a_{ii} = 0$, so nodes cannot be self-connected.

1.2. Brief Background. The concept of node centrality dates back to the 1940s and early 1950s when Bavelas [6, 7] and Leavitt [54] studied communication networks. Perhaps the simplest centrality measure, introduced by Freeman [32], is given by the *degree*,

$$\deg_i := \sum_{k=1}^{N} a_{ik} = (A\mathbf{e})_i \,, \tag{1}$$

which counts the number of edges involving node i. Here, $\mathbf{e} \in \mathbb{R}^N$ denotes the vector with all values equal to one. The importance of the degree centrality is not only practical but also conceptual. Several other centrality measures can be seen as extensions of this one. Of particular relevance for our work is the centrality measure introduced in 1953 by Katz [50], where geometrically scaled powers of the adjacency matrix are used to give a measure for the ith node according to

$$k_i := \sum_{j=1}^{N}\sum_{k=0}^{\infty} \alpha^k \left(A\right)_{ij}^k = \left(\left((I-\alpha A)^{-1} - I\right)\mathbf{e}\right)_i . \tag{2}$$

Here, I is the N-dimensional identity matrix and the fixed parameter α must be smaller than the inverse of the largest eigenvalue of A.

Although we do not consider them in this work, we mention in passing that weighted networks were studied by Hubbell [44], who produced what may be regarded as a generalization of Katz's centrality measure.

A quantum leap occurred when Bonacich [9, 10] introduced the definition of *eigenvector centrality*, in which a node's centrality is a function of the centralities of those nodes to which it is connected; more precisely,

$$b_i := \frac{1}{\lambda_1}\sum_{j=1}^{N} a_{ij} b_j = \left(\frac{1}{\lambda_1} A\mathbf{f}\right)_i , \tag{3}$$

where λ_1 and $\mathbf{f}$ are the Perron–Frobenius eigenvalue and eigenvector of A, respectively. The eigenvector centrality "can be regarded as an elegant summary of Katz's, Hoede's and Hubbell's measures" [11]. We also note that the Google search engine uses a similar philosophy when assigning *rank* to a web page [53].

Recall now that a *path* of *length* n between two distinct nodes i and j is an ordered list of distinct nodes $i, k_1, k_2, \ldots, k_{n-1}, j$ such that successive nodes in the list are connected; that is,

$$a_{i,k_1} = a_{k_1,k_2} = \cdots = a_{k_{n-2},k_{n-1}} = a_{k_{n-1},j} = 1. \tag{4}$$

We assume that the graph is connected, so that every pair of nodes can be joined by a path. The length of the shortest path between i and j is called the *pathlength* or *distance*. Two important centrality measures that use the concept of pathlength were introduced by Freeman [32]. The *closeness centrality* of node i is the sum over all other nodes j in the network of the pathlength between nodes i and j. The *betweenness centrality* is the fraction of shortest paths going through a given node.

1.3. Links with Linear Algebra. The adjacency matrix tells us directly whether nodes i and j have pathlength 1 ($a_{ij} = 1$) or higher ($a_{ij} = 0$). What happens if we square the matrix A? Writing $(A^2)_{ij}$ in the form $\sum_{k=1}^{N} a_{ik}a_{kj}$, we see that it counts the number of intermediate nodes that are connected to both i and j. In other words, $(A^2)_{ij}$ gives the number of different paths of length 2 from i to j.

To interpret higher matrix powers, we need to introduce the concept of a walk between nodes i and j, which differs from a path in that (a) nodes may be revisited along the way, and (b) we allow the case of starting and finishing at the same node, $i = j$. More precisely a *walk* of *length* n is an ordered list of nodes $i, k_1, k_2, \ldots, k_{n-1}, j$ such that successive nodes in the list are connected (4). The values $k_1, k_2, \ldots, k_{n-1}$ need not be distinct, and may include i or j. In the case where $i = j$, so the walk starts and ends at the same node, we have a *closed walk* based on node i. From the identity

$$(A^n)_{ij} = \sum_{k_1=1}^{N} \sum_{k_2=1}^{N} \cdots \sum_{k_{n-2}=1}^{N} \sum_{k_{n-1}=1}^{N} a_{i,k_1}\, a_{k_1,k_2} \cdots a_{k_{n-2},k_{n-1}}\, a_{k_{n-1},j},$$

the following simple lemma is almost immediate; a proof can be found, for example, in [17, Theorem 2.2.1].

LEMMA 1.1. *The quantity* $(A^n)_{ij}$ *counts the number of different walks* ($i \neq j$) *or closed walks* ($i = j$) *of length* n *between nodes* i *and* j.

In the next section we explain how counting walks has led to useful network measures that use the exponential of the adjacency matrix. In section 3 we then develop a general framework based on matrix functions and show that a particular case involving the resolvent can be justified from first principles. Connections with spectral methods in data mining are brought out in section 4. In section 5 we compare measures analytically and on a synthetic network, and in section 6 we look at real networks. Section 7 finishes with a brief discussion.

2. Using the Matrix Exponential.

2.1. Centrality. Suppose now that each node is to be assigned a number that quantifies its "well-connectedness." A simple choice is given by the degree (1). We note in passing that $(A^2)_{ii} = \sum_{k=1}^{N} a_{ik}a_{ki} = \deg_i$, so the degree can be characterized through the diagonal of A^2. The degree, however, paints a very localized picture of a node's importance; it does not distinguish between edges that connect to well-connected or poorly connected nodes. We may interpret $\deg_i$ as counting the number of closed walks of length 2 based on node i. This suggests that it might also be of

interest to consider how many walks of length 3 begin and end at node i. A better-connected node should have more opportunities to form triangles $i \to k_1 \to k_2 \to i$. We note from Lemma 1.1 that the number of such length-3 walks is given by $(A^3)_{ii}$. Continuing this reasoning, we could argue that $(A^n)_{ii}$, for each $n = 2, 3, \ldots$, provides a useful piece of information,[1] because it counts the number of closed walks of length n based on node i. How may we combine these counts in order to obtain a single number that summarizes well-connectedness? Shorter walks are typically more important than longer walks—information is passed more quickly and efficiently—so it is intuitively reasonable to form a length-based weighted average. Estrada and Rodríguez-Velázquez [31] put forward this viewpoint for complex networks and suggested that the number of walks of length n could be scaled by $1/(n!)$. This leads to a measure for node i of the form

$$\left(\frac{A^2}{2!} + \frac{A^3}{3!} + \cdots + \frac{A^k}{k!} + \cdots \right)_{ii}.$$

Since the relative ordering does not change if we add a constant, say, 1, to each node's value, and recalling that $a_{ii} = 0$, we may change this to

$$\left(I + A + \frac{A^2}{2!} + \frac{A^3}{3!} + \cdots + \frac{A^k}{k!} + \cdots \right)_{ii},$$

where I is an identity matrix, which, of course, may be written

$$\left(\exp(A)\right)_{ii}, \tag{5}$$

where $\exp(\cdot)$ denotes the matrix exponential [43]. This quantity, first introduced by Estrada in a different context to quantify the degree of folding in protein chains [22], was originally referred to as the *subgraph centrality* of node i [31]. The sum over all nodes of the subgraph centrality has since become known as the Estrada Index [13, 34, 38, 39, 40].

Estrada and Hatano [29] interpreted the subgraph centrality measure defined in (5) from the viewpoint of statistical mechanics and showed that it may be regarded as a partition function for the network. Subgraph centrality has been successfully applied to the identification of essential proteins in protein-protein interaction networks [25], detection of keystone species [26] and patches [27] in ecological food webs and landscapes, respectively, to the analysis of infrastructure robustness [23], and detection of good expansion properties in graphs [24].

2.2. Communicability. The idea of counting walks can be extended to the case of a pair of distinct nodes, i and j. The adjacency matrix tells us whether i and j are connected by a walk of length 1, but this does not reveal anything about the possible role that other edges might play in relating the two nodes. For example, if nodes i and j are not connected, at one extreme they may have many neighbors in common, but at the other extreme they may be widely separated in the sense of having a large pathlength. To push this idea further, we may imagine something tangible being passed around the network; perhaps a rumor, a message, a disease, a computer virus, or a drug needle. Typically the shortest possible path will not be used, but on the other hand longer walks are generally less likely [62]. For example, in the famous

[1] We also mention that A^n arises naturally when the power method is used to compute the eigenvector centrality (3).

small world experiments of Stanley Milgram [58], messages were passed along social acquaintance links by individuals who did not have knowledge of the overall topology, even though surprisingly short walks emerged on average [51]. The same phenomenon has been observed in more modern communication networks [19, 72]. This motivates the idea of using walk counts to quantify how easy it is for "information" to pass from node i to node j. Following the arguments used to derive subgraph centrality (5), we may form a weighted sum over all walks from i to j, with a length-based scaling of $1/(n!)$. This leads to the definition

$$(\exp(A))_{ij} \tag{6}$$

for the *communicability* between distinct nodes i and j. This idea was introduced by Estrada and Hatano [28], who showed that it provides a very useful means to extract information from real-life networks. An extension for weighted networks was developed in [16] and applied to networks describing anatomical connectivity in the brain.

2.3. Betweenness. In order to quantify the influence of a particular node as information flows around a network, it is reasonable to ask how the overall communicability changes when the node is removed. Fixing on node r, we will let $A - E(r)$ denote the adjacency matrix for the network that arises when all edges involving node r are removed. So $E(r) \in \mathbb{R}^{N\times N}$ has nonzeros only in row and column r, and row and column r have 1 wherever A has 1. Then the quantity

$$\frac{1}{(N-1)^2-(N-1)}\sum\sum_{i\neq j, i\neq r, j\neq r}\frac{(\exp(A)_{ij}-\exp(A-E(r))_{ij})}{\exp(A)_{ij}} \tag{7}$$

measures the overall relative change in communicability averaged over all pairs of nodes that are distinct from r. The factor $(N-1)^2-(N-1)$ represents the number of terms in the sum, so the result lies between zero and one, and, of course, we require $N \geq 3$ nodes for this to make sense. This quantity was introduced and illustrated in [30].

3. A General Framework and a New Set of Measures. The $n!$ scaling inherent in (5), (6), and (7) is natural in the sense that it leads to a simple and intuitively appealing function of the adjacency matrix. However, it is certainly possible to consider other scalings, and, as we will show below, there is an alternative that can be derived from a more fundamental graph-based perspective.

Generally, we could introduce any sequence of real numbers $\{c_n\}_{n\geq 1}$ such that the number of walks of length n is scaled by c_n. This leads to a communicability measure given by the i, j component of $\sum_{n=1}^{\infty} c_n A^n$, assuming (which we do henceforth) that the series is convergent for all adjacency matrices. Adding any coefficient c_0 we may let the function $f(x)$ be defined through the Maclaurin series $\sum_{n=0}^{\infty} c_n x^n$. In our context, we would like every walk to make a nonnegative contribution to the overall weighted sum, so we assume that $c_n \geq 0$ for all n. This motivates the following general definitions.

Centrality: The f-centrality of node i is given by $f(A)_{ii}$.

Communicability: The f-communicability of distinct nodes i and j is given by $(f(A))_{ij}$.

Betweenness: The f-betweenness of node r is given by

$$\frac{1}{(N-1)^2-(N-1)}\sum\sum_{i\neq j, i\neq r, j\neq r}\frac{(f(A)_{ij}-f(A-E(r))_{ij})}{f(A)_{ij}}. \tag{8}$$

Under the assumption that the graph is connected, there must be at least one walk of length less than N from node i to node j. Hence, we can guarantee that $f(A)_{ij} \neq 0$ in (8) with the condition $c_n > 0$ for $1 \leq n \leq N-1$.

We note that the coefficient c_0 is arbitrary in the sense that it has no effect on the communicability and betweenness (because $(c_0 I)_{ij} = 0$ for $i \neq j$) and for the centrality c_0 is simply added uniformly for each i.

In terms of the spectrum of A, f-centrality then has the form

$$\sum_{k=1}^{N} f(\lambda_k) {\mathbf{x}_i^{[k]}}^2, \tag{9}$$

and f-communicability has the form

$$\sum_{k=1}^{N} f(\lambda_k) \mathbf{x}_i^{[k]} \mathbf{x}_j^{[k]}, \tag{10}$$

where $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_N$ are the eigenvalues of A and $\mathbf{x}^{[1]}, \mathbf{x}^{[2]}, \ldots, \mathbf{x}^{[N]}$ the corresponding eigenvectors. Here, $\mathbf{x}_i^{[k]}$ denotes the ith component of $\mathbf{x}^{[k]}$.

This makes it clear that the choice of f can be regarded as a means to transform the spectrum. We note that f is not necessarily monotonic for $x < 0$, so this transformation might not preserve the original ordering of the eigenvalues.

The factorial weighting in (5), (6), and (7) has the benefits of (a) penalizing long walks, (b) giving a convergent series, and (c) leading to a well-known matrix function, but there there seems to be no a priori justification for this choice over other possibilities. We suggest here that a reasonable starting point for downweighting long walks is to consider *comparing the number of walks of length n between nodes i and j with that for the complete graph, K_N*. The justification is that because every possible edge exists, K_N clearly admits the maximum number of such walks. So we compare the actual number admitted by the network with a sharp upper bound over all networks of the same size.

How many different walks of length n are there between a distinct pair of nodes, i and j, in K_N? An exact formula is given by $\left((N-1)^n - (-1)^n\right)/N$. Similarly, for $i = j$, the number of closed walks of length n in K_N is $\left((N-1)^n - (-1)^n\right)/N + (-1)^N$. These expressions can be derived by noting from Lemma 1.1 that we are looking at elements of $(J - I)^n$, where $J \in \mathbb{R}^{N \times N}$ is the matrix of all ones. The identity $(J - I)^n = \left((N-1)^n - (-1)^n\right) J/N + (-1)^n I$ follows by induction on n, using the fact that $J^2 = NJ$. Because neither the $i = j$ nor the $i \neq j$ expression is a Maclaurin series coefficient for a simple function f, it is intuitively appealing and computationally attractive to use the value $(N-1)^{n-1}$ for the weight c_n, which is an excellent approximation for the large N case of interest. This gives us (using $c_0 = N - 1$)

$$f(x) = (N-1)\left(1 - \frac{x}{N-1}\right)^{-1}.$$

Since we are concerned only with relative sizes as i and j vary, we may rescale this to

$$f(x) = \left(1 - \frac{x}{N-1}\right)^{-1}. \tag{11}$$

We are interested in large, sparse, complex networks, so it is reasonable to assume that every node has degree much less than N and hence, in particular, $\| A \|_\infty \leq N-2$. Here, $\| A \|_\infty := \max_{j=1,2,\ldots,N} \sum_{i=1}^{N} a_{ij}$ is the infinity matrix norm, which is also the maximal nodal degree. This implies that every eigenvalue of A lies in the interval $[-N-2, N-2]$, and so $I - A/(N-1)$ cannot have an eigenvalue of zero. Hence, the function $f(x)$ in (11) can be applied to A. In terms of the spectrum of A, for $f(x)$ in (11) the f-centrality of node i may be written

$$\sum_{k=1}^{N} \frac{N-1}{N-1-\lambda_k} \mathbf{x}_i^{[k]^2}, \tag{12}$$

and the f-communicability of distinct nodes i and j has the form

$$\sum_{k=1}^{N} \frac{N-1}{N-1-\lambda_k} \mathbf{x}_i^{[k]} \mathbf{x}_j^{[k]}. \tag{13}$$

It is also worth mentioning that for any matrix $A \in \mathbb{R}^{N \times N}$, the function $g(s) = (A - sI)^{-1}$ over $s \in \mathbb{C}$ is called the *matrix resolvent*. Hence, we will refer to (12), (13), and the corresponding betweenness (8) as resolvent centrality, resolvent communicability, and resolvent betweenness, respectively. The resolvent is related to the exponential through the Laplace transform, and fascinating connections between the two functions can be found in the applied and numerical mathematics literature; see, for example, [68]. In this work we are proposing to replace a matrix exponential with a resolvent in order to obtain alternative definitions of centrality, communicability, and betweenness. In section 5 we compare the two versions more closely.

4. Connections with the Graph Laplacian and Spectral Clustering. The idea of using the dominant part of the spectrum in order to capture the essential features of a matrix is common across many areas, including numerical linear algebra [35], statistics [33], data mining [21], and machine learning [56]. In this section we make the connections more explicit by relating f-centrality and f-communicability to spectral clustering and reordering [5, 42, 66] in the case where f is monotonic.

As motivation, suppose that we wish to partition the nodes into two groups, so that nodes in the same group share many edges and nodes across different groups share few edges. If we let $\mathbf{x} \in \mathbb{R}^N$ be an *indicator vector*, with $\mathbf{x}_i = \frac{1}{2}$ indicating that node i has been assigned to the first group and $\mathbf{x}_i = -\frac{1}{2}$ indicating that node i has been assigned to the second group, then the quantity

$$\sum_{i=1}^{N} \sum_{j=1}^{N} (\mathbf{x}_i - \mathbf{x}_j)^2 a_{ij} \tag{14}$$

counts how many edges straddle the two groups. Minimizing a quantity like (14), with appropriate constraints to rule out trivial solutions, over all discrete assignments $\mathbf{x}_i = \pm\frac{1}{2}$ is generally too expensive for large networks. Instead, we may *relax* the problem by asking for $\mathbf{x}$ to take real values. This motivates the problem

$$\min_{\mathbf{x} \in \mathbb{R}^N, \|\mathbf{x}\|_2 = 1, \sum_{i=1}^{N} \mathbf{x}_i = 0} \sum_{i=1}^{N} \sum_{j=1}^{N} (\mathbf{x}_i - \mathbf{x}_j)^2 a_{ij}. \tag{15}$$

Here $\mathbf{x}$ is allowed to take real values. The constraint $\|\mathbf{x}\|_2 = 1$ eliminates the trivial solution $\mathbf{x} \equiv 0$ and the constraint $\sum_{i=1}^{N} \mathbf{x}_i = 0$ accounts for the built-in redundancy—adding a constant value to all components of $\mathbf{x}$ does not alter the objective function. Letting $D = \mathrm{diag}\,(\deg_i)$, the problem may be rewritten

$$\min_{\mathbf{x}\in\mathbb{R}^N, \|\mathbf{x}\|_2=1, \sum_{i=1}^{N} \mathbf{x}_i = 0} \mathbf{x}^T (D - A)\,\mathbf{x}. \tag{16}$$

The matrix $D - A$ appearing in (16) is known as the (unnormalized) *graph Laplacian* [42, 66]. By construction, $(D - A)\mathbf{e} = \mathbf{0}$, and hence 0 is an eigenvalue of the graph Laplacian with corresponding eigenvector $\mathbf{e}$. We are assuming that the graph is connected, and it follows that all other Laplacian eigenvalues are positive. So we may order the eigenvalues $0 = \mu_1 < \mu_2 \le \mu_3 \le \cdots \le \mu_N$, with corresponding eigenvectors $\mathbf{e} = \mathbf{v}^{[1]}, \mathbf{v}^{[2]}, \mathbf{v}^{[3]}, \ldots, \mathbf{v}^{[N]}$. It then follows that $\mathbf{v}^{[2]}$ solves the optimization problem (16) [42]. The vector $\mathbf{v}^{[2]}$ is called a *Fiedler vector* of the graph.[2] Recalling that we started with $\mathbf{x}_i = \pm\frac{1}{2}$, if the relaxed problem (16) has a similar solution to the original discrete version, in the sense that the entries split into distinctly positive and negative sets, we could argue that if $\mathbf{v}_i^{[2]}\mathbf{v}_j^{[2]} > 0$, then nodes i and j should be assigned to the same group, and if $\mathbf{v}_i^{[2]}\mathbf{v}_j^{[2]} < 0$, then they should be assigned to different groups. Moreover, since $\mathbf{v}^{[2]}$ is real-valued, rather than simply having entries of $\pm\frac{1}{2}$, we could argue that a larger positive value of $\mathbf{v}_i^{[2]}\mathbf{v}_j^{[2]}$ indicates that nodes i and j are more significantly related, overall, and a larger negative value of $\mathbf{v}_i^{[2]}\mathbf{v}_j^{[2]}$ indicates that nodes i and j are more significantly unrelated. So the off-diagonal elements of the rank-one matrix $\mathbf{v}^{[2]}{\mathbf{v}^{[2]}}^T$ can be interpreted as measuring relatedness of nodes.

Now in the case where the graph is *regular*, so the degree is uniform with $\deg_i \equiv \deg$ for $1 \le i \le N$, the graph Laplacian has the form $\deg I - A$. We see that its eigenvalues are $\mu_i = \deg - \lambda_i$, and the corresponding eigenvectors are $\mathbf{x}^{[i]} = \mathbf{v}^{[i]}$, so the dominant eigenvector of A has the form $\mathbf{x}^{[1]} = \mathbf{e}$. This carries no information that distinguishes between the nodes in the (regular) graph—the $k = 1$ term in (10) is the same for all pairs (i, j). In the case where f is monotonic, the next most dominant term, at $k = 2$, then uses a multiple of $\mathbf{v}^{[2]}{\mathbf{v}^{[2]}}^T$, precisely the information that is used in clustering via the graph Laplacian.

In addition to clustering them, a Fiedler vector may also be used to reorder the nodes, using the relation $i \le j \Rightarrow \mathbf{v}_i^{[2]} \le \mathbf{v}_j^{[2]}$; that is, the node with the most negative Fiedler vector component goes first, the node with the next most negative Fiedler vector component goes second, and so on. This idea can also be motivated from the minimization of (14), where we are trying to place nodes close together in the new ordering if they are strongly interconnected in the graph. If we continue to focus on the regular graph case, the objective function in (16) can be simplified to $-\mathbf{x}^T A\mathbf{x}$, giving the equivalent problem

$$\max_{\mathbf{x}\in\mathbb{R}^N, \|\mathbf{x}\|_2=1, \sum_{i=1}^{N} \mathbf{x}_i = 0} \sum_{i=1}^{N}\sum_{j=1}^{N} \mathbf{x}_i a_{ij} \mathbf{x}_j. \tag{17}$$

In maximizing the sum of terms of the form $\mathbf{x}_i a_{ij} \mathbf{x}_j$, we are trying to make $\mathbf{x}_i$ and $\mathbf{x}_j$ take large values of the same sign whenever nodes i and j are connected. In this way,

[2] It is possible for more than one distinct Fiedler vector to exist [4].

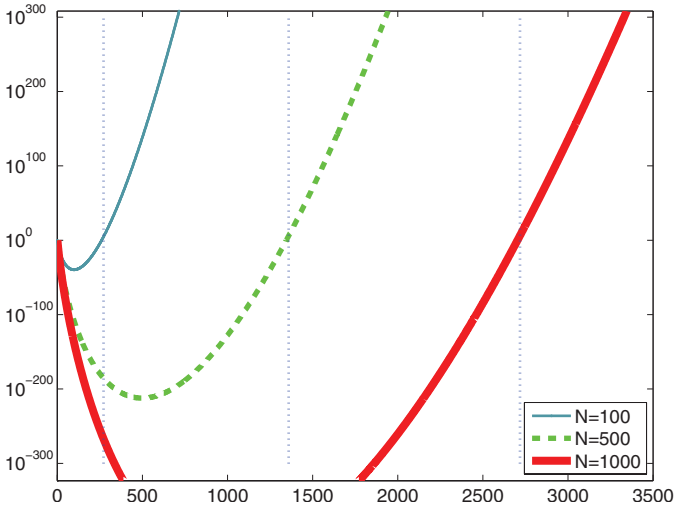

Fig. 1 *The sequence* $n!/((N-1)^{n-1})$ *for fixed values of* $N = 100$, 500, *and* 1000. *Vertical lines indicate the cutoff region at* $n = Ne$.

the most "active" or "well-connected" nodes will be assigned values farthest away from the origin, and the quantity $\mathbf{v}_i^{[2]^2}$ is a measure of how well the node has fared overall. In (9) the $k = 1$ term again does not distinguish between nodes, so, when f is monotonic, the dominant contribution to centrality will come from $\mathbf{v}_i^{[2]^2}$, precisely the term from spectral reordering that quantifies the well-connectedness of node i.

5. Resolvent versus Exponential. To understand the difference between the exponential and resolvent measures, we may compare the relative sizes of the weights $c_n = 1/n!$ and $c_n = (N-1)^{n-1}$ when the network dimension, N, is large. First we note that

$$\sum_{n=1}^{\infty} \frac{1}{n!} = e - 1 \quad \text{and} \quad \sum_{n=1}^{\infty} \frac{1}{(N-1)^{n-1}} = \frac{N-1}{N-2},$$

so both versions have an $O(1)$ amount of weight to distribute across the different walk lengths. For a given network dimension, the factorial function $n!$ clearly starts off below $(N-1)^{n-1}$ when n is small and overtakes it as n increases. Using the Stirling approximation $n! \approx \sqrt{2\pi n}(n/e)^n$, we find that $n!$ and $(N-1)^{n-1}$ are comparable when $n \approx Ne$; so the exponential-based measure is more generous than the resolvent-based measure to walks of length up to around twice the network dimension, and vice versa for longer walks. In Figure 1 we plot terms in the ratio $n!/((N-1)^{n-1})$ as a sequence in n for $N = 100$, 500, and 1000. Note that the vertical axis is logarithmically scaled. Vertical lines indicate the cutoff level $n = Ne$, where the ratio starts to exceed 1.

Using the triangle inequality and the submultiplicative inequality $\| A^n \|_\infty \leq \| A \|_\infty^n$, we see that the contribution from paths of length N or greater to the re-

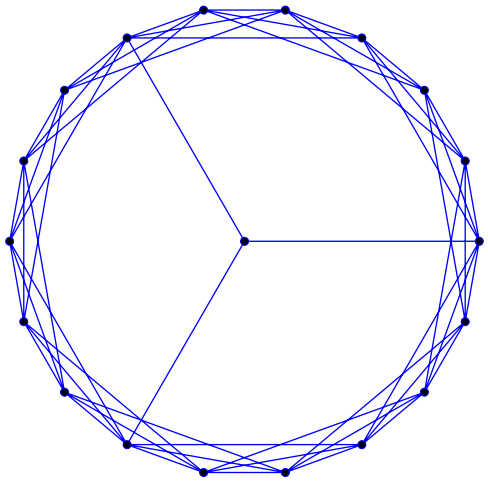

Fig. 2 *Network consisting of a $2K$-nearest neighbor periodic ring of N nodes, with an extra central "hub" that connects to H "equally spaced" nodes around the ring. All nodes in the ring have degree $2K$ except for the H nodes that connect to the hub (these have degree $2K+1$) and the hub, which has degree H. For illustration, we show the case where $N = 18$, $K = 3$, and $H = 3$.*

solvent communicability can be bounded as

$$\begin{aligned}\sum_{n=N}^{\infty}\left(\frac{A^n}{(N-1)^{n-1}}\right)_{ij} &\le \left\|\sum_{n=N}^{\infty}\frac{A^n}{(N-1)^{n-1}}\right\|_{\infty}\\ &\le \sum_{n=N}^{\infty}\frac{\|A^n\|_{\infty}}{(N-1)^{n-1}}\\ &\le \sum_{n=N}^{\infty}\frac{\|\,A\,\|_{\infty}^{n}}{(N-1)^{n-1}}\\ &\le \frac{(N-1)^2}{N-1-\|\,A\,\|_{\infty}}\left(\frac{\|\,A\,\|_{\infty}}{N-1}\right)^{N}.\end{aligned}$$

Since we are considering the regime where $\|\,A\,\|_{\infty} \ll N$, so there are few links per node, we may conclude that the walks of length $O(N)$, where the resolvent down-weights less severely than the exponential, make a negligible contribution. So, overall, we would expect the behavior on short walks, where the exponential takes more account of non-shortest-length contributions, to be the distinguishing feature.

To see the differences in practice, we give some computational results on a synthetic network whose properties we can control. The network is based on a periodic ring of N nodes, where each node is connected to its K closest nodes in a clockwise sense and its K closest nodes in a counterclockwise sense. We then add a further "hub" node, which is connected to H of the ring nodes, with equal spacing between the hub links. More precisely, for $s = 1, 2, \ldots, H$, the hub node, $N+1$, is connected to the node whose index is the closest integer to $1 + N(s-1)/H$. Figure 2 shows the case where $N = 18$, $K = 3$, and $H = 3$.

In our test we fix $N = 200$ and $K = 6$ and let H vary from 2 to 20. So, for a fixed underlying ring, we alter the degree of the hub. We focus on node $N+1$,

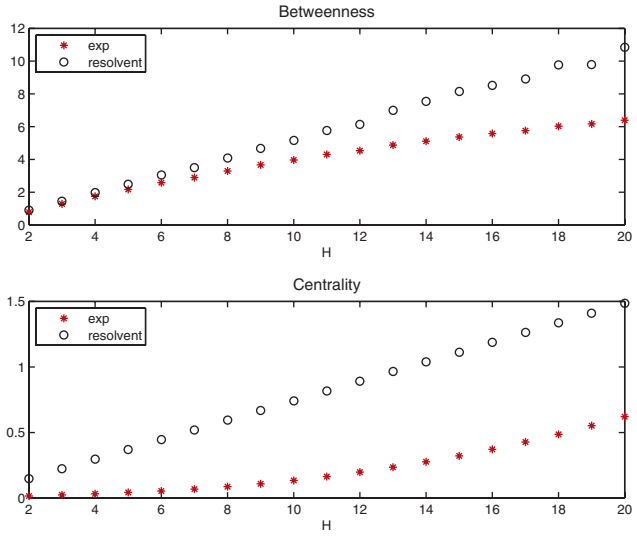

Fig. 3 *Upper picture: hub betweenness divided by node* 1 *betweenness as the hub degree, H, is varied. Lower picture: hub centrality divided by node* 1 *centrality as the hub degree, H, is varied. Asterisks are used for the exponential measure and circles for the resolvent.*

the hub, and node 1, a member of the ring that is connected to the hub. With this construction, for small H the hub has much lower degree than all other nodes in the network. However, its neighbors are spread across the underlying ring topology, so it has important connections in the sense that it creates short walks between nodes that are otherwise very far apart. Removing the hub would have a major effect on the overall ease with which information could flow around the network, so we would expect the hub to have a higher betweenness measure than its degree might suggest.

The upper plot in Figure 3 shows the betweenness for the hub relative to the betweenness for node 1. The exponential case is shown as asterisks and the resolvent case as circles. We see that for hub degree H as small as 3, both versions assign the hub a higher betweenness rating than the ring node, which has degree 13. As H is increased, the relative size of the hub node to ring node betweenness is greater for the resolvent version of the measure. An intuitive explanation for this effect is that hub removal causes many pairs of nodes to lose all short connecting walks, making a large impact on their resolvent communicability.

The lower plot in Figure 3 shows the centrality for the hub relative to the centrality for node 1 (with f shifted so that its degree-zero term in the Maclaurin expansion is zero). As before, the exponential case is shown as asterisks and the resolvent case as circles. We see that, for small hub degree H, both versions give a ratio less than 1, indicating that the hub is less central than the ring node. This makes sense, because the hub is typically taking part in longer walks than the ring node. As expected, the resolvent measure behaves more like the nodal degree, giving a ratio close to 1 at $H = 13$.

6. Tests on Real Data. We now present some computations with real networks, focusing on centrality. We emphasize that our aim here is not to judge whether one measure is "better" in any sense than another. Such issues are clearly open to inter-

pretation and require application-specific expertise; for example, protein essentiality was used as a target for centrality measures in [25]. Instead, we wish to record the correlations between the three centralities given by degree, exponential, and resolvent and to check whether they are distinct. So, our aim is to get a feel for how the different versions of centrality compare; we are not making the case for one measure over the others.

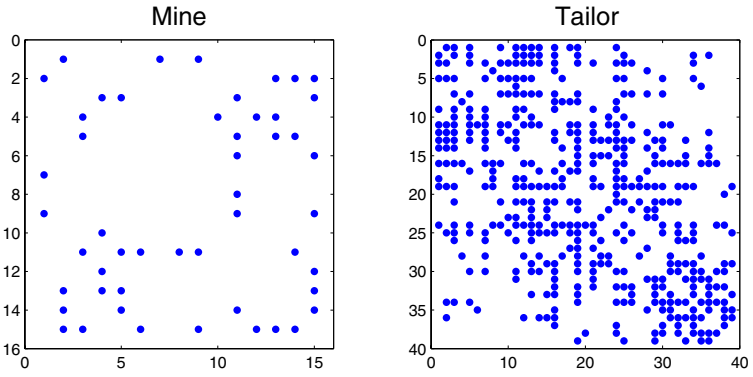

Fig. 4 *Adjacency matrices for two social interaction networks. A dot in position* (i, j) *denotes a nonzero entry in the matrix.*

6.1. Small Scale Tests. We begin with two real data sets from social science. These examples are small, so that the overall networks are easy to visualize. The two adjacency matrices are shown in Figure 4. The network on the left records interactions between 15 mine workers in Zambia [20, 48]. Two men are linked by an edge if they were observed to interact in more than one way, for example, through conversation, joking, job assistance, cash assistance, or personal assistance. On the right in Figure 4 we have a larger and denser network that records assistance-related interactions between individuals in a tailor's shop in Zambia [49]. Both data sets were downloaded from the website http://vlado.fmf.uni-lj.si/pub/networks/data/UciNet/UciData.htm.

Recall now that the "importance" of node i could be measured by the subgraph centrality $f(A)_{ii}$ or simply the degree of the node. The upper plots in Figure 5 show the exponential, resolvent, and degree measures for the mine network (left) and tailor network (right). Here we set $c_0 = 0$ in the resolvent and exponential power series and we normalize each measure so that it sums to 1 over all the nodes. The asterisks, circles, and crosses correspond to degree, exponential, and resolvent, respectively. For the mine data, we see that the resolvent closely follows the degree, but generally differs from it in the direction of the exponential. For example, nodes $2, 3, 4, 5$ all have degree 4. The exponential measure distinguishes node 4 as the least important among them, and the resolvent measure does the same, albeit less dramatically. Similarly, nodes 13 and 14 both have degree 4 and the two centrality measures rate node 14 as the more central.

We may use these measures to place the nodes in order with the most central in position 1, the next in position 2, and so on. The lower left plot in Figure 5 compares the three sets of rankings that arise for the mine network. Looking at position i on the horizontal axis, we see a circle plotted at some height j. This indicates that the node ranked ith according to degree was ranked jth according to exponential centrality. Similarly, crosses plot degree against resolvent centrality. So a straight

line of unit slope indicates that the two rankings were the same, and departure from this straight line quantifies a difference in the rankings. We note that the degree ranking is somewhat ambiguous—several nodes share the same degree so a ranking involves arbitrary tie-breaking. (Here, we use MATLAB's built-in `sort` function.) At the very least, centrality measures give a means to break these ties systematically. In the picture we see some significant departures between the two centralities and the degree for nodes ranked in positions 4–8, but these are nodes with equal degree and hence the degree ranking here is locally arbitrary.

Results for the tailor network are shown on the right in Figure 5. In the upper picture, we see larger differences between the three measures than for the smaller and sparser mine network, but once again the resolvent tends to produce a value between the degree and exponential extremes. This is also reflected in the ordering results, shown in the lower picture, and is consistent with the analysis and synthetic test in section 5.

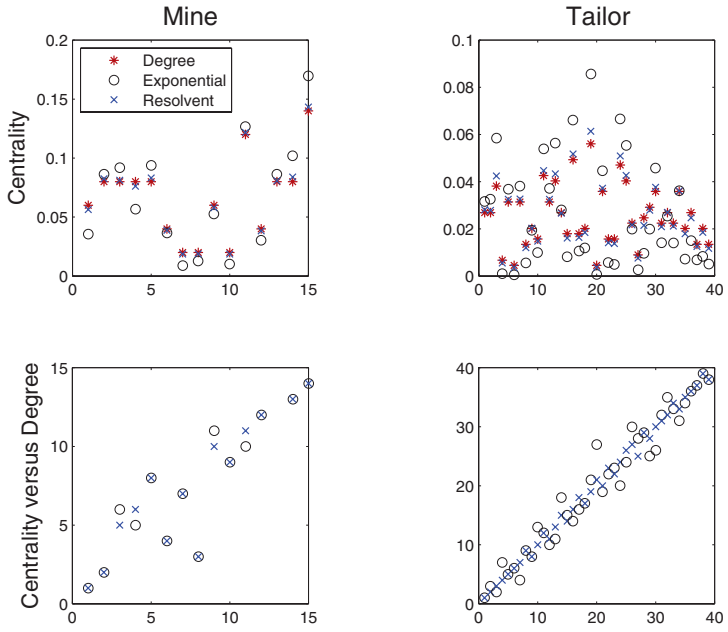

Fig. 5 *Upper picture: degree (asterisk), exponential centrality (circle), and resolvent centrality (cross), normalized to sum to* 1. *Lower picture: a circle in position* (i, j) *indicates that a node was ranked* i *in terms of degree and* j *in terms of exponential centrality. Similarly, a cross in position* (i, j) *indicates that a node was ranked* i *in terms of degree and* j *in terms of resolvent centrality. Left: mine network. Right: tailor network.*

6.2. Larger Scale Tests. We now give summary statistics on three larger networks. First, we use a food web from [55], where the 81 nodes represent marine species and links describe their trophic relationships. In the upper picture of Figure 6, for each of the $N = 81$ nodes we plot the degree on the horizontal axis against the resolvent-based centrality on the vertical axis. Because the resolvent centralities are quite compressed, we use a log scale for the vertical axis. We see from the picture that there is a very strong correlation between the two measures. The lower picture compares the degree with the exponential-based centrality, and we see a greater

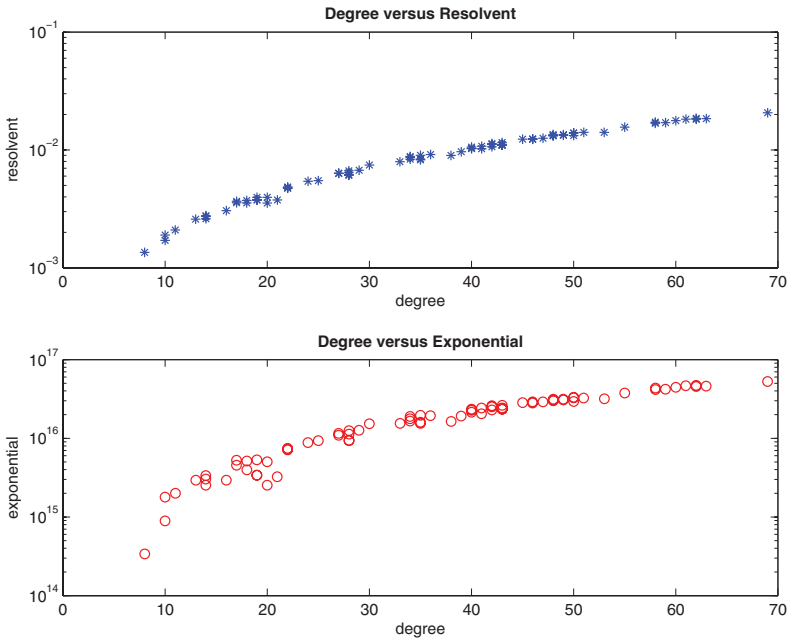

Fig. 6 *Results for shelf data. Upper: an asterisk at (x_i, y_i) indicates a node with degree x_i and resolvent centrality y_i. Lower: vertical axis now denotes exponential centrality.*

variation between the values assigned to each node. The Pearson correlation coefficients [33] are 0.9956, 0.9858, and 0.9969 for degree-resolvent, degree-exponential, and exponential-resolvent, respectively. So, as we expect from the previous analysis and examples, the resolvent measure can be regarded as lying between the degree and exponential measures, and in this network it is closer to exponential. To emphasize that the three measures are capturing genuinely different behavior, the "top ten" nodes rated from low to high, that is, from 10th place up to 1st place in terms of the three centralities, are

$$\begin{aligned} \textit{degree:}\quad & 50 < 49 \equiv 68 < 69 < 39 < 48 < 40 \equiv 41 < 42 < 43, \\ \textit{resolvent:}\quad & 50 < 49 < 69 < 68 < 39 < 41 < 48 < 42 < 40 < 43, \\ \textit{exponential:}\quad & 50 < 49 < 69 < 68 < 39 < 41 < 42 < 48 < 40 < 43. \end{aligned}$$

So although the same nodes appear in each top ten list, the ordering differs each time. (The $\equiv$ symbol indicates that nodes share the same degree, and hence there are ties in the rankings.)

Figure 7 repeats this test for a network describing Macaque cortical connectivity, from http://www.biological-networks.org/?page_id=25; see [46, 52]. Here the 95 nodes represent regions in the monkey brain and edges represent physical connections. In this case, the correlation coefficients are 0.9970, 0.9560, and 0.9628 for degree-resolvent, degree-exponential, and exponential-resolvent, so this time the resolvent is closest to degree. The ordered top ten lists are

$$\begin{aligned} \textit{degree:}\quad & 15 < 94 < 65 < 58 < 31 \equiv 39 < 38 < 59 < 93 < 68, \\ \textit{resolvent:}\quad & 13 < 6 < 65 < 39 < 58 < 31 < 38 < 59 < 93 < 68, \\ \textit{exponential:}\quad & 11 < 12 < 65 < 39 < 58 < 31 < 59 < 38 < 93 < 68. \end{aligned}$$

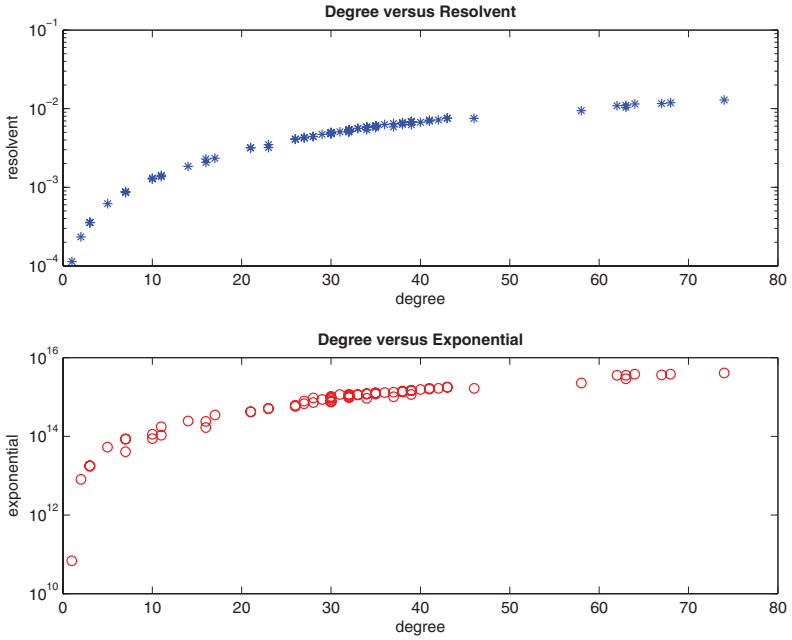

Fig. 7 *As for Figure 6 with Macaque brain data.*

We see an overall consistency between the three rankings, with some differences among the lower positions.

In Figure 8 we show results for a yeast protein-protein interaction network, taken from [12] based on data from [69]. There are 2224 proteins, and an edge denotes that a physical interaction has been recorded. In this case the degree-resolvent, degree-exponential, and exponential-resolvent correlation coefficients are 0.9999992, 0.4928, and 0.4934. The top ten ordered lists are

$$\begin{aligned} \textit{degree:}\ & 607 \equiv 1896 < 489 < 473 < 138 < 200 \equiv 739 < 1338 < 292 \equiv 535, \\ \textit{resolvent:}\ & 111 < 607 < 489 < 473 < 138 < 739 < 200 < 1338 < 535 < 292, \\ \textit{exponential:}\ & 1170 < 122 < 129 < 156 < 117 < 473 < 292 < 242 < 126 < 427. \end{aligned}$$

In this case, node 111 shares the same degree as nodes 607 and 1896, so the resolvent and degree rankings could be regarded as equivalent.

In these tests, and many others, we have found that the resolvent-based centrality measure typically gives values between the degree and exponential versions. It is usually closely aligned with the degree, especially for large networks. The resolvent-based approach offers two immediate advantages over the degree:

- being real-valued, it is more naturally suited to the task of ranking nodes than the degree, as it is less likely to require arbitrary tie-breaking;
- it readily extends to give analogous measures of betweenness and communicability, as described in section 3.

7. Discussion. There are many connections between linear algebra and graph theory, and the emerging discipline of network science draws heavily on both fields. The power series/matrix function/weighted walk count viewpoint provides useful conceptual and computational tools, and has the potential to be extended in many di-

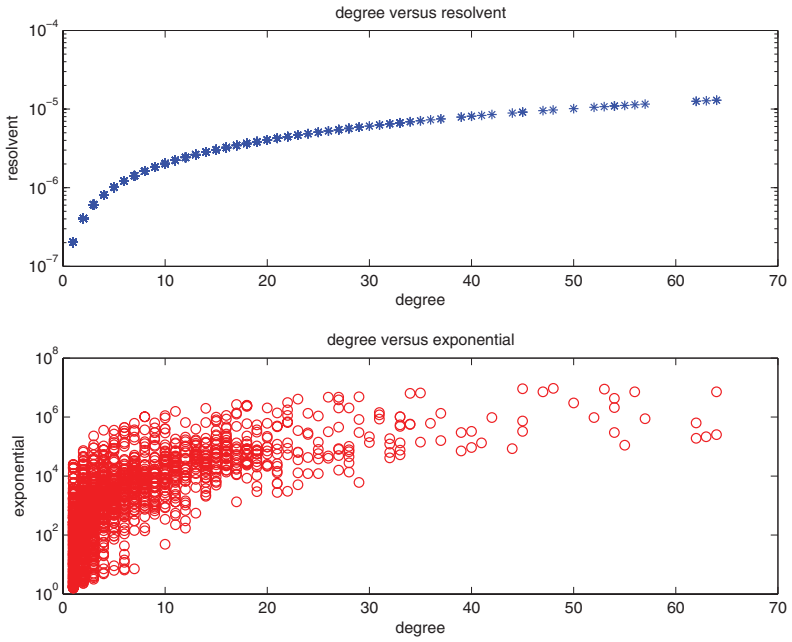

Fig. 8 *As for Figure* 6 *with protein-protein interaction data.*

rections. Our aim in this work was to put forward a unified framework for defining centrality, communicability, and betweenness measures based on a general matrix function and to point out that a new matrix resolvent version can be derived from first principle arguments, thereby avoiding the arbitrary parameter choices required by some alternative versions.

This area offers several interesting challenges, including

- relating these network properties to other concepts such as good expansion [24], lethality, or entropy [57];
- developing efficient computational algorithms that exploit sparsity and perhaps other naturally occurring structures such as small-worldness [71] or scale-freeness [3];
- characterizing other network features through matrix functions, such as bipartivity and multipartivity [30]; and
- dealing with network topology that evolves over time [36].

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