

ON THE STABILITY OF NETWORK INDICES DEFINED BY MEANS OF MATRIX FUNCTIONS*

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Abstract. Identifying important components in a network is one of the major goals of network analysis. Popular and effective measures of importance of a node or a set of nodes are defined in terms of suitable entries of functions of matrices $f(A)$. These kinds of measures are particularly relevant as they are able to capture the global structure of connections involving a node. However, computing the entries of $f(A)$ requires a significant computational effort. In this work we address the problem of estimating the changes in the entries of $f(A)$ with respect to changes in the edge structure. Intuition suggests that, if the topology of connections in the new graph \tilde{G} is not significantly distorted, relevant components in G maintain their leading role in \tilde{G} . We propose several bounds giving mathematical reasoning to such intuition and showing, in particular, that the magnitude of the variation of the entry $f(A)_{k\ell}$ decays exponentially with the shortest-path distance in G that separates either k or ℓ from the set of nodes touched by the edges that are perturbed. Moreover, we propose a simple method that exploits the computation of $f(A)$ to simultaneously compute the all-pairs shortest-path distances of G , with essentially no additional cost. As the nodes whose edge connection tends to change more often or tends to be more often affected by noise have marginal role in the graph and are distant from the most central nodes, the proposed bounds are particularly relevant.

Key words. Centrality indices, stability, decay bounds, geodesic distance, Faber polynomials.

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1. Introduction. Networks and datasets of large dimension arise naturally in a number of diversified applications, ranging from biology and chemistry to computer science, physics and engineering, [10, 1, 27, 37, 15, 40, 13] e.g. Being able to recognize important components within a vast amount of data is one of the main goals of the analysis of networks. As a network can be uniquely identified with an adjacency matrix, many efficient mathematical and numerical strategies for revealing relevant components employ tools from numerical linear algebra and matrix analysis. Important examples include locations of clusters of data points [17, 36, 39, 29], detection of communities [20, 21, 38] and ranking of nodes and edges [18, 7, 32].

To address the latter range of problems, a popular approach is to employ the concepts known as centrality and communicability of the nodes of a network. These two attributes describe a certain measure of importance of nodes and edges in a network. Many commonly used and successful models for communicability and centrality measures are based on matrix eigenvectors. These models quantify the importance of a node in terms of the importances of its neighbors, thus relying on the local behavior around the node. In this work we focus on another common class of models for centrality and communicability measures based, instead, on matrix functions [23, 11]. This latter class of models is particularly informative and effective as, unlike the eigenvector-based models previously mentioned, the use of matrix functions allows to capture the global structure of connections involving a node. However the matrix function approach requires a significantly larger computational cost. This is particularly prohibitive for example when the network changes and the important

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components have to be updated or when the network structure is affected by noise and the importance of the components can be biased. In principle each change in the network requires a complete re-computation of the matrix function to obtain the updated measure. However, in many applications one needs to know only “who are” the first few most important nodes in the graph and how stable they are with respect to edge perturbations. Moreover, the nodes whose edge connection tends to change more often or is more likely to be affected by noise are those having a marginal role in the graph [32].

Intuition suggests that, if the topology of connections in the new “perturbed” graph \tilde{G} is not significantly distorted, relevant components in the original graph G maintain their leading role in \tilde{G} . In this paper we provide mathematical support for this intuition by analyzing the stability of network measures based on matrix functions with respect to edge changes. By exploiting the theory of Faber polynomials and the recent literature on functions of banded matrices [44, 42, 9, 8, 6], we propose a number of bounds showing that the magnitude of the variation of the centrality of node k or the communicability between nodes k and ℓ decays exponentially with the distance in the graph that separates either k or ℓ from the set of nodes touched by the edges that are perturbed. This implies, for example, that if changes in the edge structure occur in a relatively small and peripheral network area – in the sense that the perturbed edges involve only nodes being far from the most relevant ones – then the set of leading components remains unchanged.

We organize the discussion as follows: The next section reviews some central concepts and properties we shall use alongside the present work, in particular the notions of f -centrality and f -communicability. Section 3 is devoted to give details about our motivating ideas. Then, in Section 4, we review the relevant theory about Faber polynomials. In Section 5 we state and prove our main results where we provide a number of bounds on the absolute variation of the centrality and the communicability measures of nodes k and ℓ based on the matrix function $f(A)$ when some edges are modified in G . The bounds are given in terms of the distances in G that separate k and ℓ from the set of perturbed edges and for two important network matrices: the adjacency matrix and the normalized (random walk) adjacency matrix. We give particular attention to the case of the exponential and the resolvent function, as they often arise in the related literature on complex networks. We also provide a simple algorithm that exploits the computation of the entries of $f(A)$ to simultaneously address the all-pairs shortest-path distances of the graph, at essentially no additional cost. Finally, in Section 6, we provide several numerical experiments where the behavior of the proposed computational strategy as well as the one of the proposed bounds is tested on some example networks, both synthetically generated and borrowed from real-world applications.

2. Network properties and matrix functions. One of the major goals of data analysis is to identify important components in a network $G = (V, E)$ by exploiting the topological structure of connections between nodes. In order to address this matter from the mathematical point of view one needs a quantitative definition of the importance of a node k or a pair of nodes (k, ℓ) , thus leading to concepts such as the nodes centrality and the nodes communicability. Despite these quantities have a long history, dating back to the early 1950s, recent years have seen the introduction of many new centrality scores based on the entries of certain function of matrices [7, 18, 19, 26]. The idea behind such metrics is to measure the relevance of a component by quantifying the number of subgraphs of G that involve a certain node or

group of nodes. In order to better perceive these concepts, we first introduce some preliminary graph notation.

Let $G = (V, E, \omega)$ be a (weighted) graph where $V = \{1, \dots, N\}$ is the finite set of nodes, $E \subseteq V \times V$ the set of edges and $\omega : E \rightarrow \mathbb{R}_+$ a positive weight function. Given two nodes $k, \ell \in V$, an ordered sequence of edges $\mathcal{W} = \mathcal{W}(k, \ell) = \{e_1, \dots, e_r\} \subseteq E$ is a walk in G from k to ℓ , if k is the starting point of e_1 , ℓ is the endpoint of e_r and, for any $i = 1, \dots, r - 1$, the endpoint of e_i is the starting point of e_{i+1} . The length of a walk is the number of edges forming the sequence (repetitions are allowed) and is denoted by $|\mathcal{W}|$. The length of the shortest walk from k to ℓ is called the (geodesic or shortest-path) distance in G from k to ℓ and is denoted hereafter by $d_G(k, \ell)$. If there is no walk in G connecting the pair (k, ℓ) , we set $d_G(k, \ell) = +\infty$. The diameter of G is the longest shortest-path distance between any two nodes.

A graph is said to be *strongly connected* if $d_G(k, \ell)$ is a finite number, for any two possibly coinciding nodes k and ℓ . Note that, in a strongly connected undirected graph without self-loops, $d_G(k, k) = 2$ for any $k \in V$. Given a set $S \subseteq V$ and a node $k \notin S$, we let

$$d_G(k, S) = \min_{s \in S} d_G(k, s) \quad \text{and} \quad d_G(S, k) = \min_{s \in S} d_G(s, k).$$

The weight of a walk \mathcal{W} is defined by

$$\omega(\mathcal{W}) = \prod_{e \in \mathcal{W}} \omega(e).$$

This quantity has a natural matrix representation. Consider the adjacency matrix $A = (a_{ij}) \in \mathbb{R}_+^{N \times N}$ of $G = (V, E, \omega)$, defined by

$$a_{ij} = \begin{cases} \omega(e) & \text{if } i, j \text{ are starting and ending points of } e \in E, \text{ respectively} \\ 0 & \text{otherwise} \end{cases}.$$

Thus, for any walk $\mathcal{W} = \mathcal{W}(k, \ell)$, there exists a sequence of nodes u_1, \dots, u_n , such that

$$(2.1) \quad \omega(\mathcal{W}) = a_{ku_1} a_{u_1 u_2} \cdots a_{u_{n-1} u_n} a_{u_n \ell}.$$

The preceding formula shows that the powers of the adjacency matrix A can be used to count the “weighted number” of walks of different lengths in G . More precisely, if n is a positive integer and $\Omega_n(k, \ell) = \{\mathcal{W}(k, \ell) : |\mathcal{W}(k, \ell)| = n\}$ is the set of walks from k to ℓ of length exactly n , then one can easily observe that $(A^n)_{k\ell} = \sum_{\mathcal{W} \in \Omega_n(k, \ell)} \omega(\mathcal{W})$. It is worth noting that, regardless of the edge weight function $\omega : E \rightarrow \mathbb{R}_+$, such characterization of the entries of A^n implies that

$$(2.2) \quad (A^n)_{k\ell} = 0, \quad \text{for every } n < d_G(k, \ell).$$

This property will be one of the key tools of our forthcoming analysis.

A matrix function can be defined in a number of different but equivalent ways (see [28] e.g.). Here we adopt the power series representation as it has a direct interpretation in terms of network properties: Given a matrix A and a function $f : \mathbb{C} \rightarrow \mathbb{C}$ being analytic on a region $\Omega \subseteq \mathbb{C}$ containing the spectrum of A , we let $f(A) = \sum_{n \geq 0} \theta_n A^n$, where $f(z) = \sum_{n \geq 0} \theta_n z^n$ is the power series representation of f in Ω . Given a function f , the importance of a node in a network can be quantified

in terms of certain entries of the matrix $f(A)$. This idea was firstly introduced by Estrada and Rodriguez-Vasquez in [19], for the particular choice $f(z) = \exp(z)$, and then developed and extended in many subsequent works, see f.i. [7, 2, 18] and the references therein. We thus adopt the following definition:

DEFINITION 2.1. *Let $A \in \mathbb{R}_+^{N \times N}$ be the adjacency matrix of a graph $G = (V, E, \omega)$. Let $f : \mathbb{C} \rightarrow \mathbb{C}$ be analytic on a set Ω containing the spectrum of A and such that, for $z \in \Omega$, $f(z) = \sum_{n \geq 0} \theta_n z^n$ with $\theta_n > 0$. The f -centrality of the node $k \in V$ is the quantity $f(A)_{kk}$. The f -communicability from node k to node ℓ is the quantity $f(A)_{k\ell}$.*

The centrality of a node is a measure of its importance as a component in the graph. Using (2.1) one easily realizes that the quantity $f(A)_{kk} = \sum_{n \geq 0} \theta_n (A^n)_{kk}$ is a weighted sum of the weights of all the possible closed walks from k to itself, the weights being given by the positive coefficients θ_n . If $f(A)_{kk}$ is large, then many closed walks consistently weighted pass by the node $k \in V$, and thus k can be recognized as an important component in G .

The communicability of a pair of nodes is a measure of the robustness of communication between the pair. Arguing as before, we can infer that, if $f(A)_{k\ell}$ is large, then many walks with a consistent weight start in k and end up in ℓ . Thus the connection between these two nodes is likely to be not affected by unpredicted breakdowns in the edge structure of the network, that is any message sent from k toward ℓ is very likely to reach its destination.

As mentioned before, typical choices of the function f in the context of networks analysis are the exponential and the resolvent functions [19, 18], respectively given by choosing $\theta_n = 1/n!$ or $\theta_n = \alpha^n$, where $0 < \alpha < \rho(A)$ and $\rho(A)$ is the spectral radius of A . Namely,

$$(2.3) \quad \exp(A) = \sum_{n \geq 0} \frac{1}{n!} A^n, \quad r_\alpha(A) = \sum_{n \geq 0} \alpha^n A^n = (I - \alpha A)^{-1}.$$

3. Motivations. This work is concerned with the problem of estimating the changes in the entries of $f(A)$ with respect to “small” changes in the entries of A . However, for our purposes, the concept of being small is not related with the norm nor the spectrum of the perturbation, whereas we assume that a small number of entries are modified in A via a sparse matrix δA . This form of perturbation has the following network interpretation: if A is a square nonnegative matrix of order N and $G = (V, E, \omega)$ is the graph associated with A , then adding the sparse noise $\delta A \in \mathbb{R}^{N \times N}$ to A is equivalent to adding, removing or modifying the weight of the edges in a set $\delta E \subseteq V \times V$, with $|\delta E| \ll |E|$. We obtain in this way a new graph $\tilde{G} = (V, \tilde{E}, \tilde{\omega})$, where $\tilde{E} = E \cup \delta E$ and $\tilde{\omega} : \tilde{E} \rightarrow \mathbb{R}_+$ coincides with ω on $\tilde{E} \setminus \delta E$. Although the norm of δA can be arbitrarily large, intuition suggests that, if the topology of connections in the new graph \tilde{G} is not significantly distorted, relevant components in G maintain their leading role in \tilde{G} . Providing mathematical evidences in support of this intuition is one of the main objectives of the present work, where we show that the magnitude of the variation of the entry $f(A)_{k\ell}$ decays exponentially with the distance in G that separates either k or ℓ from the set of nodes touched by the new edges δE .

This is of particular interest when addressing measures of f -centrality or f -communicability for large networks. To fix ideas, let us focus on the centrality case and consider the example case where the network represents a data set where interactions evolve in time. Let A be the adjacency matrix of the current graph G and

$\tilde{A} = A + \delta A$ be the adjacency of the graph \tilde{G} in the next time stamp. Computing the diagonal entries of $f(A)$ is a costly operation and, in principle, knowing the importance of nodes in \tilde{G} requires computing the entries of $f(\tilde{A})$ almost from scratch. On the other hand, very often one needs to know only “who are” the first few most important nodes in the graph, whereas the nodes whose edge connection tends to change more often are those having a marginal role in the graph [32], and typically we expect that the distance in G from important nodes and nodes having a marginal role is large.

To gain further intuition, in what follows we briefly consider an example model where an edge exists from node i to node j with a probability being exponentially dependent on the difference between the importances of i and j . This is a form of “logistic preferential attachment” model, where edge distribution follows an exponential rather than a more common power law. The reasons for this choice are purely expository, as the logistic function simplifies the computations we discuss below. Let $c : V \rightarrow [0, 1]$ be a centrality function measuring the importances of nodes. Assume that an edge from i to j exists with probability

$$\mathbb{P}(i \rightarrow j) = s_\alpha(c_j - c_i), \quad \text{where} \quad s_\alpha(x) = \frac{1}{1 + e^{-\alpha x}}.$$

The parameter $0 < \alpha \leq 1$ can be used to vary the slope of the sigmoid function s_α and thus to tune the growth rate of s_α towards 1 or 0, as x increases or decreases respectively.

This model is assuming that nodes highly ranked are very unlikely pointing to nodes with low rank, whereas the reverse implication is very likely to occur. This kind of phenomenon is relatively common in real-world networks [3] and it is at the basis of several ranking models [32].

Given a set of nodes $S \subseteq V$ let $c_S = \max_{i \in S} c_i$ be the centrality of the most influential node in S . By noting that for $x, y \in \mathbb{R}$ it holds $s_\alpha(x)s_\alpha(y) \leq s_\alpha(x + y)$, the probability $\pi_n(i, S)$ that there exists in G a walk of length n from i to the set S , can be bounded by

$$\pi_n(i, S) \leq \binom{N - |S|}{n} s_\alpha(c_S - c_i)$$

where $\binom{a}{b} = \frac{a!}{(a-b)!b!}$ is the binomial coefficient. We can thus bound the probability that a node i is at least n steps far from the set S as follows:

$$\mathbb{P}(d_G(i, S) > n) = \prod_{k=1}^n (1 - \pi_k(i, S)) \geq \left(1 - \binom{N - |S|}{n} s_\alpha(c_S - c_i)\right)^n.$$

Suppose for simplicity that the set of perturbed edges in \tilde{G} is a clique $\delta E = S \times S$. If the size of S is small enough and $c_i \gg c_S$, that is the node i is significantly more relevant than the nodes in S , then the above derivation shows that the probability that i is n steps far from S is large. We shall show in the forthcoming Section 5 that the absolute variation $|f(A)_{k\ell} - f(\tilde{A})_{k\ell}|$ decays exponentially with d_G . Thus, as claimed, in a model with such a preferential attachment edge distribution, it is expected that changes in the topology of edges involving low relevant nodes do not affect the ranking of the leading components.

4. Faber polynomials. In this section we review the definition of Faber polynomials and several of their fundamental properties. Faber polynomials extend the

theory of power series to sets different from the disk, and, inspired by the analysis made in [42], will be used in the next section for our main results.

Let Ω be a continuum with connected complement, and let us consider the relative conformal map ϕ satisfying the following conditions

$$\phi(\infty) = \infty, \quad \lim_{z \rightarrow \infty} \frac{\phi(z)}{z} = d > 0.$$

Hence, ϕ can be expressed by a Laurent expansion $\phi(z) = dz + a_0 + \frac{a_1}{z} + \frac{a_2}{z^2} + \dots$. Furthermore, for every $n > 0$ we have

$$(\phi(z))^n = d^n z^n + a_{n-1}^{(n)} z^{n-1} + \dots + a_0^{(n)} + \frac{a_{-1}^{(n)}}{z} + \frac{a_{-2}^{(n)}}{z^2} + \dots$$

The Faber polynomial for the domain Ω is defined by (see, e.g., [44])

$$\Phi_n(z) = dz^n + a_{n-1}^{(n)} z^{n-1} + \dots + a_0^{(n)}, \quad \text{for } n \geq 0.$$

If f is analytic on Ω then it can be expanded in a series of Faber polynomials over Ω , namely

THEOREM 4.1 ([44]). *Let f be analytic on Ω . Let ϕ be the conformal map of Ω , ψ be its inverse and Φ_j be the j -th Faber polynomial associated with ϕ . Then*

$$(4.1) \quad f(z) = \sum_{j=0}^{\infty} f_j \Phi_j(z), \quad \text{for } z \in \Omega;$$

with the coefficients f_j being defined by

$$f_j = \frac{1}{2\pi i} \int_D \frac{f(\psi(z))}{z^{j+1}} dz,$$

where D is the boundary of a neighborhood of the unit disc such that f in Ω can be represented in terms of its Cauchy integral on $\psi(D)$.

It immediately follows from the above theorem that, if the spectrum of A is contained in Ω and f is a function analytic in Ω , then the matrix function $f(A)$ can be expanded as follows (see, e.g., [44, p. 272])

$$(4.2) \quad f(A) = \sum_{j=0}^{\infty} f_j \Phi_j(A).$$

The field of values or numerical range of a matrix $A \in \mathbb{C}^{N \times N}$ is a convex and compact subset of \mathbb{C} defined by

$$\mathcal{F}(A) = \{x^* A x : x \in \mathbb{C}^N, \|x\|_2 = 1\}.$$

The following theorem, proved by Beckermann in [4, Theorem 1], will be particularly useful in the following section.

THEOREM 4.2. *Let A be a square matrix and let Ω a convex set containing $\mathcal{F}(A)$. Then for every $n \geq 1$ it holds*

$$\|\Phi_n(A)\| \leq 2,$$

being Φ_n the n -th Faber polynomial for the domain Ω , as previously defined.

5. Main results. Consider a function $f : \mathbb{C} \rightarrow \mathbb{C}$ and let k, ℓ be two nodes in V . Assume that the adjacency matrix A of $G = (V, E, \omega)$ is modified into the matrix $\tilde{A} = A + \delta A$ with associated graph \tilde{G} . As we discussed above, we are interested in a-priori estimations of the absolute variation of the entries of $f(\tilde{A})$ with respect to those of $f(A)$. To this end, in the following Sections 5.1 and 5.2, we develop a number of explicit bounds of the form

$$(5.1) \quad |f(A)_{k\ell} - f(\tilde{A})_{k\ell}| \leq \beta(\delta) \left(\frac{1}{\rho(\delta)} \right)^\delta,$$

where δ is a quantity measuring the distance in G from k and ℓ and the set of modified edges in \tilde{G} , $\beta(\delta) \rightarrow \beta > 0$ for $\delta \rightarrow +\infty$, and $\rho(\delta)$ depends on the function f and the field of values of A and \tilde{A} .

It is worthwhile pointing out that the bounds we propose depend on the distances between nodes in G , whereas no knowledge on the topology of \tilde{G} is required. This is particularly important as it allows us to formulate a simple algorithm that exploits the computations needed for computing the f -centrality or f -communities scores to simultaneously compute (or approximate) the distances between node pairs in G and thus, for each node k or pair of nodes k and ℓ , identifying via (5.1) the subareas of G whose change in the edge topology do not affect (or affect in minor part) the score $f(A)_{k\ell}$.

5.1. Upper bounds on network indices' stability. In order to derive our bounds for the stability of $f(A)_{k\ell}$ we employ the theory of Faber polynomials briefly discussed in Section 4. On top of being of self interest, the following lemmas are crucial to address our main Theorem 5.3.

LEMMA 5.1. *Let $G = (V, E, \omega)$ be a graph and $A \in \mathbb{R}_+^{N \times N}$ be its adjacency matrix. Consider the graph \tilde{G} , with adjacency matrix \tilde{A} , obtained by adding, erasing, or modifying the weights of the edges contained in $\delta E \subset V \times V$. If $S = \{s | (s, t) \in \delta E\}$ and $T = \{t | (s, t) \in \delta E\}$ are respectively the sets of sources and tips of δE , then*

$$(p_n(\tilde{A}))_{k\ell} = (p_n(A))_{k\ell},$$

for every polynomial p_n of degree $n \leq d_G(k, S) + d_G(T, \ell)$.

Proof. We prove it for the monomials $(\tilde{A}^n)_{k\ell} = (A^n)_{k\ell}$ concluding then by linearity. Since $(A^n)_{k\ell}$ is the weighted number of walks from k to ℓ of length n , $(\tilde{A}^n)_{k\ell} = (A^n)_{k\ell}$ whenever G and \tilde{G} have the same walks of length n from k to ℓ . Furthermore, a modified walk from k to ℓ in \tilde{G} must contain at least an edge from S to T . We conclude noticing that any walk from k to ℓ passing through S and T has length greater or equal to $d_G(k, S) + d_G(T, \ell) + 1$. \square

LEMMA 5.2. *Consider the assumptions of Lemma 5.1. Moreover, let Ω be a convex continuum containing $\mathcal{F}(A)$ and $\mathcal{F}(\tilde{A})$ and with connected complement. If f is an analytic function on Ω and $f(z) = \sum_{j=0}^{\infty} f_j \Phi_j(z)$ is its Faber expansion (4.1) for the domain Ω , then*

$$\left| \left(f(A) - f(\tilde{A}) \right)_{k\ell} \right| \leq 4 \sum_{j=\delta+1}^{\infty} |f_j|,$$

where $\delta = d_G(k, S) + d_G(T, \ell)$.

Proof. Since the coefficients f_j depend only on the set Ω and the function f they are the same for both the expansions (4.2) of $f(A)$ and $f(\tilde{A})$. Therefore, (4.2) gives

$$f(A) - f(\tilde{A}) = \sum_{j=0}^{\infty} f_j(\Phi_j(A) - \Phi_j(\tilde{A})).$$

By Lemma (5.1) we get

$$\left(\Phi_j(A) - \Phi_j(\tilde{A})\right)_{k\ell} = 0 \quad \text{for every } j \leq \delta.$$

Thus

$$\left(f(A) - f(\tilde{A})\right)_{k\ell} = \sum_{j=\delta+1}^{\infty} f_j \left(\Phi_j(A) - \Phi_j(\tilde{A})\right)_{k\ell}.$$

Since Ω is convex Theorem 4.2 concludes the proof. \square

The previous theorem allows for the claimed exponential decay bound on the absolute variation of the entries of $f(A)$ and $f(\tilde{A})$.

THEOREM 5.3. *Let Ω be a convex continuum containing $\mathcal{F}(A)$ and $\mathcal{F}(\tilde{A})$ and let f be analytic in Ω . Given a $\tau > 1$ let $D = D_\tau = \{z : |z| = \tau\}$ and ψ be as in the assumptions of Theorem 4.1. Then*

$$\left|\left(f(A) - f(\tilde{A})\right)_{k\ell}\right| \leq \mu_\tau(f) \frac{2}{\pi} \frac{\tau}{\tau - 1} \left(\frac{1}{\tau}\right)^{\delta+2},$$

with $\delta = d_G(k, S) + d_G(T, \ell)$ and

$$\mu_\tau(f) = \int_{D_\tau} |f(\psi(z))| dz.$$

Proof. By Lemma 5.2 we get $\left|\left(f(A) - f(\tilde{A})\right)_{k\ell}\right| \leq 4 \sum_{j=\delta+1}^{\infty} |f_j|$. The Faber coefficients f_j are given by

$$f_j = \frac{1}{2\pi i} \int_{D_\tau} \frac{f(\psi(z))}{z^{j+1}} dz.$$

Thus $|f_j| \leq \frac{1}{2\pi\tau^{j+1}} \mu_\tau(f)$, and

$$\begin{aligned} \left|\left(f(A) - f(\tilde{A})\right)_{k\ell}\right| &\leq \mu_\tau(f) \frac{2}{\pi} \sum_{j=\delta+1}^{\infty} \left(\frac{1}{\tau}\right)^{j+1} \\ &= \mu_\tau(f) \frac{2}{\pi} \left(\frac{1}{\tau}\right)^{\delta+2} \sum_{j=0}^{\infty} \left(\frac{1}{\tau}\right)^j \\ &= \mu_\tau(f) \frac{2}{\pi} \frac{\tau}{\tau - 1} \left(\frac{1}{\tau}\right)^{\delta+2} \end{aligned}$$

concluding the proof. \square

The theorem above shows that if k is distant from S , or T is distant from ℓ , then $f(\tilde{A})_{k\ell}$ is close to $f(A)_{k\ell}$. Moreover, the difference between the two values decreases

exponentially in $\delta = d_G(k, S) + d_G(T, \ell)$. As a limit case, if the considered graph is not connected and there is no walk either from k to m or from n to ℓ , then $\delta = +\infty$ and we deduce $f(\tilde{A})_{k\ell} = f(A)_{k\ell}$.

In order to obtain a sharp bound in Theorem 5.3 we need to choose τ appropriately. This choice clearly depends on the trade-off between $\mu_\tau(f)$, that is the possibly “large size” of f on the given region, and the exponential decay of $(1/\tau)^{\delta+2}$. Hence, Theorem 5.3 produces a family of bounds depending on the considered problem.

As we discussed in Section 2, the exponential and the resolvent functions (2.3) play a central role for f -centrality and f -communicability problems in the complex networks literature [19, 18, 7]. For this reason in what follows we focus on these two special functions and derive more precise bounds when $f(x)$ is either $\exp(x)$ or $r_\alpha(x)$.

We will use the symbol $\Re(z)$ to denote the real part of the complex number z .

COROLLARY 5.4. *Let A, \tilde{A}, S and T be as in Lemma 5.1, Ω be a set containing $\mathcal{F}(A)$ and $\mathcal{F}(\tilde{A})$, and $\delta = d_G(k, S) + d_G(T, \ell)$.*

If the boundary of Ω is a horizontal ellipse with semi-axes $a \geq b > 0$ and center c , and $\delta > b - 1$ then

$$\left| \left(\exp(A) - \exp(\tilde{A}) \right)_{k\ell} \right| \leq \frac{4e^{\Re(c)} p(\delta + 1)}{p(\delta + 1) - (a + b)/(\delta + 1)} \left(\frac{a + b}{\delta + 1} \frac{e^{q(\delta + 1)}}{p(\delta + 1)} \right)^{\delta + 1},$$

with $q(\delta) = 1 + \frac{a^2 - b^2}{\delta^2 + \delta\sqrt{\delta^2 + a^2 - b^2}}$, $p(\delta) = 1 + \sqrt{1 + (a^2 - b^2)/\delta^2}$.

If Ω is a disk of radius a and center c , and $\delta > a - 1$ then

$$\left| \left(\exp(A) - \exp(\tilde{A}) \right)_{k\ell} \right| \leq 4e^{\Re(c)} \frac{(\delta + 1)}{\delta + 1 - a} \left(\frac{ae}{\delta + 1} \right)^{\delta + 1}.$$

If Ω is a real subinterval $[c - a, c + a]$ (with $a > 0$), then for every $\delta > 0$

$$\left| \left(\exp(A) - \exp(\tilde{A}) \right)_{k\ell} \right| \leq \frac{4e^c p(\delta + 1)}{p(\delta + 1) - a/(\delta + 1)} \left(\frac{a}{\delta + 1} \frac{e^{q(\delta + 1)}}{p(\delta + 1)} \right)^{\delta + 1},$$

with $q(\delta) = 1 + \frac{a^2}{\delta^2 + \delta\sqrt{\delta^2 + a^2}}$, $p(\delta) = 1 + \sqrt{1 + (a/\delta)^2}$.

Notice that for δ big enough $p(\delta) \approx 2$ and $q(\delta) \approx 1$.

Proof. We begin with the case of Ω with boundary an horizontal ellipse. A conformal map for Ω is

$$(5.2) \quad \phi(w) = \frac{w - c - \sqrt{(w - c)^2 - \rho^2}}{\rho R},$$

and its inverse is

$$(5.3) \quad \psi(z) = \frac{\rho}{2} \left(Rz + \frac{1}{Rz} \right) + c,$$

with $\rho = \sqrt{a^2 - b^2}$ and $R = (a + b)/\rho$; see, e.g., [44, chapter II, Example 3]. Notice that

$$\max_{|z|=\tau} |e^{\psi(z)}| = \max_{|z|=\tau} e^{\Re(\psi(z))} = e^{\frac{\rho}{2} \left(R\tau + \frac{1}{R\tau} \right) + \Re(c)}.$$

Hence, since $\mu_\tau(\exp) \leq \tau \max_{|z|=\tau} |e^{\psi(z)}|$, by Theorem 5.3 we get

$$\left| \left(\exp(A) - \exp(\tilde{A}) \right)_{k\ell} \right| \leq 4 \frac{\tau}{\tau - 1} e^{\Re(c)} e^{\frac{\rho}{2} \left(R\tau + \frac{1}{R\tau} \right)} \left(\frac{1}{\tau} \right)^{\delta + 1}.$$

The optimal value of $\tau > 1$ which minimizes $e^{\frac{\rho}{2}(R\tau + \frac{1}{R\tau})} \left(\frac{1}{\tau}\right)^{\delta+1}$ is

$$\tau = \frac{\delta + 1 + \sqrt{(\delta + 1)^2 + \rho^2}}{\rho R}.$$

Moreover the condition $\tau > 1$ is satisfied if and only if $\delta + 1 > \frac{\rho}{2} \left(R - \frac{1}{R}\right) = b$. Finally, noticing that

$$\frac{\rho}{2} \left(R\tau + \frac{1}{R\tau}\right) = (\delta + 1)q(\delta + 1),$$

the proof is completed for the ellipse case.

The case in which Ω is a disk is easily obtained setting $b = a$, while the case $\Omega = [c - a, c + a]$ can be proved considering an ellipse of center c , major axis a minor axis any $b > 0$, and then letting $b \rightarrow 0$ in the bound for the ellipse case. \square

Similarly, we can derive a bound for the resolvent $r_\alpha(A) = (I - \alpha A)^{-1}$. In this case, the function $r_\alpha(z)$ is not analytic in the whole complex plane. This property has crucial effects in the approximation, as the subsequent corollary shows.

COROLLARY 5.5. *Let A, \tilde{A}, S and T be as in Lemma 5.1, Ω be a set symmetric with respect to the real axis and containing $\mathcal{F}(A)$ and $\mathcal{F}(\tilde{A})$, $\delta = d_G(k, S) + d_G(T, \ell)$, and $r_\alpha(x)$ be defined as in (2.3) with $\alpha > 0$ such that $\alpha^{-1} \notin \Omega$.*

If the boundary of Ω is a horizontal ellipse with semi-axes $a \geq b > 0$ and center c , then for $0 < \varepsilon < |\alpha^{-1} - c| - a$ and $\delta > 0$

$$\left| \left(r_\alpha(A) - r_\alpha(\tilde{A}) \right)_{k\ell} \right| \leq \frac{4}{1 - \frac{a+b}{(|\alpha^{-1}-c|-\varepsilon)p_\varepsilon}} \frac{1}{\varepsilon} \left(\frac{a+b}{|\alpha^{-1}-c|-\varepsilon} \frac{1}{p_\varepsilon} \right)^{\delta+1},$$

where $p_\varepsilon = 1 + \sqrt{1 - (a^2 - b^2)/(|\alpha^{-1} - c| - \varepsilon)^2}$.

If Ω is a disk of radius a and center c , then for $0 < \varepsilon < |\alpha^{-1} - c| - a$ and $\delta > 0$

$$\left| \left(r_\alpha(A) - r_\alpha(\tilde{A}) \right)_{k\ell} \right| \leq \frac{4}{1 - \frac{a}{(|\alpha^{-1}-c|-\varepsilon)}} \frac{1}{\varepsilon} \left(\frac{a}{|\alpha^{-1}-c|-\varepsilon} \right)^{\delta+1}.$$

If Ω is a real subinterval $[c - a, c + a]$ (with $a > 0$), then for $0 < \varepsilon < |\alpha^{-1} - c| - a$ and $\delta > 0$

$$\left| \left(r_\alpha(A) - r_\alpha(\tilde{A}) \right)_{k\ell} \right| \leq \frac{4}{1 - \frac{a}{(|\alpha^{-1}-c|-\varepsilon)p_\varepsilon}} \frac{1}{\varepsilon} \left(\frac{a}{|\alpha^{-1}-c|-\varepsilon} \frac{1}{p_\varepsilon} \right)^{\delta+1},$$

where $p_\varepsilon = 1 + \sqrt{1 - (a/(|\alpha^{-1} - c| - \varepsilon))^2}$.

Notice that since incidence matrices are real their field of values are symmetric with respect to the real axis, hence the assumption on Ω is natural. We also remark that $p_\varepsilon \approx 2$ when δ is large.

Proof. Here we prove the case of Ω with ellipse shape since the other two cases can then be derived as done in the proof of Corollary 5.4.

Let ϕ as in (5.2) and ψ as in (5.3). Since the function $(1 - \alpha z)^{-1}$ is not analytic in α^{-1} in order to fulfill the assumptions of Theorem 5.3 we assume $|\psi(z)| < \alpha^{-1}$ for every $|z| = \tau$, with $\tau > 1$.

Notice that $\frac{\rho}{2} \left(R\tau + \frac{1}{R\tau} \right)$ is the major semi-axis of the ellipse $\Gamma_\tau = \{\psi(z) : |z| = \tau\}$. Since the center of the ellipse is on the real axis, for $\varepsilon > 0$ small enough we get

$$\varepsilon = \min_{|z|=\tau_\varepsilon} |\psi(z) - \alpha^{-1}| = |\alpha^{-1} - c| - \frac{\rho}{2} \left(R\tau_\varepsilon + \frac{1}{R\tau_\varepsilon} \right),$$

for some $\tau_\varepsilon > 1$. Hence by Theorem 5.3 we get

$$\left| \left(r_\alpha(A) - r_\alpha(\tilde{A}) \right)_{k\ell} \right| \leq 4 \frac{\tau}{\tau-1} \frac{1}{\varepsilon} \left(\frac{1}{\tau_\varepsilon} \right)^{\delta+1},$$

Noticing that

$$\tau_\varepsilon = \frac{|\alpha^{-1} - c| - \varepsilon + \sqrt{(|\alpha^{-1} - c| - \varepsilon)^2 - \rho^2}}{\rho R},$$

we derive the bound. Finally, the condition $\tau > 1$ is satisfied if and only if $\varepsilon < |\alpha^{-1} - c| - a$. \square

5.2. Normalized adjacency matrices: Random walks on G . In many cases the adjacency matrix of a graph $G = (V, E, \omega)$ is “normalized” into a transition matrix, so to model a random walk process on the edges. Transition matrices (or random walks matrices) arise in many network applications, including centrality, quasi-randomness and clustering problems (e.g. [12, 14, 43, 46]).

Assume for simplicity that the graph G is unweighted, loop-free and with no dangling nodes. That is, if A is the adjacency matrix of G , then $a_{ij} \in \{0, 1\}$, $a_{ii} = 0 \forall i, j$ and, for each i , there exists at least one j such that $a_{ij} = 1$. A popular transition matrix \mathcal{A}_{out} on G describes the stationary random walk on the graph where a walker standing on a vertex i chooses to walk along one of the outgoing edges of node i , with no preference among such edges. The entries of \mathcal{A}_{out} are the probabilities of going from node i to node j in one step, which are then given by $(\mathcal{A}_{out})_{ij} = (D_{out}^{-1}A)_{ij}$, where A is the adjacency matrix of G , $D_{out} = \text{diag}(d_1^{out}, \dots, d_n^{out})$ and d_i^{out} is the number of outgoing edges from node i . Note that when the graph is not oriented the adjacency matrix A is symmetric, however the transition matrix is not. This is one of the reasons why a symmetrized version of \mathcal{A}_{out} is typically preferred in this case. Such matrix, defined by $\mathcal{A} = D_{out}^{1/2} \mathcal{A}_{out} D_{out}^{-1/2} = D_{out}^{-1/2} A D_{out}^{-1/2}$, is also known as normalized adjacency matrix of G .

In this section we discuss how the bounds of Section 5.1 transfer to \mathcal{A}_{out} and \mathcal{A} . For the sake of simplicity, let us first address the undirected case.

For a set of nodes $S \subseteq V$ let $\partial S = \{i \in V \setminus S : d_G(S, i) = 1\}$ denote the neighborhood of S . Let \mathcal{A} and $\tilde{\mathcal{A}}$ be the normalized adjacency matrices of G and \tilde{G} , respectively. Unlike the conventional adjacency matrix, the set of entries that are effected by the changes in E are not only related to δE , but to a larger set. Precisely, if the edges in δE connects the nodes within $S \subset V$, then changes in \mathcal{A} occur on the entries corresponding to the nodes in $\tilde{S} = S \cup \partial S$. Given $k \notin S$, we have

$$(5.4) \quad d_G(k, S) = d_G(k, \tilde{S}) + 1.$$

Therefore, an easy consequence of Lemma 5.1 applied to \tilde{S} implies that Theorem 5.3 holds for $|f(\mathcal{A})_{k\ell} - f(\tilde{\mathcal{A}})_{k\ell}|$ when δ is replaced by $d_G(k, S) + d_G(S, \ell) - 2$. However a more careful analysis of the structure reveals that the following lemma holds:

LEMMA 5.6. *Let $G = (V, E, w)$ be an undirected graph and $\mathcal{A} \in \mathbb{R}_+^{N \times N}$ be its normalized adjacency matrix. Consider the graph \tilde{G} , obtained by adding or erasing*

the edges between the nodes in a subset S and let $\tilde{\mathcal{A}}$ be the corresponding normalized adjacency matrix. Then, for any $k, \ell \notin S$ we have

$$(p_n(\tilde{\mathcal{A}}))_{k\ell} = (p_n(\mathcal{A}))_{k\ell},$$

for every polynomial p_n of degree $n \leq d_G(k, S) + d_G(S, \ell) - 1$.

Proof. A walk from k to ℓ in \tilde{G} contains a modified edge only if it passes through at least one modified edge in S or through at least one re-weighted edge connecting S and ∂S . Therefore, any modified walk must go from k to ∂S , then from ∂S to S , then from S to ∂S , and finally from ∂S to ℓ . Therefore, due to the identity (5.4), the length of any modified walk must be equal or longer than

$$d_G(k, \bar{S}) + d_G(\bar{S}, \ell) + 2 = d_G(k, S) + d_G(S, \ell).$$

The proof thus follows as the one of Lemma 5.1. \square

Hence, following the same arguments as the one in Section 5, we can extend to \mathcal{A} the bounds of Theorem 5.3, Corollary 5.4 and Corollary 5.5 by replacing δ with $\delta - 1$.

Let us now consider the case of a directed network and let us thus transfer Lemma 5.1 to the transition matrix \mathcal{A}_{out} . Arguing as above we obtain

LEMMA 5.7. *Let $G = (V, E, w)$ be a directed graph and $\mathcal{A}_{out} \in \mathbb{R}_+^{N \times N}$ be the its transition matrix. Consider the graph \tilde{G} , obtained by adding or erasing the edges in $\delta E \subset V \times V$, and let $\tilde{\mathcal{A}}_{out}$ be the corresponding transition matrix. If $S = \{s | (s, t) \in \delta E\}$ and $T = \{t | (s, t) \in \delta E\}$ are respectively the sets of sources and tips of δE , then*

$$(p_n(\tilde{\mathcal{A}}_{out}))_{k\ell} = (p_n(\mathcal{A}_{out}))_{k\ell},$$

for every polynomial p_n of degree $n \leq d_G(k, S) + \min\{d_G(T, \ell), d_G(S, \ell) - 1\}$.

Proof. Consider $\partial_{out}S = \{i \in V \setminus S : d_G(S, i) = 1\}$, the out neighborhood of S . A walk from k to ℓ in \tilde{G} contains a modified edge only if it passes through at least one modified edge in S or through at least one re-weighted edge connecting S and $\partial_{out}S$. Therefore, any modified walk must go from k to S , then it may go from S to T through a modified edge, or it can go to any node in $\partial_{out}S$. In the first case, the length from k to ℓ of the walk must be greater or equal than

$$d_G(k, S) + d_G(T, \ell) + 1.$$

In the second case, the length of the walk must be greater or equal than

$$d_G(k, S) + d_G(S, \ell).$$

The proof thus follows as the one of Lemma 5.1. \square

Hence, we can extend to \mathcal{A}_{out} the bounds of Theorem 5.3, Corollary 5.4 and Corollary 5.5 by replacing δ with $\min\{\delta, d_G(k, S) + d_G(S, \ell) - 1\}$.

5.3. On the field of values of adjacency matrices. Two quantities play a key role in the computation of the bounds we proposed: the shortest-path distances between pairs of nodes and the shape of the field of values of A and \tilde{A} . Next subsection deals with the former whereas we devote the present subsection to the latter.

Let A be a $N \times N$ real matrix with nonnegative entries. The numerical radius of A is the quantity

$$\nu(A) = \max\{|w| : w \in \mathcal{F}(A)\},$$

whereas, the Hermitian part of A is the Hermitian matrix defined by $H_A = (A + A^*)/2$. As for the spectrum of A , a Perron-Frobenius theory for the field of values $\mathcal{F}(A)$ has been developed in relatively recent years (see e.g. [35, 34]). We recall henceforth two results which are useful for our scopes:

1. When $A \geq 0$, the numerical radius $\nu(A)$ is the maximal element of $\mathcal{F}(A)$, attained by the maximal eigenvector of H_A . Precisely, for $A \geq 0$, we have

$$(5.5) \quad \nu(A) = \rho(H_A).$$

2. The shape of the field of values $\mathcal{F}(A)$ for nonnegative matrices can be characterized in terms of the index of imprimitivity of A , defined as the number of eigenvalues of A having maximal modulus. In fact, if $A \geq 0$ is irreducible, then the maximal elements of $\mathcal{F}(A)$ are of the form

$$\nu(A) \exp(2i\pi p/k), \quad p = 1, 2, \dots, k-1$$

being k the index of imprimitivity of A .

Point 1 shows that, for nonnegative matrices $A \in \mathbb{R}_+^{N \times N}$, it is always possible to compute a set Ω containing the field of values of A or of \tilde{A} , by letting $\Omega = \{\zeta \in \mathbb{C} : |\zeta| \leq \nu\}$ where ν is $\nu(A)$ or $\nu(\tilde{A})$, respectively. Moreover, point 2 above shows that if the imprimitivity index of A is large, then the ball $\{\zeta \in \mathbb{C} : |\zeta| \leq \nu(A)\}$ is a tight approximation of the field of values $\mathcal{F}(A)$.

The normalized adjacency matrix \mathcal{A} has the desirable property of being diagonally similar to a stochastic matrix. This implies that $\nu(\mathcal{A}) = \nu(\tilde{\mathcal{A}}) = 1$. For general nonnegative matrices, instead, the field of values can be large. However, due to (5.5), the numerical radii $\nu(A)$ and $\nu(\tilde{A})$ can be well approximated by standard eigenvalues techniques such as the power method or the Lanczos process. The computational cost of this operation is much smaller than the effort required to compute the entries of the matrix functions $f(A)$ or $f(\tilde{A})$. Moreover, if δA is sparse enough, we expect $\nu(A)$ and $\nu(\tilde{A})$ to be close. This claim is also supported by the following Theorem 5.8, where the case of a single-entry perturbation is discussed.

THEOREM 5.8. *Let $A \geq 0$ and let $\tilde{A} = A + \mathbb{1}_m \mathbb{1}_n^T$. Then*

1. $0 \leq \nu(\tilde{A}) - \nu(A) \leq 1/2$ and, if $H_{\tilde{A}}$ is irreducible, then $\nu(\tilde{A}) - \nu(A) > 0$.
2. Assume H_A irreducible. For any nonnegative function $f : \mathbb{C} \rightarrow \mathbb{R}_+$, such that $f(\nu(A)) \neq 0$ we have

$$0 < \nu(\tilde{A}) - \nu(A) \leq \frac{\sqrt{f(A)_{mm} f(A)_{nn}}}{f(\nu(A))} + O\left(\frac{1}{4}\right)$$

Proof. As $\tilde{A} \geq A \geq 0$, then $H_{\tilde{A}} \geq H_A \geq 0$ and, by the Perron-Frobenius theorem and point 1 above, we have $\nu(\tilde{A}) \geq \nu(A)$. As, by assumption, $\tilde{A} \neq A$, then $H_{\tilde{A}} \neq H_A$ and, again, the Perron-Frobenius theorem applied to H_A and $H_{\tilde{A}}$ ensures the strict inequality if $H_{\tilde{A}}$ is irreducible. Observe that $H_{\mathbb{1}_m \mathbb{1}_n^T}(\mathbb{1}_m + \mathbb{1}_n) = (\mathbb{1}_m + \mathbb{1}_n)/2$, implying that $\rho(H_{\mathbb{1}_m \mathbb{1}_n^T}) = \|H_{\mathbb{1}_m \mathbb{1}_n^T}\|_2 = 1/2$. By the Bauer-Fike theorem (see [25] f.i.) applied to $H_{\tilde{A}} = H_A + H_{\mathbb{1}_m \mathbb{1}_n^T}$ we get

$$|\nu(A) - \nu(\tilde{A})| \leq \|A - \tilde{A}\|_2 = \|H_{\mathbb{1}_m \mathbb{1}_n^T}\|_2 = 1/2$$

completing the proof of the first statement. To address the second statement note that, as H_A is irreducible, $\nu(A) = \rho(H_A)$ is a simple eigenvalue and the corresponding

eigenvector x with $x^*x = 1$ is entry-wise positive. Thus we can use a standard eigenvalue perturbation argument (see e.g. [47]) to get

$$(5.6) \quad \nu(\tilde{A}) - \nu(A) = (x^* H_{\mathbb{1}_m \mathbb{1}_n^T} x) \|H_{\mathbb{1}_m \mathbb{1}_n^T}\|_2 + O(\|H_{\mathbb{1}_m \mathbb{1}_n^T}\|_2^2) = x_m x_n + O(1/4)$$

Let y_2, \dots, y_n be the orthonormal eigenvectors of H_A corresponding to the eigenvalues $\lambda_2, \dots, \lambda_n$, with $\lambda_j \neq \nu(A)$. Then, for any $1 \leq i \leq n$, we have

$$f(A)_{ii} = f(\nu(A))x_i^2 + \sum_{j>1} f(\lambda_j)(y_j)_i^2 \geq f(\nu(A))x_i^2.$$

As a consequence $x_i \leq \sqrt{f(A)_{ii}/f(\nu(A))}$ and, together with (5.6), we conclude. \square

5.4. Computing node distances by Krylov methods. The bounds proposed so far rely on the geodesic distances between pair of nodes in the graph. Computing such distances is a classical problem in graph theory and several efficient and parallelizable algorithms are available [45]. In this section, however, we propose a simple numerical strategy that exploits the computation of $f(A)_{k\ell}$, to simultaneously approximate the distances $d_G(m, \ell)$ and $d_G(k, m)$ for any node m , at essentially no attentional cost. As we will discuss in what follows, the procedure is well suited for undirected graphs and allows to compute small distances exactly, whereas provides a lower bound when $d_G(m, \ell)$ (resp. $d_G(k, m)$) is too large.

Computing the f -communicability or f -centrality of a network can be a computationally expensive task, especially for large graphs. An established and efficient strategy to address this quantities exploits the fact that $f(A)_{k\ell}$ can be written as the quadratic form $\mathbb{1}_k^T f(A) \mathbb{1}_\ell$ and thus employs Lanczos-type algorithms [30, 31] both for symmetric ([24, 5]) and non-symmetric matrices ([22, 41]).

The non-Hermitian Lanczos algorithm produces two basis $\{v_0, \dots, v_{n-1}\}$ and $\{w_0, \dots, w_{n-1}\}$ for the Krylov subspaces $\mathcal{K}_n(A, v_0)$ and $\mathcal{K}_n(A^T, w_0)$, respectively. If no breakdowns arise, the j -th vectors v_j and w_j are obtained at the j -th step of the algorithm. Moreover, they are biorthogonal ($w_j^* v_j = 1$) and such that

$$v_j = p_j(A)v_0 \quad \text{and} \quad w_j = p_j(A^T)w_0,$$

with p_j a polynomial of degree exactly j . We remark that the Hermitian Lanczos algorithm can be used when A is symmetric and $v_0 = w_0$. For symmetric matrices and the case $v_0 \neq w_0$, a similar strategy can be employed (see [24, Ch. 7] for details). In the following we treat only the non-Hermitian Lanczos algorithm. Everything can be easily transferred to the Hermitian case by letting $w_j = v_j$.

In order to approximate $f(A)_{k\ell}$ the method requires to set $v_0 = \mathbb{1}_\ell$ and $w_0 = \mathbb{1}_k$. We then get the following result:

THEOREM 5.9. *Let $\{v_0, \dots, v_{n-1}\}$ and $\{w_0, \dots, w_{n-1}\}$ be the basis of $\mathcal{K}_n(A, \mathbb{1}_\ell)$ and $\mathcal{K}_n(A^T, \mathbb{1}_k)$ obtained by the non-Hermitian Lanczos algorithm. Then for every $m = 1, \dots, N$ the distance $d_G(m, \ell)$ (resp. $d_G(k, m)$) is equal to the first index j for which the m -th element of v_j (resp. w_j) is nonzero.*

Proof. We prove the result for $d_G(m, \ell)$. The proof can be easily transferred to $d_G(k, m)$. As we already discussed, $(A^j)_{m\ell}$ is the overall weight of the walks of length j from m to ℓ . Therefore, if $d_G(m, \ell) < j$, then $(p_j(A))_{m,\ell} = 0$. Moreover, since p_j has degree exactly j , if $d_G(m, \ell) = j$ then $(p_j(A))_{m,\ell} = \alpha(A^j)_{m,\ell} \neq 0$ for some $\alpha \neq 0$, concluding the proof. \square

Hence, we can modify the non-Hermitian Lanczos algorithms to compute the distance vectors

$$\vec{d}_k = \begin{pmatrix} d_G(k,1) \\ \vdots \\ d_G(k,N) \end{pmatrix}, \quad \overleftarrow{d}_\ell = \begin{pmatrix} d_G(1,\ell) \\ \vdots \\ d_G(N,\ell) \end{pmatrix}.$$

The idea is to add the following pseudo-code to the Lanczos algorithm (we assume to stop it at the $(n-1)$ -th iteration).

First, initialize the variables `is_zero_k`, `is_zero_l`, `d_k` and `d_l` as follows

```

for i=1,...,N
  is_zero_k(i) = TRUE
  is_zero_l(i) = TRUE
  d_k(i) = n    % vector of the distances from k
  d_l(i) = n    % vector of the distances to l
end

```

and then modify the method by adding the procedure below, to derive the distances from the nonzero pattern of v_j and w_j , at each step of the scheme

```

for j=1,...,n-1 % Iteration of Lanczos algorithm
  compute vector v_j and w_j
  for m=1,...,N
    if v_j(m) > 0 && is_zero_k(m)
      d_k(m) = j
      is_zero_k(m) = FALSE
    end
    if w_j(m) > 0 && is_zero_l(m)
      d_l(m) = j
      is_zero_l(m) = FALSE
    end
  end
end
proceed with the rest of the algorithm
end

```

Notice that if n is smaller or equal than the diameter of the graph, there can be null elements in v_j for $j = 0, \dots, n-1$. Nevertheless, for all these elements, n is a lower bound for the distance, which can then be used to approximate δ in Theorem 5.3. On the other hand, let us remark that many real-world networks have a small diameter, thus we expect the proposed technique to be able to actually compute the desired distances in typical applications. Also note that by using this strategy, computing the diagonal of $f(A)$ allows to simultaneously address the all-pair shortest-path distances of the graph. This is particularly effective when dealing with undirected graphs. In that case, in fact, the entries $f(A)_{kk}$ can be computed with the Hermitian Lanczos method which further ensures no breakdowns. Table 1 in the next section shows how this strategy behaves on four sample undirected networks, where the diagonal of the exponential function is approximated by the Hermitian Lanczos method and the number of maximal iterations varies.

6. Numerical examples. In this section we illustrate the behavior of the proposed bounds on some example networks.

The first explanatory example graph we consider is represented in Figure 1. The considered graph G is made by two simple cycles (closed undirected paths) with 111 nodes each, and by one directed edge \vec{e} from node 111 to node 112.

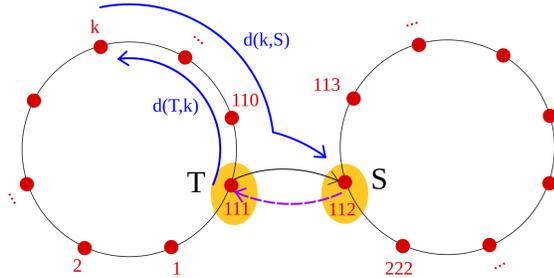


FIG. 1. Example: two cycles connected by a directed bridge (n, m) in which we add the edge in the opposite direction (m, n) .

Since there are no closed walks passing through \vec{e} , all the nodes in G have the same f -centrality. The graph is then perturbed by the insertion of one single new directed edge \overleftarrow{e} from node 112 to node 111. This new edge “closes the two-directional bridge” between the two circles, resulting into a perturbation of the f -centrality scores of the nodes. In Figure 2 we plot in red crosses the values $|\exp(A)_{kk} - \exp(\tilde{A})_{kk}|$ (left plot) and those of $|r_\alpha(A)_{kk} - r_\alpha(\tilde{A})_{kk}|$ with $\alpha = 3$ (right plot), for $k = 1, \dots, 222$. With blue circles, instead, we represent the bound in Corollaries 5.4 (left plot) and 5.5 (right plot) for every admissible k . As we can see the behavior of the decays of the differences is well approximated by the bounds. Moreover, we observe that the exponential decay for the exponential centrality variation as well the linear decay of the resolvent one are captured by the bound.

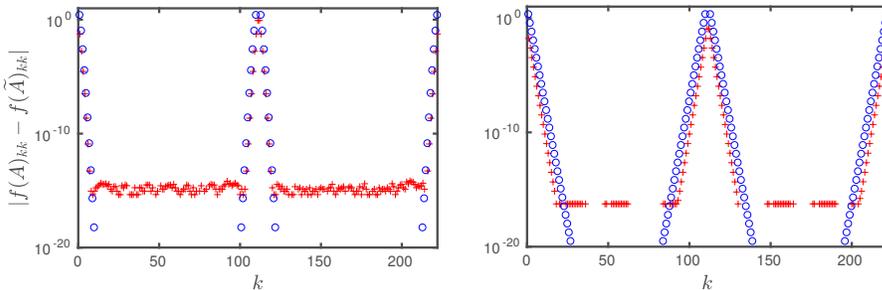


FIG. 2. In the ordinate: $|f(A)_{kk} - f(\tilde{A})_{kk}|$ (red crosses) when adding the edge \overleftarrow{e} in the graph of Figure 1 and the bounds (blue circles) of Corollaries 5.4 and 5.5. In the abscissa: k , the nodes of the graph. From left to right: variation of exponential centrality $f(x) = \exp(x)$; variation of resolvent centrality $f(x) = r_3(x)$.

In the following we present four examples of real-world undirected networks whose diameter is proportional to the logarithm of the number of nodes. Our analysis is meant to show the correlation between the variation of the network centralities and the variation of the distances in G with respect to the set of perturbed edges. For

this reason, normalized adjacency matrices \mathcal{A} are considered below, so to guarantee the field of values of both the original and the perturbed matrices to be constrained within the unit segment $[-1, 1]$.

The considered network data are borrowed from [16, 33] and are briefly described below:

Gnutella A snapshots of the Gnutella peer-to-peer file sharing network in August, 8, 2002. Nodes represent hosts in the Gnutella network topology and edges represent connections between the Gnutella hosts. Number of nodes: 6300, Number of edges: 41297, Diameter: 10;

Facebook This dataset consists of anonymous “friends circles” from Facebook. Facebook data was collected from survey participants. Number of nodes: 4038, Number of edges: 176167, Diameter: 10;

GRCQ General Relativity and Quantum Cosmology (GR-QC) collaboration network. Data are collected from the e-print arXiv and covers scientific collaborations between authors papers submitted to GR-QC category. The data covers papers in the period from January 1993 to April 2003. Number of nodes: 5242, Number of Edges: 14496, Diameter: 17;

Erdős Erdős collaboration network. Number of nodes: 472, Number of edges: 2628, Diameter: 11.

For each network we compute (approximate) the exponential centrality index $\exp(\mathcal{A})_{kk}$, $k = 1, \dots, n$, by running n iterations of the Lanczos algorithm. By using the method presented in Subsection 5.4, for every ℓ we can compute $d_n(k, \ell)$: an approximation of $d_G(k, \ell)$. If $d_G(k, \ell) \leq n$, then $d_n(k, \ell) = d_G(k, \ell)$. Otherwise, if $d(k, \ell) > n$ then $d_n(k, \ell) = n \leq d_G(k, \ell)$.

We compared the proposed methods with $d^M(k, \ell)$: the distance between k and ℓ computed by the Matlab function `distances`. Note that, $d^M(k, k) = 0$ for every node k , whereas $d_n(k, k)$ is either n or the minimal length of a closed walk passing through k . Moreover, when k and ℓ are disconnected, $d_n(k, \ell) = n$ for every n , while `distances` correctly sets to ∞ the distance between disconnected nodes.

In order to evaluate the proposed method, we consider the quantity

$$\varrho_n(G) = \frac{\#\{(k, \ell) \mid d_n(k, \ell) \neq d^M(k, \ell), k \neq \ell, d_G(k, \ell) < \infty\}}{\#\{(k, \ell) \mid k \neq \ell, d_G(k, \ell) < \infty\}},$$

which depends on the number of pairs (k, ℓ) for which $d_n(k, \ell) \neq d^M(k, \ell)$ (excluding the disconnected and the coincident nodes). Table 1 presents $\varrho_n(G)$ for some values of n and for the networks listed above. The table clearly shows that for a small number of Lanczos iterations we are able to determine most of the distances. Moreover, when n is greater or equal to the diameter of the network we always have $d_n(k, \ell) = d^M(k, \ell)$, for every $k \neq \ell$ and $d_G(k, \ell) < \infty$.

Now, for each network, we select the 10 nodes having smallest centrality $\exp(\mathcal{A})_{kk}$ and we perturb the edge topology of the graph by adding all the missing edges among those nodes (obtaining a clique connecting all the “less important” nodes).

The plots of Figure 3 represent the actual variation of network exp-centrality values $|\exp(\mathcal{A})_{kk} - \exp(\tilde{\mathcal{A}})_{kk}|$ (red crosses) and the bound in Corollary 5.4 (blue circle). Let us point out that in the plots shown, we are relabeling the nodes according with the distance from (and to) the set S of modified nodes: the larger is the node index k the farther k is from S . The results show that the proposed bounds, although not tight, well approximate the actual behavior of the variation of $f(\mathcal{A})_{kk}$. This allows to predict the nodes whose centrality index remains effectively unchanged under perturbations

n	Erdős	Facebook	GRQC	Gnutella
7	$1.7188e - 02$	$1.6729e - 02$	$2.5187e - 01$	$5.1500e - 04$
9	$5.4461e - 04$	$7.2177e - 04$	$3.0759e - 02$	$5.1438e - 08$
11	0	0	$2.3687e - 03$	0
13	0	0	$1.0956e - 04$	0
15	0	0	$5.4373e - 06$	0
17	0	0	0	0

TABLE 1

Values of $\varrho_n(G)$ for $n = 7, 9, 11, 13, 15, 17$ and for the networks: Erdős, Facebook, GRQC, and Gnutella.

of the original graph topology. For example, the exp-centrality of all the nodes from 3000 onwards in GRQC is guaranteed to be unchanged up to 10 digits of precision.

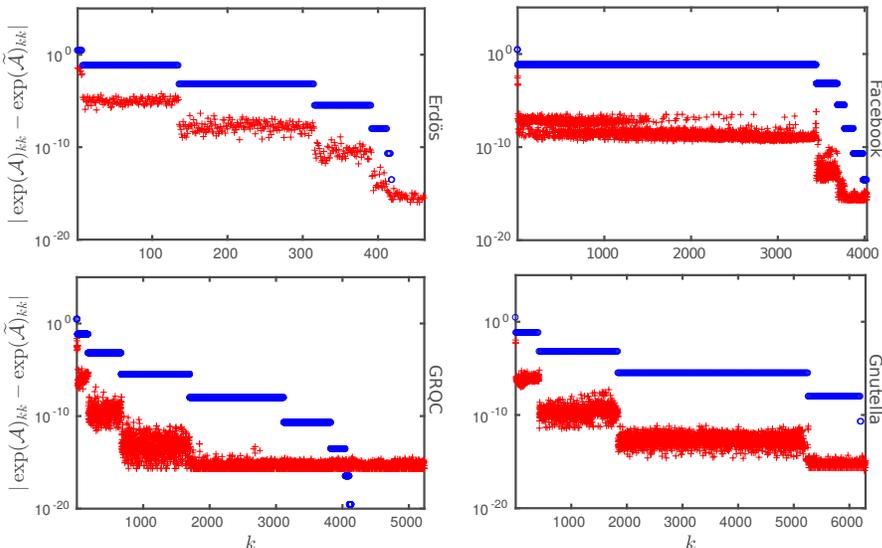


FIG. 3. Absolute variation $|\exp(A)_{kk} - \exp(\tilde{A})_{kk}|$ when k ranges from 1 to N . The perturbed edges are $\delta E = S \times S$, where S is the set of 10 nodes with least exp-centrality. Nodes in the plot are ordered so that the larger is k the farther it is from S . Red crosses show the actual difference whereas the blue circles show the bound of Corollary 5.4.

7. Conclusion. Centrality and communicability indices based on function of matrices are among the most effective measures of the importance of nodes and of the robustness of edges in a network. These quantities are defined as the entries $f(A)_{k\ell}$ where $f(A)$ is a suitable function of a matrix A describing the structure of the network G . In this work we address the somewhat natural problem of understanding the stability of such indices with respect to perturbations in the edge topology of the graph. Our analysis reveals that the absolute variation of $f(A)_{k\ell}$ decays exponentially with respect to the distance in G that separates k and ℓ from the set of nodes touched by the perturbed edges. The knowledge of this behavior can be of help in several practical applications. In fact, if A is modified into $\tilde{A} = A + \delta A$, the entries of $f(\tilde{A})$ should in principle be re-computed from scratch. However, we propose a simple numerical strategy that allows to compute the distances between nodes in G simul-

taneously with the computation of the entries of $f(A)$, with essentially no additional cost. In particular, computing the diagonal of $f(A)$ for undirected networks (the network f -centrality scores) allows to compute the all-pairs shortest-path distances in the graph. Thus, using the proposed bounds, we are able to predict the magnitude of variation in the f -centralities of G when changes occur in a localized set of edges or, viceversa, for each node k we can locate a set of nodes whose change in the edge topology affects the score $f(A)_{kk}$ by a small order of magnitude.

Examples of application include the case where the edge topology is evolving in time and changes in G happen more frequently in network subareas being peripheral with respect to the subset of nodes one is actually interested in, or where the information on the edge structure of peripheral nodes is not fully reliable or, equivalently, is likely to be affected by noise.

Finally, the results proposed are numerically tested on some example networks borrowed from real-world applications. Our experiments show that the proposed bounds well resemble the actual behavior of the variation of $f(A)_{k\ell}$ although being some orders of magnitude larger. A clear margin for improvements and further work is thus left open to determine a better constant $c > 2$ to be added in the exponent $\delta + c$ of Theorem 5.3.

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