Matrix Functions and Network Communicability Measures

Michele Benzi

Abstract In recent years, functions of matrices have played an increasingly important role in the analysis of graphs and networks, especially in the definition of powerful centrality and communicability measures and in the analysis of diffusion processes, both local and nonlocal. These techniques are having a significant impact in a variety of applications, ranging from social network analysis to chemical physics to the neurosciences. This contribution provides a succinct overview of how matrix functions can be used in the analysis of communicability in complex networks.

1 Introduction

Network science provides conceptual and quantitative tools for analyzing and understanding the structure, function and dynamics of large and complex interconnected systems. It has had a tremendous impact on virtually every area of knowledge, from the natural and life sciences to the social sciences, from engineering to the humanities, and it has become indispensable for understanding a wide range of phenomena arising in fields like sociology, biology, ecology, engineering, computer and information sciences, economics, finance, and many others (Barabasi 2002; Boccaletti et al. 2006; Brandes and Erlebach 2005; Estrada 2012d; Newman 2003, 2018).

Since the beginnings of social network analysis in the late 1940s, tools from graph theory, linear algebra, probability and statistics have been essential to this field (Rapoport 1963; Katz 1953; Seeley 1949). In particular, quantities defined in terms of matrices associated to graphs (such as the adjacency matrix and the graph Laplacian) have been used to define computable metrics for the structural analysis of both static and dynamic networks, such as centrality and communicability measures. The quantitative analysis of networks often translates into classical problems of numerical linear algebra such as matrix factorizations, solving sparse linear systems, computing eigenvalues and eigenvectors, and the evaluation of functions of matrices.

M. Benzi (✉)
Scuola Normale Superiore, Pisa, Italy
e-mail: michele.benzi@sns.it

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These problems can be challenging in view of their possibly very large size, and require state-of-the-art techniques for their efficient solution.

This contribution surveys the use of matrix functions to define and investigate various notions of *communicability* in networks. Roughly speaking, communicability allows one to quantify how well (or poorly) two distinct nodes in a network can exchange information. This notion is closely related both to node centrality (which measures the importance of individual nodes) and to global measures of graph connectivity. Communicability can be defined in terms of graph walks (expressed by suitable functions of the adjacency matrix) but it can also be measured by means of diffusion processes and random walks on the graph, which are best expressed in terms of functions of the graph Laplacian.

For earlier (and more in-depth) surveys of matrix functions in network analysis the reader is referred to Estrada and Higham (2010) and to Benzi and Boito (2020).

2 Background on Graphs and Linear Algebra

This section provides the basic graph theory and linear algebra notions used in the sequel. Good reference works include Diestel (2000), Horn and Johnson (2013), Higham (2008); see also Estrada and Knight (2015).

2.1 Graphs and Matrices

A *directed graph* or *digraph*, G is defined by a set of n nodes (also called vertices) V and a set of edges $E = \{(i, j)|i, j \in V\}$. If $(i, j) \in E$ implies $(j, i) \in E$, then G is *undirected* and the edges are formed by unordered pairs of vertices.

In a directed graph, the *out-degree* of a vertex i, denoted by d_i^{out}, is the number of edges with i as the starting node, i.e., the number of edges in E of the form (i, k). The *in-degree* of node i is the number d_i^{in} of edges of the form (k, i). If G is undirected, then $d_i^{\text{out}} = d_i^{\text{in}} = d_i$, the *degree* of node i. An undirected graph G is d*-regular* if all the nodes have the same degree d.

A *walk* of length k in G is a list of nodes $i_1, i_2, \ldots, i_k, i_{k+1}$ such that for all $1 \leq j \leq k$ there is a (directed) edge from i_j to i_{j+1}. A walk is *closed* when $i_1 = i_{k+1}$. A walk with no repeated nodes is called a *path*, and a *cycle* is a closed walk with no repeated nodes, except for the first and last one. In a *weighted graph*, a weight $w_{ij} \in \mathbb{R}^+$ is assigned to each edge $(i, j) \in E$. If all the weights are taken equal to 1, the graph is *unweighted*. For ease of exposition, here G will be generally assumed to be unweighted, but most results extend to the weighted case with straightforward modifications.

A *loop* in a graph is an edge from a node i to itself. A graph is *simple* if it has no loops, no multiple edges, and its edges are unweighted. An undirected graph is

connected if there exists a path between every pair of nodes. A directed graph is *strongly connected* if there exists a directed path between every pair of nodes.

In an undirected graph G, the *geodesic distance* between two nodes is the length of the shortest path joining them. If no such path exists, they distance between the nodes is set to infinity. The *diameter* of G is equal to the maximum distance between any two nodes in G; note that G has finite diameter if and only if it is connected.

A graph is called *bipartite* if its set of nodes V is the disjoint union of two non-empty sets V_1 and V_2 such that each edge connects a node from V_1 and a node from V_2. Given a directed graph, we can define an associated undirected bipartite graph as follows. Take two copies V and V' of the set of nodes of the original graph, and define edges according to the following rule: a node $i \in V$ and a node $j' \in V'$ are connected if and only if there is an edge from node i to node j in the directed graph.

The *adjacency matrix* $A = (a_{ij})$ associated with a simple graph G is an $n \times n$ matrix such that

$$a_{ij} = \begin{cases} 1 \text{ if } (i, j) \text{ is an edge in } G, \\ 0 \text{ otherwise.} \end{cases}$$

More generally, if the graph is weighted then $a_{ij} = w_{ij} > 0$ whenever $(i, j) \in E$. Recall that a square matrix A is *reducible* if there is a permutation matrix P such that

$$PAP^T = \begin{bmatrix} B & C \\ 0 & D \end{bmatrix}$$

with B and D square matrices. If no such P exists, A is said to be *irreducible*. It is well known that the adjacency matrix of a graph G is irreducible if and only if G is strongly connected.

Note that the in- and out-degrees of a node i can be computed as the i-th entries of the vectors $A^T\mathbf{1}$ and $A\mathbf{1}$, respectively, where $\mathbf{1}$ denotes the vector of all ones.

For an unweighted graph, the powers of the associated adjacency matrix A have an important property: each entry $[A^k]_{ij}$ counts the number of walks of length k from node i to node j. In particular, the diagonal entries $[A^k]_{ii}$ count the number of *closed* walks of length k passing through node i. This notion can easily be extended to weighted graphs.

If G is undirected, then its adjacency matrix A is symmetric and has nonnegative entries, with zeros on the main diagonal. The eigenvalues of A are real; we will label them in nondecreasing order as $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. The matrix A can be diagonalized as $A = Q\Lambda Q^T$, where $\Lambda = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$, the matrix $Q = [\mathbf{q}_1, \mathbf{q}_2, \ldots, \mathbf{q}_n]$ is orthogonal and $\mathbf{q}_i$ is an eigenvector associated with λ_i. If G is connected, the Perron-Frobenius theorem (Horn and Johnson 2013) implies that $\lambda_1 > \lambda_2$. Moreover, the *dominant eigenvector* $\mathbf{q}_1$ can be chosen to have positive entries: we write $\mathbf{q}_1 > \mathbf{0}$.

If G is a strongly connected digraph, its adjacency matrix A is irreducible. Let $\rho(A)$ be the spectral radius of A. Then, again by the Perron-Frobenius theorem, $\lambda_1 = \rho(A)$ is a simple eigenvalue of A and the eigenvector associated with λ_1 can be chosen to be positive. If A is diagonalizable, then there exists an invertible matrix

X such that $A = X\Lambda X^{-1}$, where $\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$ with $\lambda_1 \geq |\lambda_i|$ for $2 \leq i \leq n$, and the columns of X are corresponding eigenvectors. If, on the other hand, A is not diagonalizable, it can still be put into Jordan canonical form:

$$A = XJX^{-1} = X \begin{bmatrix} \lambda_1 & \mathbf{0}^T \\ \mathbf{0} & \hat{J} \end{bmatrix} X^{-1}.$$

Here J is the Jordan matrix of A, where for ease of notation the 1×1 block corresponding to the eigenvalue λ_1 appears first. The first column $\mathbf{x}_1$ of X is the dominant right eigenvector of A.

Besides the diagonal form and the Jordan form of A, another basic tool is the *singular value decomposition* (Golub and Van Loan 2013). Any matrix $A \in \mathbb{R}^{m\times n}$ of rank r can be decomposed as $A = U\Sigma V^T$, where $U \in \mathbb{R}^{m\times m}$ and $V \in \mathbb{R}^{n\times n}$ are orthogonal matrices, and $\Sigma \in \mathbb{R}^{m\times n}$ is zero except for its first r diagonal entries $\sigma_1, \ldots, \sigma_r$. Here $\sigma_1, \ldots, \sigma_r$ are positive real numbers and are called the *singular values* of A. The columns $\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_m$ of U are the *left singular vectors* of A, whereas the columns $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n$ of V are the *right singular vectors* of A. The singular values are uniquely determined by A, but the singular vectors, in general, are not. When A has rank $r < \min(m, n)$ it is often useful to consider the *compact singular value decomposition* of A. This is given by $A = U_r \Sigma_r V_r^T$, where $U_r = [\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_r] \in \mathbb{R}^{m\times r}$, $V_r = [\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_r] \in \mathbb{R}^{n\times r}$, and $\Sigma_r = \mathrm{diag}(\sigma_1, \sigma_2, \ldots, \sigma_r) \in \mathbb{R}^{r\times r}$ is the leading $r \times r$ block of Σ.

If the undirected graph G is bipartite, with $V = V_1 \cup V_2$, there exists an ordering of the nodes such that the adjacency matrix of G takes the form

$$A = \begin{bmatrix} 0 & B \\ B^T & 0 \end{bmatrix},$$

where B is $|V_1| \times |V_2|$. It is well known (see, e.g., Golub and Van Loan 2013) that the nonzero eigenvalues of A are of the form $\lambda_i = \pm\sigma_i$, where the σ_i are the singular values of B.

If G is a digraph with n nodes, the associated undirected bipartite graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ has $2n$ nodes and its adjacency matrix is of the form

$$\mathcal{A} = \begin{bmatrix} 0 & A \\ A^T & 0 \end{bmatrix},$$

where A is the $n \times n$ adjacency matrix of G.

The *Laplacian matrix* associated with an undirected, unweighted graph G is defined as $L = D - A$, where A is the adjacency matrix of G and $D = \mathrm{diag}(d_1, \ldots, d_n)$ is the *degree matrix* of G.

For directed graphs, one may replace D by either the matrix of in-degrees $D^{\mathrm{in}} = \mathrm{diag}(d_1^{\mathrm{in}}, \ldots, d_n^{\mathrm{in}})$ or the matrix of out-degrees $D^{\mathrm{out}} = \mathrm{diag}(d_1^{\mathrm{out}}, \ldots, d_n^{\mathrm{out}})$, resulting in two distinct notions of Laplacian matrix, L_{in} and L_{out}, the second one being usually preferred.

For an undirected graph, the Laplacian L is a singular (since $L\mathbf{1} = \mathbf{0}$), symmetric, positive semidefinite M-matrix (Berman and Plemmons 1994). The algebraic multiplicity of the zero eigenvalue is equal to the number of connected components of the graph. In particular, the graph is connected if and only if the zero eigenvalue of the Laplacian is simple (i.e., if and only if L has rank $n - 1$). The smallest nonzero eigenvalue of the Laplacian of a connected graph is known as its *algebraic connectivity* (Fiedler 1973), and the corresponding eigenvector as its *Fiedler vector*. Loosely speaking, the algebraic connectivity of G measures how hard it is to disconnect G into two subgraphs of comparable size by removing selected edges: the larger the algebraic connectivity, the harder it is to disconnect G into two roughly equal subgraphs by removing a small number of edges. The sign of the entries of the Fiedler vector can be used to assign nodes of G to either subgraph. Hence, the graph Laplacian plays a role in the important problem of graph partitioning.

For a directed graph, both L_{in} and L_{out} are singular M-matrices, with $\mathbf{1}^T L_{\text{in}} = \mathbf{0}^T$ and $L_{\text{out}}\mathbf{1} = \mathbf{0}$. If G is strongly connected, then L_{in} and L_{out} have rank $n - 1$; the converse, in general, is not true.

The notion of *normalized Laplacian* is also widely used in the literature. The symmetric normalized Laplacian is defined as $\mathcal{L} = D^{-\frac{1}{2}} L D^{-\frac{1}{2}}$, where all nodes are assumed to have positive degree; if some nodes have zero degree, $D^{-1/2}$ is defined as the diagonal matrix such that $[D^{-1/2}]_{ii} = 1/\sqrt{d_i}$ if $d_i > 0$, and $[D^{-1/2}]_{ii} = 0$ if $d_i = 0$. As an effect of diagonal scaling, the eigenvalues of $\mathcal{L}$ belong to the interval $[0, 2]$. In the directed case, additional notions of normalized Laplacian $\mathcal{L}_{\text{in}} = I - D_{\text{in}}^{-1} A$ and $\mathcal{L}_{\text{out}} = I - A^T D_{\text{out}}^{-1}$ are also of interest.

2.2 Functions of Matrices

Several, essentially equivalent definitions of a matrix function exist (Higham 2008). A rather general definition is the one based on the diagonal or Jordan form. Let A be an $n \times n$ matrix (real or complex), assumed for now to be diagonalizable. Therefore $A = X\Lambda X^{-1}$, where $\Lambda = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$ is a diagonal matrix containing the eigenvalues of A, and X is invertible. Let $f(z)$ be a (real or complex) function that is well-defined on the eigenvalues of A. Then $f(A)$ is defined as

$$f(A) = X f(\Lambda) X^{-1},$$

where $f(\Lambda) = \text{diag}(f(\lambda_1), f(\lambda_2), \ldots, f(\lambda_n))$.

If A is not diagonalizable, let $A = XJX^{-1}$ be its Jordan decomposition. The Jordan matrix J has a block diagonal structure $J = \text{diag}(J_1, J_2, \ldots, J_m)$, with one or more blocks J_k associated with each distinct eigenvalue of A. Let J_k be one such block of size $\nu \times \nu$, with eigenvalue λ; then $f(J_k)$ is defined as

$$f(J_k) = \begin{bmatrix} f(\lambda) & f'(\lambda) & \frac{f''(\lambda)}{2!} & \dots & \frac{f(\lambda)^{(v-1)}}{(v-1)!} \\ & f(\lambda) & f'(\lambda) & \dots & \frac{f(\lambda)^{(v-2)}}{(v-2)!} \\ & & \ddots & \ddots & \vdots \\ & & & f(\lambda) & f'(\lambda) \\ & & & & f(\lambda) \end{bmatrix}.$$

Now set $f(J) = \mathrm{diag}(f(J_1), f(J_2), \dots, f(J_m))$ and

$$f(A) = Xf(J)X^{-1}.$$

It can be shown that this definition is independent of the choice of X. Note that here $f(z)$ must be assumed to be differentiable a sufficient number of times at each eigenvalue of A. More precisely, denote with m_i the *index* of λ_i, i.e., size of the largest Jordan block in which the eigenvalue λ_i appears. If, for each distinct eigenvalue λ_i of A, the function f and its derivatives of order up to $m_i - 1$ are defined for $\lambda = \lambda_i$, f is said to be *defined on the spectrum of* A, and $f(A)$ is well-defined.

If $f(z)$ has a Taylor series expansion

$$f(z) = \sum_{k=0}^{\infty} a_k (z - z_0)^k$$

with radius of convergence R, this property can be used to give an alternative definition of $f(A)$. Suppose that each eigenvalue λ_i of A is either contained in the interior of the convergence disk $|z - z_0| < R$, or is on the boundary of the disk and the series for $f^{(m_i-1)}(\lambda)$ is convergent at $\lambda = \lambda_i$, with m_i the index of λ_i. Then $f(A)$ is well-defined and it is given by

$$f(A) = \sum_{k=0}^{\infty} a_k (A - z_0 I)^k.$$

Note that the converse is also true, i.e., if $f(A)$ can be expressed through the Taylor series of $f(z)$, then the eigenvalues of A satisfy the conditions stated above.

The notion of matrix function can be extended to rectangular matrices via the singular value decomposition (Hawkins and Ben-Israel 1973). Take $A \in \mathbb{R}^{m\times n}$ and let $A = U_r \Sigma_r V_r^T$ be its compact singular value decomposition. If f is a scalar function such that $f(\sigma_i)$ is defined for $i = 1, \dots, r$, then the *generalized matrix function* $f^\diamond$ induced by f is defined as

$$f^\diamond(A) = U_r f(\Sigma_r) V_r^T,$$

where $f(\Sigma_r) = \mathrm{diag}(f(\sigma_1), \dots, f(\sigma_r))$. If A is square, $f^\diamond(A)$ does not necessarily coincide with the standard matrix function $f(A)$; however, if A is symmetric positive definite (or semidefinite and $f(0) = 0$), then $f^\diamond(A)$ reduces to $f(A)$.

3 Matrix Functions for Communicability Measures

A fundamental problem in the structural analysis of networks is that of quantifying how well different parts of a network, such as individual nodes or groups of nodes, are connected to one another. This problem is of great importance, for instance, in the design and analysis of robust infrastructural networks, in the study of urban traffic, in anatomy and medicine (especially brain networks), in the study of vulnerability of financial networks, in bibliometry, in community detection, in the study of the chemico-physical properties of molecular networks, and in many other fields. Matrix functions provide an elegant mathematical framework for tackling this problem.

3.1 Network Communicability

The notion of *communicability* between two nodes, first introduced by Estrada and Hatano (2008), provides an effective measure of the connectivity between pairs of nodes. The underlying intuition is that two nodes i and j are well-connected if there are many walks in G connecting i and j, with shorter walks being given more weight than longer ones. Having in mind the interpretation of the entries of A^k in terms of graph walks, Estrada and Hatano proposed the following definition of communicability between two nodes $i, j \in V$:

$$[\mathrm{e}^{\beta A}]_{ij} = \delta_{ij} + [A]_{ij} + \frac{1}{2!}[A^2]_{ij} + \cdots = \sum_{k=0}^{\infty} \frac{\beta^k}{k!}[A^k]_{ij}\,. \tag{1}$$

Here $\beta > 0$ is the *inverse temperature*, which can be used to tune the relative contributions of short and long walks (Estrada and Hatano 2007; Estrada et al. 2012). When $i = j$ we obtain a measure of the centrality of node i, known as *subgraph centrality*, see Estrada and Rodríguez-Velázquez (2005). In other words, $[\mathrm{e}^{\beta A}]_{ii}$ is a measure of the importance, or influence, of node i in the graph. Of course, other functions besides the matrix exponential can be used. For example, the off-diagonal entries of the resolvent $f(A) = (I - \alpha A)^{-1}$, with $0 < \alpha < \frac{1}{\lambda_1}$, can be used to define the *Katz communicability* between nodes (Katz 1953). An *eigenvector-based communicability* can be obtained by taking the product $x_1(i)x_1(j)$ of the ith and jth entries of the (positive) dominant eigenvector $\mathbf{x}_1$ of a (strongly) connected network, normalized so that $\|\mathbf{x}_1\|_2 = 1$. Again, for $i = j$ we obtain a well-known centrality measure, the *eigenvector centrality* of node i (Bonacich 1987). Eigenvector communicability can be interpreted as a measure of communicability that takes into account longer walks: for a connected undirected graph, it can be obtained as the limit of the expression (1), normalized by $\mathrm{e}^{\beta\lambda_1}$, as $\beta \to \infty$. The same applies to the Katz communicability (multiplied by $(1 - \alpha\lambda_1)$) in the limit $\alpha \to \frac{1}{\lambda_1}^-$. At the other extreme we have the simplest and most local notion of communicability between nodes, taking the values 1 or 0 depending on whether or not there is an edge

between nodes i and j. This can be seen as the limit, as $\beta \to 0+$ or $\alpha \to 0+$, of the two parameter-dependent communicability measures based on $e^{\beta A}$ and $(I - \alpha A)^{-1}$, respectively; see the analysis in Benzi and Klymko (2015). For intermediate values of α and β, these communicability measures are able to take into account the effect of short, medium, and long range interaction between nodes.

The exponential-based communicability (1) has been used very effectively in a number of fields. For example, it has been used to develop algorithms for the community detection problem (Estrada 2011; Estrada and Hatano 2009; Xu 2020) and, more generally, for the identification of sparse and dense subgraphs of large graphs (Fioriti and Chinnici 2014). Other applications of exponential communicability include: the analysis of urban traffic flow and other transportation networks (Akbarzadeh and Estrada 2018; Mussone and Notari 2019); the study of anatomical networks (Ostachuk 2024) and especially brain networks, including the identification of anomalies in the brains of patients affected by stroke, Type 2 diabetes and other conditions (Betzel et al. 2016; Crofts and Higham 2009; Crofts et al. 2011; Gravert et al. 2017; de Reus and van den Heuvel 2014; Pião Azevedo et al. 2024; Veergossen et al. 2019); the modeling of cancer spread (Gladilin 2017); models of concept learning by weighted networks (Koponen and Nousiainen 2014); the characterization of water molecules in the high-density and low-density phases (Benzi et al. 2023; Faccio et al. 2022, 2023); the modeling of fracture networks in rocks (Santiago et al. 2016); the study of the spread of contagion in financial networks (Bartesaghi et al. 2020; Silva et al. 2017); the analysis of the influence of papers in citation networks (Zhao et al. 2019); and many others.

3.2 Total Node Communicability as a Centrality Measure

Exponential-based communicability can also be used to introduce a node centrality measure, the *total communicability* of a node, defined as the sum of the communicabilities of a node with all the nodes in the network, including itself (Benzi and Klymko 2013):

$$\mathrm{TC}(i) = \sum_{j=1}^{n} [e^{\beta A}]_{ij} = [e^{\beta A}\mathbf{1}]_i \tag{2}$$

(recall that the row sums of a matrix function $f(A)$ are the components of the vector $f(A)\mathbf{1}$). A significant advantage of this centrality measure over those based on the diagonal entries of $f(A)$ (like subgraph centrality) is the fact that using Krylov subspace methods, the action of a matrix function on a vector can be computed much faster than the n diagonal entries of $[f(A)]_{ii}$ for large n; see for example (Benzi et al. 2023).

It must be mentioned, however, that centrality measures based on the diagonal entries $[f(A)]_{ii}$ can have a higher discriminating power than those based on the row sums $[f(A)\mathbf{1}]_i$. Indeed, if a graph G is d-regular, then $A\mathbf{1} = d\mathbf{1}$ and therefore also

$f(A)\mathbf{1} = f(d)\mathbf{1}$. Hence, all nodes in G get the same centrality score and no measure of this kind is able to distinguish one node from the others (the same holds, of course, for degree and eigenvector centrality). On the other hand, there are examples of regular graphs for which the subgraph centrality $C(i) = [\mathrm{e}^A]_{ii}$ is able to distinguish the nodes (Estrada and Rodríguez-Velázquez 2005). Generally speaking, however, real-world networks are not regular and, very often, subgraph centrality and total node communicability will identify the same nodes as the most central. Thus, in the case of large networks the use of the more easily computable total communicability can be advantageous.

A global measure of the ability of a network to exchange information (broadly understood) can be obtained by summing up all the total communicabilities of the nodes in G; normalizing by the number of nodes results in the *total network communicability* (see Benzi and Klymko 2013):

$$\mathrm{TC}(G) = \frac{1}{n}\sum_{i=1}^{n}\sum_{j=1}^{n}[\mathrm{e}^{\beta A}]_{ij} = \frac{1}{n}\mathbf{1}^T\mathrm{e}^{\beta A}\mathbf{1}\,. \tag{3}$$

Not surprisingly this quantity, which can be interpreted as the *average communicability* of a node, is maximized by K_n, the complete graph with n nodes. The total network communicability can be interpreted as a measure of network connectivity, and in this regard it plays a role similar to that of the *Estrada index*:

$$EE(G) = \sum_{i=1}^{n}[\mathrm{e}^{\beta A}]_{ii} = \mathrm{Tr}\,(\mathrm{e}^{\beta A})\,,$$

which is, however, more expensive to compute. Both measures can be used to compare different network structures (with the same number of nodes and edges), for example to design highly efficient networks, see the next subsection.

3.3 Network Modification Techniques

Network efficiency and robustness are of great importance in the design and realization of actual networks, both in nature and in different fields of engineering. A network with high communicability is likely to be efficient in the routing of messages or in the transportation of goods, and also to be robust against localized loss of connectivity (e.g., edge removal) due either to random accidents or to deliberate, malicious attacks. In some situations high connectivity can have undesirable effects, e.g., in the spreading of diseases, financial crises or computer viruses. In public health campaigns and law enforcement or anti-terrorism operations, it is desirable to disrupt or weaken an existing highly connected network. Highly sparse networks that display excellent connectivity properties are known in the computer science literature as *expander graphs*; we refer to Hoory et al. (2006) for an outstanding survey.

A natural application of total network communicability and similar global connectivity measures is in the comparison of different network designs, or in the modification of an existing network in order to achieve a desired goal. The following problems are often considered:

1. *Network rewiring*: given a sparse network $G = (V, E)$ with $|E| = m$, choose which k existing edges ($k \ll m$) to rewire so as to increase, or decrease, the total network communicability as much as possible.
2. *Network updating*: given $G = (V, E)$ as above and a budget of $k \ll m$ edges, choose which k pairs of unconnected nodes in G to connect so as to increase the total network communicability as much as possible.
3. *Network downdating*: given G as above, choose which k existing edges ($k \ll m$) to delete so as to decrease the total communicability as little or as much as possible; the first problem corresponds to the goal of having similar connectivity at a lower cost (fewer edges), the second to the goal of disrupting or weakening an existing network in order to drastically reduce its effectiveness with minimal effort.

In all these problems, the total network communicability can be used as an objective function $f : G \longrightarrow \mathbb{R}$ to evaluate the relative effectiveness of different rewiring, updating, or downdating strategies. This is not the only measure of connectivity available; for example, the spectral radius of A, the algebraic connectivity or the Estrada index can also be used, and these measures are all correlated. A nice feature of the total communicability is that it is easy to approximate, often at a cost of $O(n)$ (i.e., linear in the number of nodes). This fact is exploited in Arrigo and Benzi (2016a), where several heuristics are implemented and compared in the solution of the updating/downdating problems described above (the rewiring problem is similar and can be dealt with using similar techniques). These heuristics only require the identification of a small fraction of nodes in G having the highest centrality (for example, eigenvector or total communicability centrality) and are faster, sometimes by orders of magnitude, than previously proposed methods. As shown in Arrigo and Benzi (2016a), a large increase in total communicability (as well as in other measures) is obtained by connecting highly central nodes that are not already connected by an edge; conversely, deleting edges that connect highly central nodes tends to induce large drops in total communicability. If the goal is to delete as many edges as possible without disconnecting the network and with minimal decrease in total communicability, the best strategy is the removal of edges connecting peripheral nodes (i.e. nodes not in the subset of highly central nodes). The connectivity of the network after each edge removal can be checked in time that is typically linear in n, for a sparse network; see Arrigo and Benzi (2016a) and the references therein for details.

Edge rewiring, addition and deletion translate into low-rank modifications of the adjacency matrix. The problem of updating/downdating a matrix function after a low-rank change has been investigated in Beckermann et al. (2018) and Pozza and Tudisco (2018), with an eye to applications in network analysis, such as assessing the stability of node rankings under network modifications.

3.4 Communicability Distance

Communicability between nodes can also be used to define a metric (on undirected graphs) which is often more useful than the standard (geodesic) distance. Estrada (2012a, 2012c) has shown that letting

$$d_c(i,j) = \sqrt{C(i,i) + C(j,j) - 2C(i,j)}\,, \quad \text{where} \quad C(i,j) = [\mathrm{e}^A]_{ij}\,, \qquad (4)$$

defines a distance on the set of nodes of an undirected graph G. To see this, let $A = QDQ^T$ be the spectral decomposition of the adjacency matrix A, and let $\mathbf{u}_j$ denote the jth column of Q^T. Letting $\mathbf{x}_j = \mathrm{e}^{D/2}\mathbf{u}_j$, we have

$$d_c(i,j)^2 = (\mathbf{x}_i - \mathbf{x}_j)^T(\mathbf{x}_i - \mathbf{x}_j) = \|\mathbf{x}_i - \mathbf{x}_j\|_2^2\,,$$

showing that $d_c(i,j)$ is just the Euclidean distance of the vectors $\mathbf{x}_i, \mathbf{x}_j \in \mathbb{R}^n$. A similar distance based on the resolvent $(I - \alpha A)^{-1}$ instead of the matrix exponential has been introduced in Chebotarev (2012).

The exponential-based communicability distance has several interesting applications, for example in the analysis of urban traffic modeling (Akbarzadeh and Estrada 2018; Silver et al. 2018). The related notion of *communicability angles* has been shown to be able to identify the critical (i.e., most diffusive) links in consensus dynamics (Estrada et al. 2015). A notion of *spatial efficiency* based on the communicability geometry is introduced and applied to a variety of real-world networks in Estrada and Hatano (2016). Extensions of communicability geometry to multiplex networks are described in Estrada (2019), with applications to the study of the neuronal network of the worm *C. elegans*.

3.5 Communicability in Digraphs

In the case of directed networks it is necessary to take into account the directionality of communication between nodes. A simple approach is to define the communicability of two nodes as was done in the undirected case, via (1). The lack of symmetry in A, and therefore in e^A (or, more generally, in $f(A)$) is just a reflection of the fact that in a directed graph, sending information from node i to node j may be easier (or harder) than from node j to node i. Taking row sums of $f(A)$ corresponds to a total communicability measure that corresponds to the centrality of nodes as *hubs* (i.e., broadcasters of information), while taking column sums of $f(A)$ results in a centrality measure of nodes as *authorities* (i.e., receivers of information). Note that using the diagonal entries (which are more expensive to compute) does not allow one to distinguish these two roles played by the nodes.

In some situations it is desirable to distinguish further between four types of communicability: broadcaster-to-receiver, broadcaster-to-broadcaster, receiver-to-

receiver, and receiver-to-broadcaster. Such measures have been first introduced in Benzi et al. (2013), using the bipartite model of a directed graph described in Sect. 2. Let

$$\mathcal{A} = \begin{bmatrix} 0 & A \\ A^T & 0 \end{bmatrix} \tag{5}$$

be the adjacency matrix of the bipartite graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ obtained from the original digraph with adjacency matrix A. In this model, the first n nodes contained in $\mathcal{V}$ are regarded as the original nodes of the digraph when they play the role of broadcasters of information, while the last n copies contained in $\mathcal{V}$ correspond to the same nodes regarded as receivers.

As shown in Benzi et al. (2013, Proposition 1), the exponential of the symmetric matrix $\mathcal{A}$ is given by

$$\mathrm{e}^{\mathcal{A}} = \begin{bmatrix} \cosh(\sqrt{AA^T}) & U \sinh(\Sigma) V^T \\ V \sinh(\Sigma) U^T & \cosh(\sqrt{A^T A}) \end{bmatrix}, \tag{6}$$

where $A = U \Sigma V^T$ is an SVD of A. The entries of this matrix are nonnegative and may be used to quantify how effectively the nodes communicate when they are acting as broadcasters or receivers of information in G. Specifically, it is shown in Benzi et al. (2013) that the main diagonal of the first diagonal block $\cosh(\sqrt{AA^T})$ contains the centralities of the nodes in the original network in their role of hubs, whereas the diagonal entries of the second block $\cosh(\sqrt{A^T A})$ provide the centralities for the nodes in their role of authorities. When the largest singular value of A is well-separated from the remaining ones, these rankings are close to those given by Kleinberg's HITS algorithm (Kleinberg 1999); see Benzi et al. (2013). Similarly to the off-diagonal entries of the matrix exponential of an undirected graphs, the off-diagonal entries of these diagonal blocks are measures of the communicability of pairs of nodes, both acting as broadcasters (respectively, receivers) of information. Finally, the entries in the off diagonal block $U \sinh(\Sigma) V^T$ (a generalized matrix function!) and its transpose $V \sinh(\Sigma) U^T$ provide information on the communicability of pairs of nodes considered as hub-authority pairs.

As before, one can also define global communicability measures for digraphs that take into account the dual role of each node in G. Indeed, the *total hub communicability* and *total authority communicability* of G, defined as $\mathrm{T_h C}(A) = \mathbf{1}^T \cosh(\sqrt{AA^T})\mathbf{1}$ and $\mathrm{T_a C}(A) = \mathbf{1}^T \cosh(\sqrt{A^T A})\mathbf{1}$, respectively, account for the overall ability of the network of exchanging information when all its nodes are playing the same role of broadcasters ($\mathrm{T_h C}(A)$) or receivers ($\mathrm{T_a C}(A)$). Using these measures, network updating/downdating strategies based on edge modifications have been introduced in Arrigo and Benzi (2016b).

4 Temporal Communicability

Many real-life complex systems evolve in time: taking this additional feature into account leads to models based on *temporal networks*. Given a (fixed) set of n nodes, a temporal network is an ordered sequence $\{G^{[k]}\}_{k=1,\ldots,M}$ of graphs sharing the given set of nodes. For simplicity, the graphs here are assumed to be simple, undirected, and unweighted. Each graph $G^{[k]}$ records the state of the network at time t_k, where $t_1 < t_2 < \cdots < t_M$ are time points, and is represented by an associated symmetric adjacency matrix $A^{[k]}$.

Communicability measures based on counting walks can be extended to temporal networks through the use of *dynamic walks*. A dynamic walk is a sequence of edges connecting nodes in the network, with the added constraint that the sequence of edges must respect the time ordering. Nodes participating in many dynamic walks are capable of communicating well with other nodes in the network, and can therefore spread or receive information effectively not only across a given graph but also over time.

Denote with $\rho(A^{[k]})$ the spectral radius of the kth adjacency matrix, and by $\rho^* = \max_k\{\rho(A^{[k]})\}$ the maximum spectral radius over all the adjacency matrices. The *dynamic communicability matrix* is defined in Grindrod et al. (2011) as

$$Q = (I - \alpha A^{[1]})^{-1}(I - \alpha A^{[2]})^{-1} \cdots (I - \alpha A^{[M]})^{-1}, \tag{7}$$

where the parameter α satisfies $0 < \alpha < 1/\rho^*$, so that each resolvent in (7) can be expanded in a convergent power series in the corresponding adjacency matrix. Writing each resolvent as a geometric series and expanding the product in (7), we see that Q contains all terms of the form

$$\alpha^{\ell}(A^{[t_{k_1}]}A^{[t_{k_2}]} \cdots A^{[t_{k_\ell}]}), \tag{8}$$

where $t_{k_1} \le t_{k_2} \le \cdots \le t_{k_\ell}$. Each entry (i, j) in the product $A^{[t_{k_1}]}A^{[t_{k_2}]} \cdots A^{[t_{k_\ell}]}$ counts the number of dynamic walks of length ℓ from node i to node j, where the k-th edge of the walk comes from time-step t_k. Hence, Q_{ij} is a weighted sum of dynamic walks of all possible lengths from node i to node j, where walks of length ℓ are weighted by a factor α^{ℓ}. Hence, Q_{ij} is a measure of communicability between nodes i and j, with node i in the role of broadcaster and node j as the receiver. The i-th row sum

$$\mathrm{BC}(i) = \sum_{j=1}^{n} Q_{ij} = [Q \cdot \mathbf{1}]_i$$

is a measure of how well node i broadcasts information to the rest of the network, and is a measure of *broadcast centrality*. On the other hand, the j-th column sum

$$\mathrm{RC}(j) = \sum_{i=1}^{n} Q_{ij} = [Q^T \cdot \mathbf{1}]_j$$

measures how well node j receives information from all other nodes in the network and provides a measure of *receive centrality*. It is worth noting that, in general, the broadcast and receive centrality of each node are different, since the matrix Q is not symmetric. Observing that each adjacency matrix is symmetric, we have

$$Q^T = \left((I - \alpha A^{[1]})^{-1}(I - \alpha A^{[2]})^{-1} \cdots (I - \alpha A^{[M]})^{-1}\right)^T = \\ = (I - \alpha A^{[M]})^{-1}(I - \alpha A^{[M-1]})^{-1} \cdots (I - \alpha A^{[1]})^{-1},$$

showing that broadcast and receive centralities are related by a reversal of the time ordering. An application of dynamic communicability to a real-world temporal network arising in the study of a contagion model is described in Chen et al. (2017).

It is interesting to note that using the matrix exponential instead of the resolvent produces a temporal communicability matrix that fails to satisfy certain combinatorial and consistency requirements: as a consequence, not all walks of the same length are given equal weight, as shown in Arrigo et al. (2022).

5 Modeling Diffusion on Graphs

Many types of phenomena in network analysis can be modeled as diffusion processes on graphs. Diffusion, both standard and non-local, yields another perspective on network connectivity and communicability.

5.1 Functions of the Graph Laplacian: The Heat Equation

So far, the main focus of this survey has been on functions of the adjacency matrix, which have a direct interpretation in terms of graph walks. In many situations, however, it is natural to consider functions of $L = D - A$, the graph Laplacian of G. More specifically, the Laplacian (or one of its normalized versions) is used in the study of diffusion processes and random walks on graphs, both time-discrete and time-continuous. Such random walks represent an essential tool for exploring network structure. Similarly, the behavior of the solution of evolution equations involving graph Laplacians, such as the heat equation, provide important information on the network. Among the simplest such equations is the initial value problem for the heat equation on G:

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = -L\,\mathbf{x}, \quad t > 0; \quad \mathbf{x}(0) = \mathbf{x}_0. \tag{9}$$

This is a system of linear ordinary differential equations, where the unknown vector-valued function $\mathbf{x}(t)$ can be interpreted as the concentration of some substance on the nodes of G, or maybe as the "temperature" of each node, at time t. The initial distribution $\mathbf{x}_0$ is usually a nonnegative vector, often normalized so that $\|\mathbf{x}_0\|_1 = 1$. In this case, it can be interpreted as a probability distribution on the nodes of G. It is well known that the solution of (9) is unique and is given for all $t \geq 0$ by

$$\mathbf{x}(t) = \mathrm{e}^{-tL}\mathbf{x}_0 = S(t)\,\mathbf{x}_0\,,$$

where we have set $S(t) = \mathrm{e}^{-tL}$.

The family $\{S(t)\}_{t\geq 0}$ forms a continuous one-parameter commutative semigroup with $-L$ as its infinitesimal generator, i.e.,

$$S'(0) = \lim_{t\to 0+} \frac{1}{t}\,(S(t) - I) = -L\,.$$

It is easily seen that for all $t \geq 0$, $S(t)$ is a *doubly stochastic* matrix; i.e., it is a nonnegative matrix with row and columns sums equal to 1 (recall that $S(t)$ is symmetric, since G is undirected). This implies that for all $t > 0$ the solution vector $\mathbf{x}(t) = S(t)\mathbf{x}_0$ is a probability distribution on G; in particular, the ℓ^1-norm of $\mathbf{x}(t)$ remains constant and equal to 1. Hence, the evolution of $\mathbf{x}(t)$ describes a continuous time random walk on G. For a connected graph, L is irreducible and there is a unique steady-state distribution $\mathbf{x}_* = \lim_{t\to\infty} \mathbf{x}(t)$. This asymptotic distribution is easily found to be the unique positive solution to the homogeneous linear system $L\mathbf{x} = \mathbf{0}$ satisfying $\|\mathbf{x}_*\|_1 = 1$, i.e., the uniform distribution $\mathbf{x}_* = \frac{1}{n}\mathbf{1}$. In other words, at steady state the system is in "thermal equilibrium". The rate of convergence of $\mathbf{x}(t)$ to $\mathbf{x}_*$ depends on the topology of the graph and is largely determined by the algebraic connectivity of G. This can be seen by considering the eigendecomposition of the graph Laplacian:

$$L = Q\Lambda Q^T = \sum_{k=1}^{n} \lambda_k\,\mathbf{q}_k\mathbf{q}_k^T\,. \tag{10}$$

For a connected graph the eigenvalues of L satisfy $0 = \lambda_1 < \lambda_2 \leq \cdots \leq \lambda_n$ and the eigenvector associated with the simple zero eigenvalue, normalized in the ℓ^2-norm, is $\mathbf{q}_1 = \frac{1}{\sqrt{n}}\mathbf{1}$. Therefore

$$\mathrm{e}^{-tL}\mathbf{x}_0 = \frac{1}{n}(\mathbf{1}^T\mathbf{x}_0)\mathbf{1} + \sum_{k=2}^{n} \mathrm{e}^{-t\lambda_k}(\mathbf{q}_k^T\mathbf{x}_0)\mathbf{q}_k \longrightarrow \frac{1}{n}\mathbf{1} \quad \text{for} \quad t\to\infty \tag{11}$$

if $\mathbf{x}_0$ is nonnegative and has unit 1-norm.

It is clear from (11) that the rate of convergence to equilibrium depends primarily on the smallest nonzero eigenvalue λ_2 of L, i.e., on the algebraic connectivity of G. The larger is λ_2, the faster the convergence to equilibrium. Among al possible graphs with n nodes the fastest convergence to steady-state is obtained, of course, for

the complete graph K_n nodes, in which every node is connected to any other node. Indeed, the Laplacian of this graph has only two distinct eigenvalues, 0 and n (the maximum possible value), and equilibrium is reached extremely fast. The already mentioned expander graphs provide more interesting examples of highly connected graphs; these are graphs that are at the same time highly sparse and have a relatively large value of λ_2.

The use of diffusion models based on the *fractional graph Laplacian* has also been proposed, due to its ability to generate random walks that can efficiently explore large networks (Riascos and Mateos 2014, 2021). For $\alpha \in (0, 1)$, the fractional graph Laplacian is defined by

$$L^\alpha = Q\Lambda^\alpha Q^T , \tag{12}$$

where Λ^α is the diagonal matrix with entries given by $\lambda_1^\alpha = 0, \lambda_2^\alpha, \ldots, \lambda_n^\alpha$ (cf. (10)). In this definition, the principal (positive) branch of the αth root λ_i is chosen. If G is connected, L^α is a full matrix: in other words, L^α is a *non-local operator*. It turns out that the matrix L^α, like L itself, is a singular M-matrix. If Δ denotes the diagonal matrix containing the diagonal entries of L^α, the matrix $S = I - L^\alpha \Delta^{-1}$ is column stochastic and is the transition matrix of a discrete time random walk on G. Since S is dense, the random walk on G is not constrained to move from node to neighboring node, but has a nonzero probability of "jumping" from one node to any other node, including very distant ones. Furthermore, the probability of making long-range jumps may be non-negligible, making the random walk associated with $S = I - L^\alpha \Delta^{-1}$ more efficient in the exploration of a large and sparse network compared to the "local" random walk associated with $I - LD^{-1}$, especially when the diameter of G is not small. Similar considerations apply to the continuous-time non-local diffusion process

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = -L^\alpha \mathbf{x}, \quad t > 0, \quad \mathbf{x}(0) = \mathbf{x}_0 , \tag{13}$$

or the analogous one based on the normalized fractional Laplacian. These results can be extended, at least in part, to directed graphs using the nonsymmetric Laplacian $L_{\text{out}} = D - A$ (where D is the diagonal matrix of outdegrees); see Benzi et al. (2020). (It should be mentioned that a different and sometimes advantageous approach to speeding up network navigation has been proposed in Estrada et al. (2017, 2018) by means of the *k-path Laplacian*, a natural generalization of the graph Laplacian first introduced in Estrada (2012b).)

It is natural to use the exponentials e^{-tL} (or e^{-tL^α}, for $0 < \alpha < 1$) to define diffusion-based communicability measures. In the case of a d-regular graph, for which $L = dI - A$, the Laplacian-based communicability between nodes i and j is just

$$[\mathrm{e}^{-tL}]_{ij} = \mathrm{e}^{-td}[\mathrm{e}^{tA}]_{ij} ,$$

and therefore it reduces, up to a node-independent factor, to the (standard) exponential-based communicability (1), with $\beta = t$. On the other hand for non-regular graphs, or in the case of the fractional Laplacian, this commuicability mea-

sure is different from (1). It has a simple physical interpretation: it is the amount of substance found on node j at time t given that all the substance was initially concentrated on node i. In terms of (continuous time) random walks, it is the probability of being at node j at time t starting from node i at time $t = 0$.

For a connected, undirected graph, the diagonal entries of $S(t) = \mathrm{e}^{-tL}$ decrease monotonically from the value 1 for $t = 0$ to the asymptotic value $\frac{1}{n}$ for $t \to \infty$, while the off-diagonal entries increase, also monotonically, from the value 0 for $t = 0$ to the value $\frac{1}{n}$ as $t \to \infty$ (see (11). To prove monotonicity, note that

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e}^{-tL} = -L\mathrm{e}^{-tL} = -\sum_{k=2}^{n} \lambda_k \mathrm{e}^{-t\lambda_k}\, \mathbf{q}_k \mathbf{q}_k^T \,,$$

therefore

$$\frac{\mathrm{d}}{\mathrm{d}t}[\mathrm{e}^{-tL}]_{ii} = -\sum_{k=2}^{n} \lambda_k \mathrm{e}^{-t\lambda_k}\, q_k(i)^2 < 0\,,$$

whereas for $i \neq j$ there holds for all $t > 0$

$$\frac{\mathrm{d}}{\mathrm{d}t}[\mathrm{e}^{-tL}]_{ij} = -\sum_{k=2}^{n} \lambda_k \mathrm{e}^{-t\lambda_k}\, q_k(i) q_k(j) > -\sum_{k=2}^{n} \lambda_k\, q_k(i) q_k(j) = -[L]_{ij} \geq 0\,.$$

Clearly, relatively large values of $[\mathrm{e}^{-tL}]_{ij}$ for small t indicate that nodes i and j exhibit good communicability. In other words, a fast convergence of $[\mathrm{e}^{-tL}]_{ij}$ to the limit $\frac{1}{n}$ indicates a good communicability between the two nodes. Similar considerations apply if L is replaced by L^α with $0 < \alpha < 1$.

6 Computational Aspects

For small to moderate size networks (say, up to a few thousand nodes), it is possible to compute each individual entry of the matrix function $f(A)$ or $f(L)$ using a variety of methods. For undirected graphs, using the eigendecomposition of the matrix is often the easiest way to carry out the desired calculation. For directed graphs the computation of matrix functions is somewhat more delicate, but a number of techniques are available for handling small to moderate size problems, see Higham (2008). Similarly, for generalized matrix functions one can simply compute the (compact) SVD of A to obtain $f^\diamond(A)$.

In the case of large-scale networks, on the other hand, it is generally impossible to compute every entry of a matrix function. Even if A is sparse, the matrix $f(A)$ is generally a dense matrix and therefore impossible to store for large n. Fortunately, in the case of large-scale graphs it is seldom required to compute all the entries of a matrix function; as we have seen, typical calculations require computing the

action of a matrix function on a vector, or a subset of selected entries (for example the ones on the main diagonal). For these tasks there are efficient algorithms which use the matrix A (or L) only in the form of matrix-vector products. Moreover, such computations may not need to be very accurate: for instance, centrality measures are generally used to identify the top-ranked nodes, so there is no need to compute the centrality indices of all the nodes with high accuracy. Bounds on selected entries of $f(A)$ are often sufficient. Methods based on quadrature rules and the Lanczos process (Golub and Meurant 2010) can be used to obtain bounds or estimates on the individual entries of $f(A)$ (see, e.g., Benzi and Boito 2010), while computing the action of a matrix function on a vector can be done efficiently by means of Krylov subspace methods. In the case of generalized matrix functions, efficient techniques have been developed in Arrigo et al. (2016). We refer to Benzi and Boito (2020) for a more detailed discussion of these aspects.

7 Conclusions

As shown in this concise survey, communicability is by now an established tool in the analysis and design of large, complex networks from a variety of domains, with new applications being found all the time. Efficient algorithms exist for the computation of communicability measures, based on state-of-the art developments in numerical linear algebra. Progress in this field will bring about the ability to perform computations on networks of increasing size and complexity.

Future work is likely to focus on the development of matrix and tensor functions arising in the study of temporal networks, and on the extension of existing techniques to more sophisticated network models, such as multiplex and other multilayer networks. The case of temporal networks is also in need of further development.

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