Discovering important nodes of complex networks based on Laplacian spectra

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***Abstract*—Knowledge of the Laplacian eigenvalues of a network provides important insights into its structural features and dynamical behaviours. Node or link removal caused by possible outage events, such as mechanical and electrical failures or malicious attacks, significantly impacts the Laplacian spectra. This can also happen due to intentional node removal against which, increasing the algebraic connectivity is desired. In this article, an analytical metric is proposed to measure the effect of node removal on the Laplacian eigenvalues of the network. The metric is formulated based on the local multiplicity of each eigenvalue at each node, so that the effect of node removal on any particular eigenvalues can be approximated using only one single eigen-decomposition of the Laplacian matrix. The metric is applicable to undirected networks as well as strongly-connected directed ones. It also provides a reliable approximation for the "Laplacian energy" of a network. The performance of the metric is evaluated for several synthetic networks as well as the American Western States power grid. Results show that this metric has a nearly perfect precision in correctly predicting the most central nodes, and significantly outperforms other comparable heuristic methods.**

***Index Terms*—Complex network, Graph theory, Laplacian spectrum, Local multiplicity, Node-removal attack.**

I. Introduction

MANY real systems can be modelled as networks, where a number of agents (nodes) or even dynamical subsystems interact through an often complex graph of connection links [1]. Statistical properties of the network's nodes and links are often a major determinant of the behaviour of the networked system. In other words, not all nodes have the same importance for networks' dynamical behaviours, such as consensus or synchronization [2]. Nodes with considerable impacts on the structure or specific collective behaviour of a network are often called "central". The centrality of nodes and identification of which nodes are more central than others have been key issues in network analysis. For example, a criminal network may be broken to smaller components or groups with less corruptive potential when appropriate central nodes are identified and removed [3]. Central nodes are clearly important in the synchronization problem [4], and in the concern of network robustness against disturbances and attacks [5], [6]. Much research effort has been devoted to investigating impacts of adding or removing nodes and edges on performance measures from the graph-theoretic perspective, such as deleting the minimum number of nodes or links to make a graph embeddable onto a surface [7] or to optimise a manufacturing process [8].

Well-known examples of structural centrality measures include degree, betweenness and closeness centrality metrics, i.e. nodes having high degree, betweenness or closeness are regarded as those with particularly high impacts [9]. As an example, these metrics are applied to find the most influential people in the communication network of hijackers participating in the September 11, 2001 attacks [3], [11]. However, in relation to node centrality to dynamical behaviours, often these structural measures have poor performances [12].

Another interesting class of centrality measures is based on the spectral properties of the connectivity matrix. Spectrum-based centrality measures, which are based on the eigenvalues or eigenvectors of the Laplacian or the adjacency matrix of the network, have recently attracted particular attention in analysis and control of dynamical networks [13]–[20]. For example, the second smallest eigenvalue of the Laplacian matrix, known also as the algebraic connectivity, shows how close the network is to disconnection and also how synchronisable it is [43]. Or, the largest eigenvalue of the adjacency matrix, often referred to as the spectral radius, can well describe virus or rumour spreading through a network [21], [22]. Laplacian spectrum-based methods can assess the ability of a linear multi-agent system, connected over a directed graph, to achieve consensus [23]–[25]. The best set of control nodes to achieve synchronisation over the widest range of coupling strengths has been recently identified using eigen-decomposition of the Laplacian matrix of the network [12], [18]. A subgraph centrality measure is proposed in [26] based on the spectrum of the adjacency matrix, which can be useful in some applications.

Identifying central nodes of a network using spectrum-based measures has shown promising results in different applications [27]. For example, synchronisability and convergence performances of a network may be enhanced by sequentially targeted node removal to increase the algebraic connectivity [28]. A similar approach can be applied as a failure or attack

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tolerant mechanism for dynamical networks [23]. For example, identifying and protecting central nodes can improve resilience and reliability of power systems [10]. Node centrality can also be defined based on the Laplacian energy $E_L(G)$, which is sum of the squared eigenvalues of the Laplacian matrix $\boldsymbol{L}$ of the graph G [29]. The importance of a node is then reflected by the drop of $E_L(G)$ when the node is removed. This centrality measure has applications in identification of central nodes in different terrorist social networks [30], data clustering for measuring the similarity between data and their classification [31], as well as in air-traffic network optimisation [32]. Although identifying central nodes using Laplacian energy yields reliable results especially for social networks, it requires multiple eigen-decompositions of the Laplacian matrix, and thus is computationally expensive for large-scale networks.

Compared to the adjacency matrix, the effect of a node or link removal on the Laplacian spectra has been less studied analytically [3], [27]. A weak interlacing theorem is proposed in [33] where an upper and a lower bound on Laplacian eigenvalues are introduced when a node is removed. The relationship between spectral node centrality in undirected networks and eigenvectors of the Laplacian matrix has been studied analytically [34] and through extensive numerical simulations [35]. Despite the above research progress, there is still a lack of an analytical easy-to-compute metric to rank the nodes based on their impacts on the Laplacian spectra in large-scale networks. This paper develops a new metric to rank nodes based on their impacts on an individual eigenvalue of the Laplacian matrix. The metric is based on the concept of the *local multiplicity* of each eigenvalue at each node in the network. Using this metric, a clear ranking can be obtained that separates nodes for any eigenvalue of the Laplacian matrix. It will be shown that nodes with higher local multiplicity have larger spectral impact on the Laplacian matrix. This metric is therefore applicable to studying many dynamical performances and collective behaviours of the underlying dynamical network. Indeed, identifying central nodes of a network is just one application of the results of this paper. The proposed metric is also computationally cost-effective as it performs node ranking for all eigenvalues using only a single eigen-decomposition of the Laplacian matrix. The metric is applicable to weighted or unweighted undirected graphs as well as strongly-connected directed graphs. Simulations demonstrate its high precision in various networks with different topologies.

The rest of the paper is organised as follows. The mathematical concept of local multiplicity is introduced in Section II. Based on that, a new node centrality metric is introduced in Section III. The metric is applied to directed and undirected networks with scale-free, Watts-Strogatz or Erdös-Rényi structures to rank their nodes based on their impacts on the algebraic connectivity λ_1, spectral radius λ_N and Laplacian energy $E_L(G)$. It is also applied to identify nodes with maximum spectral impact on the power grid of the Western States of the United States of America. A brief conclusion is given in Section V.

Preliminaries

In this paper, vectors and matrices are shown in bold italic. The set of real numbers is denoted by $\mathbb{R}$, and $\mathbf{1}$ is the vector with all elements being 1. The inner product of vectors $\boldsymbol{x}$ and $\boldsymbol{y}$ is $\langle \boldsymbol{x}, \boldsymbol{y} \rangle = \boldsymbol{x}^\top \boldsymbol{y}$, and $\boldsymbol{e}_u$ is the canonical basis vector of $\mathbb{R}^N$ in which the u^{th} entry is 1 and all other entries are zero. The Kronecker delta is denoted by δ_{ij}, i.e. $\delta_{ij} = 1$ if $i = j$ and $\delta_{ij} = 0$ otherwise. The u^{th} entry of vector $\boldsymbol{x}$ is denoted by $\boldsymbol{x}_u$, and $\boldsymbol{E}_{uu}$ is the $(u, u)^{th}$ element of the matrix $\boldsymbol{E}$. Finally, G and $\overrightarrow{G}$ stand for an undirected and directed graph, respectively. $G\backslash u$ shows the graph G when node u is removed from it. Throughout the paper, it is always assumed that $G\backslash u$ is a connected graph.

II. Introduction to local multiplicity

Consider an undirected network $G = (V, E)$ with a set V of N nodes and a set E of links, with loops allowed, where each link (i, j) between nodes i and j is associated with a weight $w_{ij} = w_{ji}$ (if there is no loop at i, set $w_{ii} = 0$). The *Laplacian matrix* $\boldsymbol{L} = (l_{ij})$ is a zero row-sum matrix with entries

$$l_{ij} = \begin{cases} d(i), & \text{if } i = j, \\ -w_{ij}, & \text{if } i \sim j, \\ 0, & \text{otherwise.} \end{cases} \tag{1}$$

where $i \sim j$ means that there is a link between nodes i and j, and $d(i) = \sum_{j \sim i} w_{ij}$ is the *weighted degree* of node i. Sometimes, it is convenient to consider the so-called *normalized Laplacian matrix* $\boldsymbol{\mathcal{L}} = (\ell_{ij})$ with entries

$$\ell_{ij} = \begin{cases} 1 - \frac{w_{ii}}{d(i)}, & \text{if } i = j, \\ -\frac{w_{ij}}{\sqrt{d(i)d(j)}}, & \text{if } i \sim j, \\ 0, & \text{otherwise.} \end{cases} \tag{2}$$

The spectrum of the Laplacian matrix $\boldsymbol{L}$ is the set of eigenvalues $0 = \lambda_1 < \lambda_2 < \cdots < \lambda_d$, together with their algebraic (or geometric) multiplicities $m_i = m(\lambda_i)$ for $i = 1, 2, \ldots, d$,

$$\operatorname{sp}(\boldsymbol{L}) = \{\lambda_1^{m_1}, \lambda_2^{m_2}, \ldots, \lambda_d^{m_d}\}, \tag{3}$$

where m_i is the number of repeats of λ_i. The eigenvalues λ_i, for $i = 1, 2, \ldots, d$, are the roots of the characteristic polynomial $\psi_G(\lambda) = \det(\lambda \boldsymbol{I} - \boldsymbol{L})$ of G, and they are all real since $\boldsymbol{L}$ is symmetric. It is known that $m_1 + m_2 + \cdots + m_d = N$ and, for connected graphs, $m_1 = 1$. For each eigenvalue λ_i, $i = 1, 2, \ldots, d$, let $\boldsymbol{U}_i$ be a matrix which columns form an orthonormal basis of the eigenspace $\mathcal{E}_i = \operatorname{Ker}(\boldsymbol{L} - \lambda_i \boldsymbol{I})$. The dimension of $\mathcal{E}_i$ is called the geometric multiplicity of λ_i.

Definition 1. *The orthogonal projection of $\mathbb{R}^N$ onto the eigenspace $\mathcal{E}_i$ is represented by the following matrix $\boldsymbol{E}_i$, called a* principal idempotent *of $\boldsymbol{L}$,*

$$\boldsymbol{E}_i = \frac{1}{\phi_i} \prod_{\substack{j=1 \\ j \neq i}}^{d} (\boldsymbol{L} - \lambda_j \boldsymbol{I}), \quad \textit{where} \quad \phi_i = \prod_{\substack{j=1 \\ j \neq i}}^{d} (\lambda_i - \lambda_j). \tag{4}$$

Alternatively, the principal idempotents of $\boldsymbol{L}$ can be represented as $\boldsymbol{E}_i = \boldsymbol{U}_i \boldsymbol{U}_i^\top$.

Theorem 1. *[37] The idempotents satisfy the following properties.*

(i) $\boldsymbol{E}_i\boldsymbol{E}_j = \delta_{ij}\boldsymbol{E}_i$.
(ii) $\boldsymbol{L}\boldsymbol{E}_i = \lambda_i\boldsymbol{E}_i$,
(iii) $\boldsymbol{I} = \sum_{i=1}^{d}\boldsymbol{E}_i$,
(iv) *If $f(x)$ is a rational function defined at each eigenvalue of $\boldsymbol{L}$, then $f(\boldsymbol{L}) = \sum_{i=1}^{d} f(\lambda_i)\boldsymbol{E}_i$.*

Corollary 1 (Spectral decomposition). *[37] The spectral decomposition of the Laplacian matrix is $\boldsymbol{L} = \sum_{i=1}^{d}\lambda_i\boldsymbol{E}_i$.*

Proof. Apply Theorem 1(iv) with $f(x) = x$. □

Corollary 2. *A spectral decomposition of the u^{th} canonical vector is $\boldsymbol{e}_u = \sum_{i=1}^{d}\boldsymbol{z}_{ui}$ with $\boldsymbol{z}_{ui} = \boldsymbol{E}_i\boldsymbol{e}_u$.*

Proof. Simply multiply both sides of Theorem 1(iii) by $\boldsymbol{e}_u$. □

Definition 2. *[38] The local multiplicity of the eigenvalue λ_i at node u, denoted by m_{ui}, is defined as the square norm of the projection of the canonical vector $\boldsymbol{e}_u \in \mathbb{R}^N$ onto the eigenspace $\mathcal{E}_i$. That is,*

$$m_{ui} \equiv m_u(\lambda_i) = \|\boldsymbol{E}_i\boldsymbol{e}_u\|^2 = \langle\boldsymbol{E}_i\boldsymbol{e}_u, \boldsymbol{e}_u\rangle = (\boldsymbol{E}_i)_{uu}. \quad (5)$$

The local multiplicities play the same role as the (standard) multiplicities when the graph is 'seen' from a 'base vertex'. In particular, for any node u, the local multiplicities of all eigenvalues sum up to 1:

$$\sum_{i=1}^{d} m_{ui} = 1. \quad (6)$$

In addition, the multiplicity of an eigenvalue is the sum of all its local multiplicities, namely [37]:

$$\sum_{u\in V} m_{ui} = m_i \quad \text{for } i = 1, 2, \ldots, d. \quad (7)$$

From a geometrical point of view, the local multiplicity m_{ui} corresponds to $\cos^2\beta_{ui}$, where β_{ui} is the angle between $\boldsymbol{e}_u$ and $\mathcal{E}_i$, as shown in Fig. 1 [40]. The local multiplicity concept has already been applied to different graphs considering eigenvalues of the adjacency matrix [38], [39], and it is extended to the Laplacian matrix in this paper. For example, it is known that the number of walks with length ℓ between nodes u and v in G having the adjacency matrix $\boldsymbol{A}$, is the $(u, v)^{th}$ element of $\boldsymbol{A}^\ell$. On the other hand, the number of circuits of length d through node u is:

$$\mathcal{C}_\ell(u) = \sum_{i=0}^{d} m_{ui}\mu_i, \quad (8)$$

where, now, $\mu_0 > \mu_1 > \cdots > \mu_d$ are the eigenvalues of the adjacency matrix with local multiplicities m_{ui}, for $i = 0, 1, \ldots, d$, at node u. In the next section, the local multiplicity concept is applied to discover spectrally important nodes of a complex network.

III. Node Ranking Using the Local Multiplicity

The importance of node u can be measured by its impact on a specific eigenvalue $\lambda_i (1 \le i \le d)$ of the Laplacian matrix of the graph when the node is removed. It is noted that the study of the impact of a node being removed from a graph, by considering its Laplacian spectrum, is more complicated than the case of the adjacency matrix where a removing node is represented by a simple row-column removal. Here, the removal of node u from a network is represented as removing the canonical basis $\boldsymbol{e}_u$ from $\mathbb{R}^N$. The idea of ranking nodes using local multiplicities is to measure the impact of such a removal on the kernel space of λ_i. Thus, the proposed metric can be applied to any eigenvalue and any graph topology.

Lemma 2. *[41] Any real symmetric matrix, as the Laplacian $\boldsymbol{L}$ or the adjacency matrix $\boldsymbol{A}$, has an orthogonal basis composed of its eigenvectors.*

It follows from this lemma that, for any undirected graph, resulting in symmetric $\lambda_i\boldsymbol{I} - \boldsymbol{L} (i = 1, 2, \ldots, d)$, the columns of $\boldsymbol{U}_i$ form an orthogonal set. Thus, $\boldsymbol{E}_i$ is a projection matrix corresponding to an orthogonal projection onto the eigenspace $\mathcal{E}_i$. The idea is to project the canonical basis of the vector space $\mathbb{R}^N$ onto $\mathcal{E}_i$ for any desired $i = 0, 1, \ldots, d$ and then rank the projected canonical basis vectors. The vector $\boldsymbol{e}_u$, related to node u of the graph with maximum projection size on $\mathcal{E}_i$, is a candidate for removal if the maximum impact on λ_i is desirable. On the other hand, suppose $\boldsymbol{e}_u$ and $\boldsymbol{e}_v$ are the u^{th} and the v^{th} canonical bases of $\mathbb{R}^N$ corresponding to nodes u and v, respectively. Consider the case where the angle between $\boldsymbol{e}_v$ and $\mathcal{E}_i$ is bigger than that of $\boldsymbol{e}_u$, that is, $\beta_2 > \beta_1$, namely $(\boldsymbol{E}_i)_{vv} < (\boldsymbol{E}_i)_{uu}$. This means that the removal of node u impacts λ_i more than the removal of v due to the following theorem.

Theorem 3. *The larger the u-local multiplicity $m_{ui} = (\boldsymbol{E}_i)_{uu}$ is, the higher $\Delta\lambda_i$, caused by removing the node u, will be.*

Proof. This can be justified by using the adjacency matrix $\boldsymbol{A}$, with spectrum $\{\mu_0^{m_0}, \mu_1^{m_1}, \ldots, \mu_d^{m_d}\}$, and characteristic polynomial $\psi_G(\lambda) = \det(\lambda\boldsymbol{I} - \boldsymbol{A})$. Then, since the adjacency matrix of $G\backslash u$ is obtained from $\boldsymbol{A}$ by deleting the u^{th} row and column, the characteristic polynomial of the node-removed subgraph is the (u, u)-cofactor of $(\lambda\boldsymbol{I} - \boldsymbol{A})$. Indeed, recall that the inverse of a square matrix $\boldsymbol{M}$ is $\boldsymbol{M}^{-1} = \frac{1}{\det M}\operatorname{adj}(\boldsymbol{M})$, where $\operatorname{adj}(\boldsymbol{M})$ is the adjoint (or transpose of the cofactor matrix) of $\boldsymbol{M}$. Then, in the present case with $\boldsymbol{M} = \lambda\boldsymbol{I} - \boldsymbol{A}$, one has:

$$\begin{aligned}\psi_{G\backslash u}(\lambda) &= \det(\lambda\boldsymbol{I} - \boldsymbol{A})((\lambda\boldsymbol{I} - \boldsymbol{A})^{-1})_{uu} \\ &= \psi_G(\lambda)((\lambda\boldsymbol{I} - \boldsymbol{A})^{-1})_{uu} = \psi_G(\lambda)\sum_{j=0}^{d}\frac{m_u(\mu_j)}{\lambda - \mu_j},\end{aligned} \quad (9)$$

where Theorem 1(iv) has been used with $f(x) = \psi_G(\lambda)\sum_\lambda \frac{1}{\lambda - x}$, which is well-defined when λ is an eigenvalue of $\boldsymbol{A}$. For the Laplacian, the reasoning is similar, but (9) is only an approximation if the network has many nodes. The reason is that, in the principal submatrix obtained by deleting the u^{th} row and column of the Laplacian, each v^{th} diagonal entry, with v being adjacent to u, should be decreased by one unity. However, if the network has many nodes, the two matrices (the obtained principal submatrix and the Laplacian of $G\backslash u$) are very similar in the sense that the matrix norm of its difference is small.

From (9), one can deduce the known result (see, for instance, [37]) that the (not necessarily distinct) eigenvalues of the adjacency matrix of $G\backslash u$, say $\tau_1 \leq \tau_2 \leq \cdots \leq \tau_{N-1}$, interlace the eigenvalues $\omega_1 \leq \omega_2 \leq \cdots \leq \omega_N$ of the adjacency matrix of G. That is,

$$\omega_1 \leq \tau_1 \leq \omega_2 \leq \tau_2 \leq \cdots \omega_{N-1} \leq \tau_{N-1} \leq \omega_N.$$

where we have used the symbol ω instead of μ to represent non-repetitive eigenvalues of the adjacency matrix. This is because the numerators (local multiplicities) of the (partial fraction expansion of the) function

$$\zeta(\lambda) = \frac{\psi_{G\backslash u}(\lambda)}{\psi_G(\lambda)} = \sum_{j=0}^{d} \frac{m_u(\mu_j)}{\lambda - \mu_j} \tag{10}$$

are non-negative (and sum up to 1). Then, the derivative $\zeta'(\lambda)$ is negative for all real values of λ, except where it has asymptotes, that is at the zeros of $\psi_G(\lambda)$. In particular, there must be a zero of $\psi_{G\backslash u}(\lambda)$, say $\tau = \mu'_i$, between each pair of consecutive zeros μ_i and μ_{i+1}, of $\psi_G(\lambda)$. So, we are interested in knowing what is the vertex u that results in the maximum increment $\Delta_i = \mu'_i - \mu_i$. But, when $\Delta_i \neq 0$ (which usually happens in the case when the multiplicity of μ_i is one), we observe that the sum of the two terms $\frac{m_{ui}}{\lambda-\mu_i}$ and $\frac{m_{u,i+1}}{\lambda-\mu_{i+1}}$ in (10), where $m_{ui} + m_{u,i+1} \leq 1$, gives rise to a greater Δ_i (μ'_i closer to μ_{i+1}) when m_{ui} is large, as we claimed. Of course, this is an approximation suggested by the simpler case of having only two terms, where the function $\xi(\lambda) = \frac{m_{ui}}{\lambda-\mu_i} + \frac{1-m_{ui}}{\lambda-\mu_{i+1}}$ has a zero at $\mu'_i = \mu_i + m_{ui}(\mu_{i+1} - \mu_i)$. Since the u-local multiplicities sum up to 1, a more involved analysis shows that, in general, the same relationship between u-local multiplicities of μ_i and large increments Δ_i holds. We can use a similar reasoning by using the Laplacian, and conclude the proof. □

Corollary 3. *Let $\boldsymbol{x}_i$ be the eigenvector associated with the eigenvalue λ_i of a network with simple spectrum without repeated eigenvalue. Removing node u with maximum $(\boldsymbol{x}_i)_u^2$ results in maximum impact on λ_i.*

Proof. For a network with simple spectrum, one has $\mathrm{Ker}(\lambda_i \boldsymbol{I} - \boldsymbol{L}) = \langle \boldsymbol{x}_i \rangle$, which means that $\mathcal{E}_i$ is generated only by the eigenvector $\boldsymbol{x}_i$. This results in $(\boldsymbol{E}_i)_{uu} = (\boldsymbol{x}_i)_u^2$, meaning that the u^{th} diagonal element of $\boldsymbol{x}_i \boldsymbol{x}_i^\top$ reflects the impact on λ_i caused by the removal of node u. □

Remark 1. *In our previous work [12], we identified node u with the maximum $(\boldsymbol{x}_N)_u^2$, where $\boldsymbol{x}_N$ is associated with the largest (positive) eigenvalue of $\boldsymbol{L}$, as the best node to be controlled for achieving synchrony over the widest range of coupling parameters. In this paper, it is proposed to remove node u with the maximum $(\boldsymbol{E}_i)_{uu}$ when the highest impact on the i^{th} eigenvalue of the Laplacian (or the adjacency matrix) is desired. One can see that the present paper, where the study is not restricted to any specific eigenvalue, is a generalization of our previous work. The new metric is also applicable to graphs with repeated eigenvalues in the corresponding Laplacian matrix.*

Remark 2. *Suppose $0 = \lambda_1 < \lambda_2 \leq \lambda_3 \leq \cdots \leq \lambda_N$ are eigenvalues of the Laplacian matrix of the graph G and $0 = \lambda'_1 < \lambda'_2 \leq \cdots \leq \lambda'_{N-1}$ are those for $G\backslash u$. Following the above discussions, one has $\Delta\lambda_i = \lambda'_i - \lambda_i$ for $i = 2, 3, \cdots, N-1$, where the maximum happens when node u with maximum m_{ui} is removed. For $i = N$, define the variation of spectral radius as $\Delta\lambda_N = \lambda_N - \lambda'_{N-1}$. From the discussions on Eq. (10), one has $\lambda'_{N-1} = \lambda_{N-1} + m_{u(N-1)}(\lambda_N - \lambda_{N-1})$, which can be written as $(\lambda_N - \lambda'_{N-1}) = (\lambda_N - \lambda_{N-1}) - m_{u(N-1)}(\lambda_N - \lambda_{N-1}) = (\lambda_N - \lambda_{N-1})(1 - m_{u(N-1)})$. On the other hand, it has been shown that $m_{u(N-1)} + m_{uN} \leq 1$; thus, $\Delta\lambda_N \geq m_{uN}(\lambda_N - \lambda_{N-1})$, which means that node u with maximum m_{uN} can cause the maximum variation of the spectral radius.*

Example 1. A fully connected undirected graph of $N = 100$ nodes is considered with random weights $w_{ij} = w_{ji} \in (0, 1]$ on all (i, j) links. By performing an eigen-decomposition of the Laplacian matrix, the principal idempotents $\boldsymbol{E}_2$ and $\boldsymbol{E}_N$, associated with the Kernel spaces of λ_2 and λ_N respectively, are calculated. For the u^{th} node, the u^{th} diagonal elements of $\boldsymbol{E}_2$ and $\boldsymbol{E}_N$ are listed in Table I, in the columns of local multiplicities m_{u2} and m_{uN}. The increments $\Delta\lambda_2 = \lambda'_2 - \lambda_2$ and $\Delta\lambda_N = \lambda_N - \lambda'_{N-1}$ are calculated for removing each node of the graph, where the prime refers to the graph after removing the node. Table I compares local multiplicities m_{u2} and m_{uN} with $\Delta\lambda_2$ and $\Delta\lambda_N$. It shows that the local multiplicity m_{u2} of λ_2 takes the maximum of 0.7382 at node 65. At the same time, $\Delta\lambda_2 = 0.5137$ at this node, which is also the maximum in the $\Delta\lambda_2$ column. A similar result is obtained at node 54 for m_{uN} and $\Delta\lambda_N$. It is therefore concluded that m_{u2} and m_{uN} can precisely identify nodes whose removal result in maximum $\Delta\lambda_2$ and $\Delta\lambda_N$, respectively. It is worth noting that m_{u2} can identify the node whose removal results in a positive increase of λ_2, $\Delta\lambda_2 > 0$, despite the fact that other removed nodes normally decrease it. Thus, this approach suggests a useful method for increasing the algebraic connectivity of a graph by node removal.

This example is presented only to clarify how the performance of our proposed metric can be studied. Performance acceptance test of the metric absolutely requires extensive simulations in networks with different SF, WS and ER topologies, which will be presented in section IV.

A. Dealing with directed graphs

The majority of research activities in spectral graph theory deals with undirected graphs, where eigenvalues are real, and eigenvectors form an orthogonal basis. In directed graphs, however, eigenvalues of the Laplacian matrix are typically not real. Besides, eigenvectors corresponding to these eigenvalues may not form an orthogonal basis. This means that the local multiplicity metric of Definition 2 cannot be directly applied to directed graphs.

In order to extend the above metric to digraphs, suppose that w_{ij} is the weight of the link from node i to node j in the directed graph $\overrightarrow{G} = (V, E)$. Then, define the probability transition matrix $\boldsymbol{P} = (p_{ij})$, in which $p_{ij} = w_{ij}/d^+(i)$. $d^+(i)$ is the *outdegree* of node i, that is, $d^+(i) = \sum_{i \to j} w_{ij}$, where

Table I: Comparing the local multiplicity of λ_2 and λ_N at each node with $\Delta\lambda_2$ and $\Delta\lambda_N$ when the node is removed.

Node #	m_{u2}	m_{uN}	$\Delta\lambda_2$	$\Delta\lambda_N$
1	0.0002	0.0018	-0.3614	0.2308
2	0.0001	0.0001	-0.2153	0.6545
3	0.0003	0.0006	-0.6379	0.6555
⋮	⋮	⋮	⋮	⋮
53	0.0002	0.0005	-0.6562	0.6952
54	0.0002	**0.7381**	-0.4374	**1.0222**
55	0.0019	0.0001	-0.4256	0.3933
⋮	⋮	⋮	⋮	⋮
64	0.0021	0.0072	-0.7388	0.3877
65	**0.7382**	0.00003	**0.5137**	0.3989
66	0.0010	0.0015	-0.2238	0.7669
⋮	⋮	⋮	⋮	⋮
99	0.0036	0.0002	-0.0840	0.5156
100	0.00003	0.0017	-0.4498	0.2180

$i \to j$ shows that there is an arc from node i to node j. Clearly, $\boldsymbol{P}\mathbf{1} = \mathbf{1}$. The Perron-Frobenius theorem states that, if $\overrightarrow{G}$ is strongly connected and aperiodic, then there exists a unique positive vector $\boldsymbol{\phi} = (\phi_u)$, also called Perron vector, which satisfies $\boldsymbol{\phi}\boldsymbol{P} = \boldsymbol{\phi}$ and $\boldsymbol{\phi}\mathbf{1}^\top = 1$ [42]. Define the diagonal matrix $\boldsymbol{\Phi}$ with non-zero elements being the square roots of the elements of $\boldsymbol{\phi}$, that is, $(\boldsymbol{\Phi})_{uu} = \phi_u^{1/2}$. The *directed Laplacian* of $\overrightarrow{G}$ is then defined as

$$\overrightarrow{\boldsymbol{\mathcal{L}}} = \boldsymbol{\mathcal{L}}(\overrightarrow{G}) = \boldsymbol{I} - \frac{1}{2}\left(\boldsymbol{\Phi}\boldsymbol{P}\boldsymbol{\Phi}^{-1} + \boldsymbol{\Phi}^{-1}\boldsymbol{P}^\top\boldsymbol{\Phi}\right). \tag{11}$$

The following lemma relates $\overrightarrow{\boldsymbol{\mathcal{L}}}$ to the Laplacian matrix of the corresponding undirected graph.

Lemma 4. *[42] Let $\overrightarrow{G}$ be an aperiodic strongly connected weighted directed graph and let H be a weighted undirected graph, on the same vertex set as $\overrightarrow{G}$, and with weights defined by $w_{ij} = \phi_i p_{ij} + \phi_j p_{ji}$. Then,*

$$\boldsymbol{\mathcal{L}}(\overrightarrow{G}) = \boldsymbol{\mathcal{L}}(H). \tag{12}$$

In other words, the strongly connected weighted digraph $\overrightarrow{G}$ is converted to an undirected weighted connected graph with the normalized Laplacian matrix $\boldsymbol{\mathcal{L}}(H)$. We will show by simulations that this transformation preserves the centrality of nodes in terms of their local multiplicities. That is, central nodes of $\boldsymbol{\mathcal{L}}(\overrightarrow{G})$ are the same as those of $\boldsymbol{\mathcal{L}}(H)$.

From the analytical results of this section, it can be concluded that the concept of local multiplicity, if extended to the Laplacian matrix, can be applied to identify the most influential nodes from a graph spectrum perspective, which are indeed vital nodes in collective dynamical behaviour of networked systems. Simulations provided in the next section convincingly support these findings.

IV. Simulation Results

In this study, synthetic networks with typical Barabási-Albert (BA) scale-free, Watts-Strogatz (WS) small-world, and Erdös-Rényi (ER) random network structures are considered. BA networks are constructed using the preferential attachment algorithm of the original model, by first constructing a fully-connected network with a number of nodes, and then adding nodes and creating links to old nodes with a probability proportional to their degrees [49]. The probability of creating a link between the newly added node and the existing node i is $(d(i)+B)/\Sigma_j(d(j)+B)$, where $d(i)$ is the degree of node i and B is a constant controlling the heterogeneity of the network: as B increases, heterogeneity of the network decreases. WS networks are constructed starting from a ring network, where nodes are connected to their m nearest neighbours, and then by rewiring all the links with the same probability p [50]. ER networks are constructed by independently placing a link between any pair of nodes with probability p. In the case of directed graphs, 30% of links of the generated graph are randomly chosen and random directions are placed on them. Also, for weighted cases, a random weight value taken from the range $(0, 1]$ is assigned to each link of the underlying network.

A. Relationship between the spectral impact and local multiplicity

The main claim of this paper is that removing node u with higher local multiplicity of λ_i, i.e. higher $(\boldsymbol{E}_i)_{uu}$, impacts λ_i more than when other nodes are removed. Here, it is studied for λ_2 and λ_N in synthetic networks with different BA, WS and ER topologies. $(\boldsymbol{E}_2)_{uu}$ is first calculated for all nodes of the network by using the equation $\boldsymbol{E}_2 = \boldsymbol{U}_2\boldsymbol{U}_2^\top$. The increment $\Delta\lambda_2$ is also measured for all nodes by removing them one by one and performing an eigenvalue calculation. This process is repeated for $(\boldsymbol{E}_N)_{uu}$ and $\Delta\lambda_N$ and results are shown in Fig. 2(a). This figure shows that $\Delta\lambda_2$ $[\Delta\lambda_N]$ is a monotonically increasing function of $(\boldsymbol{E}_2)_{uu}[(\boldsymbol{E}_N)_{uu}]$ regardless of the network topology. Fig. 2(a) also shows that spectral impact of a node removal on networks with BA and ER topologies is stronger than those with WS topology which is in accordance with small-world features of the WS networks. The relationship between $\Delta\lambda_2$ $[\Delta\lambda_N]$ and $(\boldsymbol{E}_2)_{uu}[(\boldsymbol{E}_N)_{uu}]$ become close to linear for large enough values of the local multiplicity.

To further study the relationship between local multiplicity of nodes and their Laplacian spectral impact, the Kendall's rank correlation τ between the vector containing local multiplicity of nodes and that of $\Delta\lambda_N$ caused by removing each node is considered. Figure 3 shows the results on SF, WS and ER networks with $N = 200$ nodes and different topologies. The correlation value in SF networks is larger than 50% almost always, regardless of the average degree and heterogeneity of the graph. Smaller, yet rather strong, correlation exists in WS and ER networks.

B. Algebraic connectivity

Here, we begin by studying the impact of a node removal on the algebraic connectivity of a graph, i.e. λ_2 of its Laplacian matrix. Features of λ_2, such as being monotone increasing in the link set [43], make it a reliable measure of how well-connected a graph is [44]. Practically, modification of the algebraic connectivity λ_2 can be easier done by removing than by

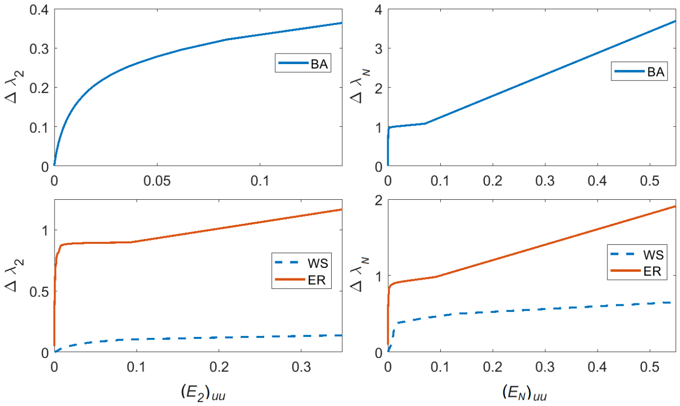

Figure 1. The relationship between the local multiplicity $(\boldsymbol{E}_2)_{uu}[(\boldsymbol{E}_N)_{uu}]$ and $\Delta\lambda_2$ $[\Delta\lambda_N]$ caused by the removal of node u, in networks with BA, WS and ER topologies. Results are averaged over 1000 iterations.

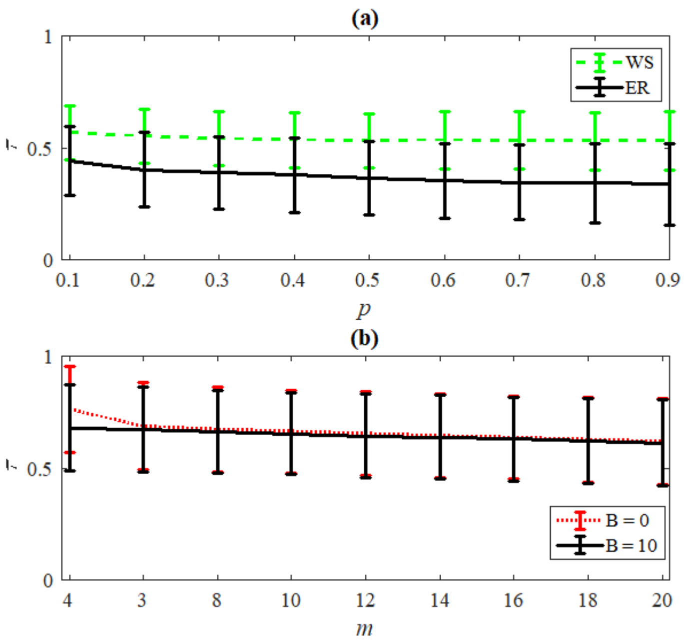

Figure 2. Kendall's rank correlation between node centrality and $\Delta\lambda_N$ caused by removing each node of a network with (a) WS or ER, and (b) SF topologies.

adding nodes [28]. Therefore, targeted node removal for maximum increase in λ_2 is of particular interest. The maximum local multiplicity of λ_2 is applied to identify the node when the maximum influence on λ_2 by node removal is desired. First, calculate $\boldsymbol{E}_2 = \boldsymbol{U}_2\boldsymbol{U}_2^\top$ using eigen-decomposition of the Laplacian, and then rank the nodes based on the diagonal elements of $\boldsymbol{E}_2$, i.e. $(\boldsymbol{E}_2)_{uu}$. The performance is compared using some heuristic methods including various metrics of degree-, betweenness- and closeness-centrality.

To study the precision of the new metric proposed in this paper, the node whose removal causes the maximum variation in λ_2 is first obtained. To this end, we follow the time-consuming process of removing nodes one by one and measuring $\Delta\lambda_2$. The nodes are then ranked based on $\Delta\lambda_2$ to obtain a ground-truth for comparing the performances of other metrics. Then, we remove the node u which is identified by our computationally efficient metric and $\Delta\lambda_2^u$ is calculated. Finally, the precision of the new metric is calculated as $P = [\Delta\lambda_2^u - \min(\Delta\lambda_2)]/[\max(\Delta\lambda_2) - \min(\Delta\lambda_2)]$, so that $P \in [0, 1]$. For example, $P = 90\%$ shows that if the node predicted by our metric is removed, $\Delta\lambda_2$ will be 90% of the maximum possible value, within the interval $[\min\Delta\lambda_2, \max\Delta\lambda_2]$, that may happen by a node removal in the network. This precision is also calculated for heuristic centrality metrics. Although these heuristics are not directly related to the algebraic connectivity by their definitions, they are still the first that comes to mind when one is looking for vital nodes. Figure 4 compares the precisions of the proposed metric with that of the heuristic centrality measures in BA scale-free networks. It clearly shows almost 100% identification of the node with the maximum impact on λ_2 using local multiplicity, regardless of the level of network heterogeneity (Figs. 4(A) to (C)). Degree centrality shows a poor performance in dense networks while betweenness and closeness centrality measures are not much sensitive to the average degree.

The performances of the new metric on WS and ER networks are again close to perfect, and much better than the heuristics (Fig. 5). Among the heuristic methods, degree and betweenness centrality measures show almost the same precision, which is less than 50% for $p > 0.2$. Closeness centrality has the poorest performance with precision less than 20%. We further studied the performance of our proposed metric in networks with different assortativity level. To this end, Erdös-Rènyi networks with different assortativity levels are generated and the metric is applied to them in order to identify the node with maximum impact on the algebraic connectivity λ_2 (Fig. 6). Assortativity shows the tendency of nodes of a complex network to get connected to similar nodes [45], e.g. nodes with the same degree in the case of degree assortativity. Pearson correlation quantifies degree assortativity: It is zero for no assortative mixing and positive or negative for assortative or disassortative mixing, respectively [45].

In Fig. 6, assortativity of the network is changed from $\sigma = -0.5$ to $\sigma = +0.5$, where σ is the Pearson correlation, by performing degree-preserving random rewiring on an initial ER graph. It shows that the performance of our proposed metric is better in disassortative networks. Its performance drops in assortative networks while it is still better than 90%. Precisions of other heuristics methods are less than 30%.

The precision of the proposed local multiplicity-based metric in finding the node with the maximum impact on λ_2 is also studied in directed graphs. Figures 7 and 8 show the precisions of our proposed metric in directed and weighted networks with BA, WS and ER topologies, respectively. A directed and weighted network is first converted to its undirected underlying graph using the Lemma 3 in Section III. The central node is then selected from ranking nodes based on local multiplicities of λ_2 at each of them. In other words, the node with maximum impact on λ_2 of the normalized Laplacian matrix of the undirected graph is the most influential one of its directed peer. Figure 7 shows that the accuracy of this approach in predicting the most influential node in directed BA graphs

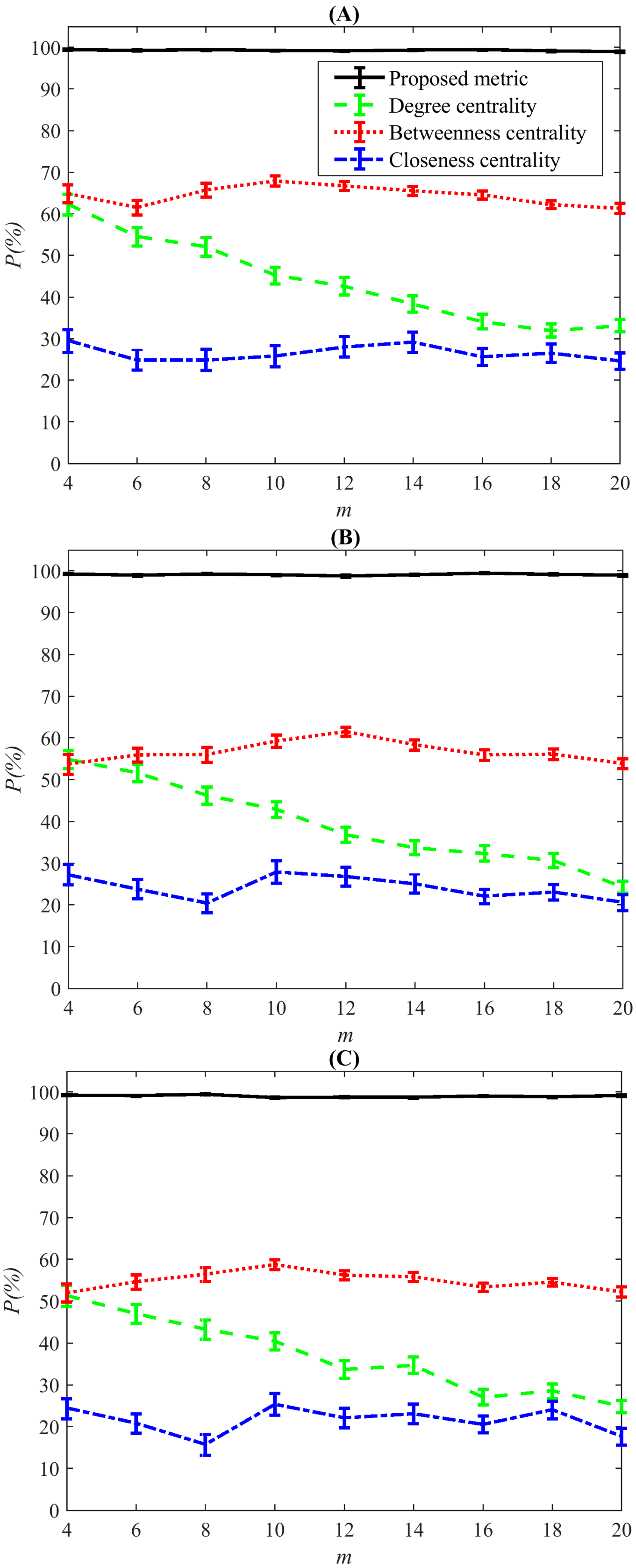

Figure 3. The precision of the proposed local multiplicity-based metric in predicting the node with the maximum influence on λ_2 in networks with BA topology having average degree m and (A) $B = 0$, (B) $B = 5$, and (C) $B = 10$.

increases in networks with high average degree values. Results are not sensitive to the network heterogeneity and an accuracy higher than 90% can be achieved for dense networks. Figure 8 shows that the proposed metric works more accurately for directed WS networks than ER networks, and the results are not much sensitive to the value of p in these networks.

C. Spectral radius

Here, finding the node whose removal causes the maximum reduction in the spectral radius, i.e. the largest eigenvalue of the Laplacian matrix of a graph, is studied. The precision of the proposed local multiplicity-based metric is again compared with heuristic methods. The way of calculating the precision P is the same as that for the algebraic connectivity. Here, only results in directed and weighted networks are presented, since the proposed metric works perfectly and outperforms the others.

Figures 9 and 10 depict this comparison in synthetic directed and weighted networks with BA, WS and ER topologies, respectively. From these figures, one can conclude that the performance of the proposed metric is always better than 70%, regardless of the network structure, level of heterogeneity and the average degree. Interestingly, the performance of the metric on BA networks is not particularly sensitive to the level of the heterogeneity. While the accuracy in directed WS graphs is not much sensitive to the value of p, the accuracy in ER graphs improves as the randomness increases.

D. Laplacian centrality

Laplacian centrality of a node [27] has been introduced based on the concept of Laplacian energy, which is defined as $E_L(G) = \Sigma_i \lambda_i^2$ for the graph G with eigenvalues λ_i of the Laplacian matrix. Central nodes are those whose removal causes higher energy drops. Thus, ranking nodes based on their importance needs N eigen-decompositions of the Laplacian matrix, where N is the number of nodes. This is a computationally expensive process for large networks. Here, based on the concept of local multiplicity, a new function is defined as $\bar{E}_L(G) = \Sigma_i (\boldsymbol{E}_i)_{uu}$. We show that $\bar{E}_L(G)$ is a computationally simple yet precise enough approximation for $E_L(G)$.

To study the precision of $\bar{E}_L(G)$ in finding central nodes, we first construct the ground-truth by measuring the drop in Laplacian energy $E_L(G)$ after removing each node. Then, we apply $\bar{E}_L(G)$ which can clearly rank nodes faster. Columns (A) and (B) in Fig. 11 show how precise $\bar{E}_L(G)$ can identify the central node for Laplacian energy in BA, WS and ER networks, respectively. For example, $P = 60\%$ shows that the impact of the node predicted by $\bar{E}_L(G)$ on the Laplacian energy, when the node is removed, is 60% of maximum possible energy drop. Upper panel of Fig. 11(A) shows that in BA networks, the precision of $\bar{E}_L(G)$ in finding the most important node is at least 60% on average, regardless of the heterogeneity level of the network. This precision increases as the average degree of the network increases. The Kendall correlation τ between ranks by using $\bar{E}_L(G)$ and $E_L(G)$ is also displayed in the lower panel of Fig. 11(A), showing

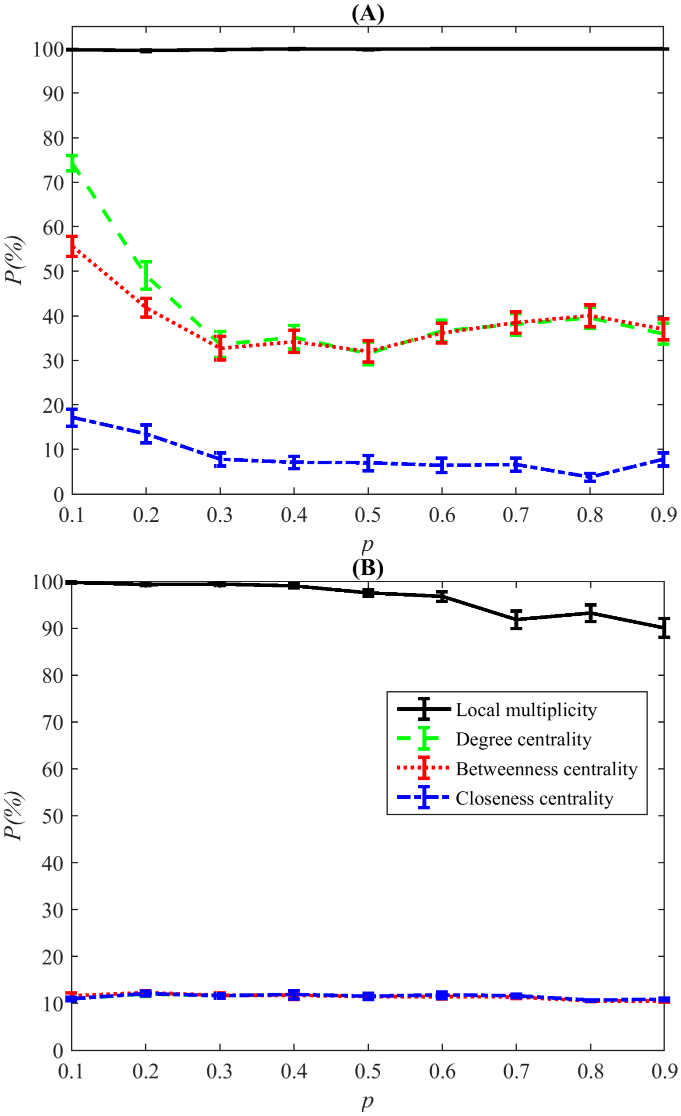

Figure 4. The precision of the proposed local multiplicity-based metric in predicting the node with the maximum influence on λ_2 in networks with $N = 200$ nodes and with (A) WS and (B) ER topologies.

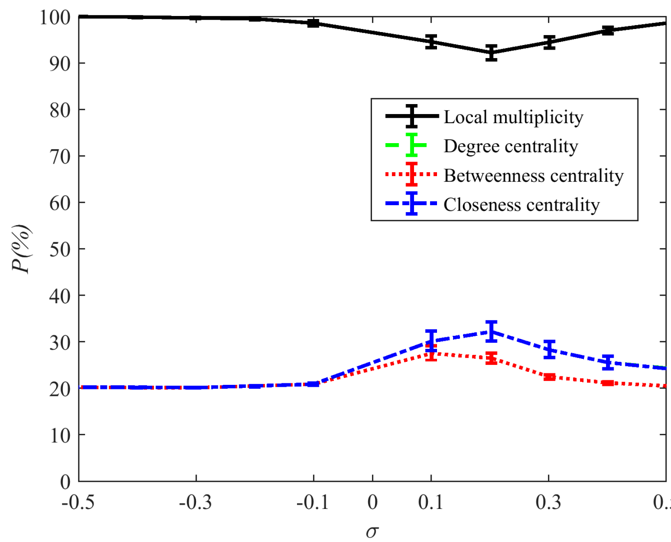

Figure 5. Precision in finding the node whose removal causes a maximum impact on algebraic connectivity in random ER networks with wiring probability $p = 0.5$ and different assortativity level σ.

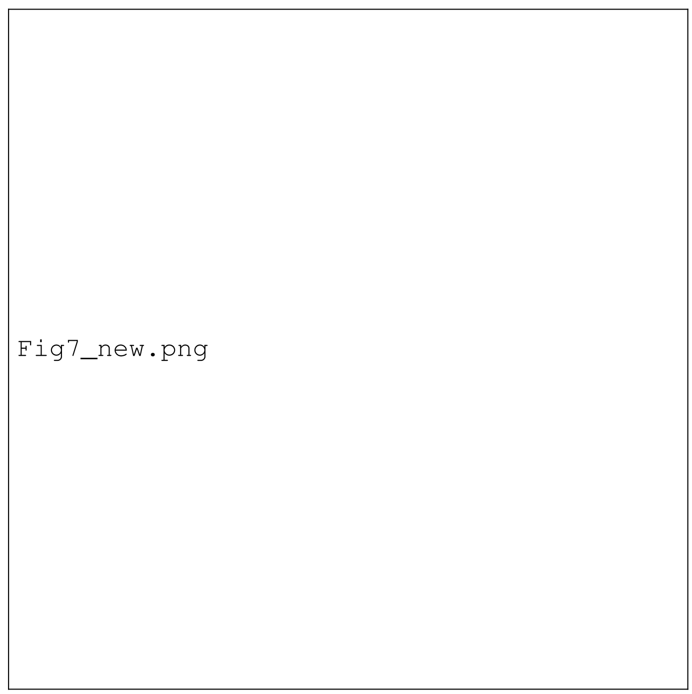

Figure 6. The precision of the proposed local multiplicity-based metric in predicting the node with the maximum influence on λ_2 in directed weighted networks with BA topology and average degree m.

the correlation of almost 80% in networks with high average degree values.

The precision of this approximation is better in WS and ER networks (Fig. 11(B)). The upper panel of Fig. 11(B) shows that the precision of the proposed metric is always better than 75%, while it performs more precisely for ER networks. The precision of $\bar{E}_L(G)$ in WS networks decreases slightly as the network topology becomes closer to random. The Kendall correlation between ranks by $E_L(G)$ and $\bar{E}_L(G)$ is higher than 80% in ER and better than 70% in WS networks, as shown in the lower panel of Fig. 11(B). These correlations are all averaged over 100 realisations.

Figures 12 and 13 show the results when simulations are repeated in directed and weighted networks with BA, WS and ER topologies. In BA networks (Fig. 12), the precision of $\bar{E}_L(G)$ in approximating $E_L(G)$ increases as the number of links in the network increases. Here, the precision is always higher than 90%, regardless of the heterogeneity level of the network. Figure 13 depicts that the proposed metric works perfectly for WS and ER networks. Based on the present study, one can consider $\bar{E}_L(G)$ as a computationally cost-effective alternative for $E_L(G)$ in ranking nodes based on the Laplacian centrality.

E. Application on an example power grid

To study a real network, we apply our metric to the power grid of the Western States of the United States of America, which includes $N = 4941$ nodes and $E = 6594$ links, which

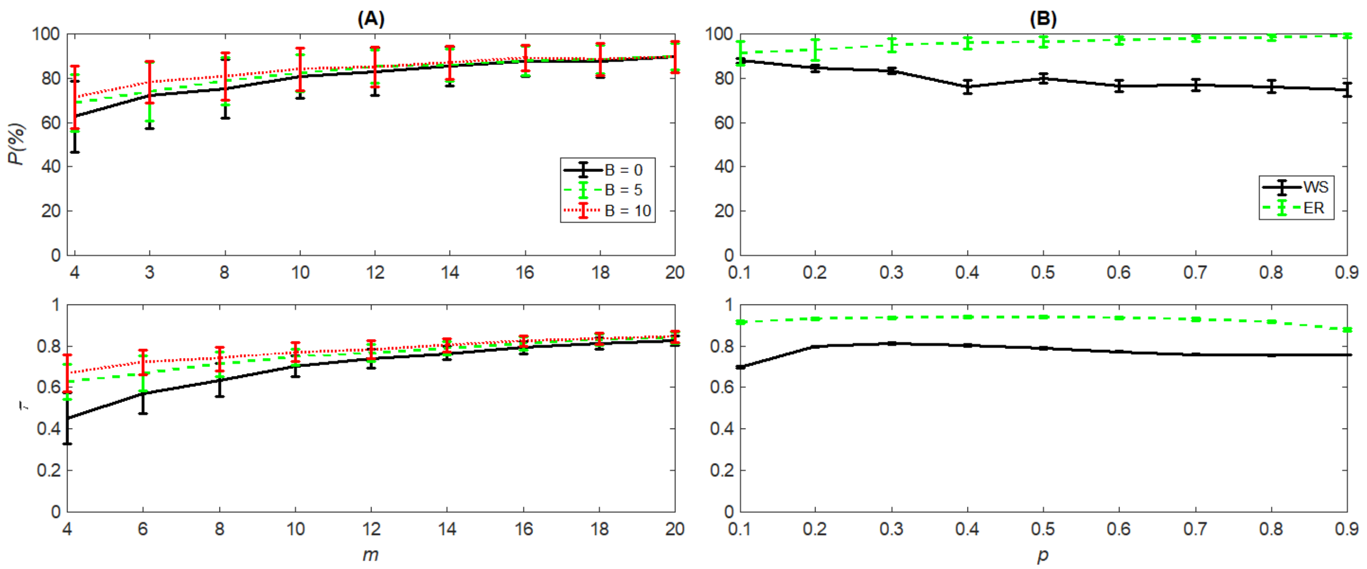

Figure 10. The precision of the $\bar{E}_L(G)$ in predicting central nodes based on the Laplacian centrality concept. Networks with $N = 200$ nodes and BA topologies are reported in column (A) where those with WS and ER topologies are in column (B). In each column, the upper figure is precision of $\bar{E}_L(G)$ and the lower one is the Kendall correlation between rankings of $\bar{E}_L(G)$ and $E_L(G)$. Results are averaged over 100 realizations.

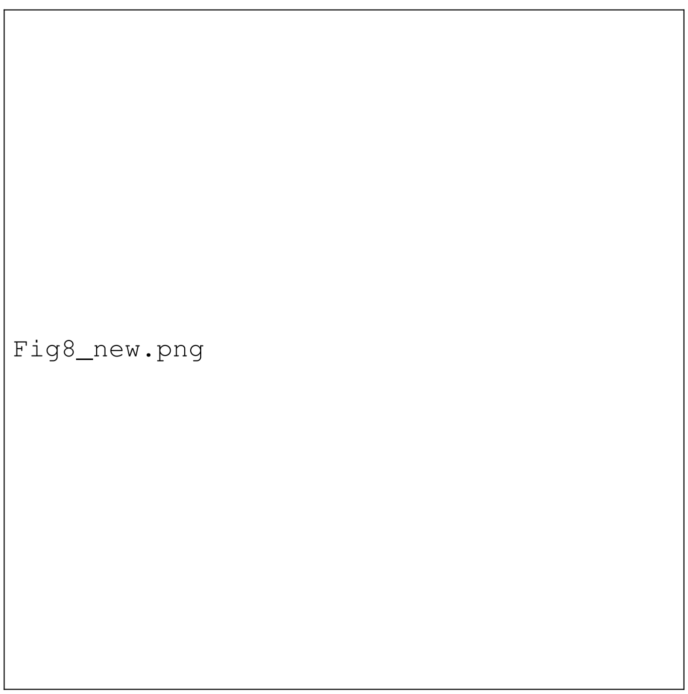

Figure 7. The precision of the proposed metric in predicting the node with the maximum influence on λ_2 in directed weighted networks with WS and ER topologies.

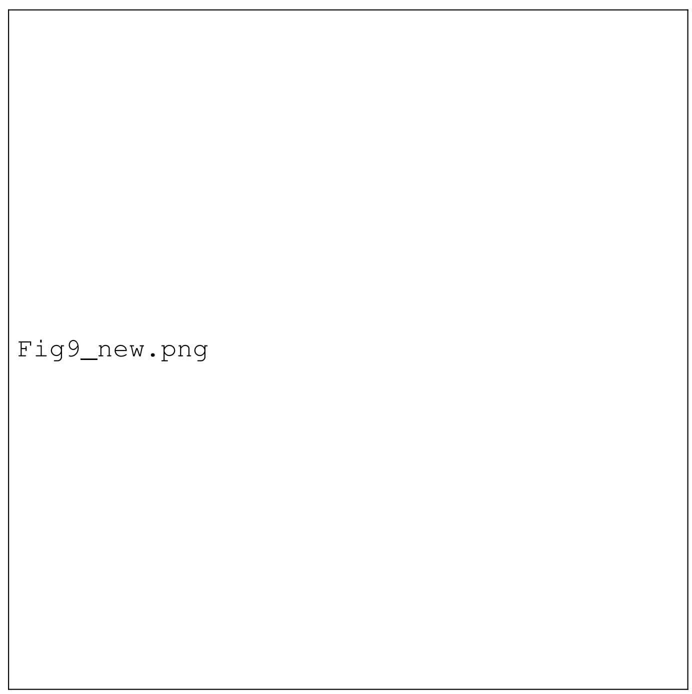

Figure 8. The precision of the proposed metric in predicting the node with maximum influence on λ_N in directed weighted networks with BA topology with $N = 200$ nodes and average degree m.

are randomly weighted. The topology of a power network affects its performance in voltage and frequency stability [46]–[48]. Here, we apply our local multiplicity (LM) based metric to find nodes with maximum impact on λ_2 and λ_N of the power grid, and compare its performance with degree (Deg) and betweenness centrality (BC) metrics. The same process explained in parts *A* and *B* is performed to achieve the ground-truth and derive the precision of our local multiplicity-based metric. Table II shows that our metric can identify the most influential node on λ_2 with precision $P = 66\%$, meaning that the predicted node has 66% of the maximum possible impact on λ_2 in this network. The precision is perfect in the case of λ_N. The degree centrality metric works almost perfectly in identifying the most influential node on λ_N, but its performance is rather weak (36%) in the case of λ_2. The BC shows very good performance for λ_2 and the least

Fig10_new.png

Figure 9. The precision of the proposed metric in predicting the node with the maximum influence on λ_N in directed weighted networks with WS and ER topologies and $N = 200$ nodes.

Fig12_new.png

Figure 11. The precision of the $\bar{E}_L(G)$ in predicting central nodes based on the Laplacian centrality concept in directed weighted scale-free networks with $N = 200$ nodes and different heterogeneity levels.

Fig13_new.png

Figure 12. The precision of the $\bar{E}_L(G)$ in predicting central nodes based on the Laplacian centrality concept in directed weighted WS and ER networks with $N = 200$ nodes.

Table II: Identification of the most influential nodes for the American Western States power grid. τ_1 is the Kendall correlation between the whole ranking vector and the ground-truth and τ_2 is that for 25% top-rank nodes.

	Metric	$P(\%)$	τ_1	τ_2
λ_2	LM	66	0.48	0.69
	Deg	36	0.16	0.21
	BC	49	0.26	0.46
λ_N	LM	100	0.42	0.62
	Deg	98	0.06	0.11
	BC	60	0.03	0.03

precision for λ_N compared to other metrics. The Kendall correlation between the ground-truth vector and vector ranked by our metric is 0.48 for λ_2 and 0.42 for λ_N, confirming the significant correlation. This correlation calculation is also repeated for the top 25% of nodes which results in correlations of 0.69 and 0.62 for λ_2 and λ_N, respectively. This means that our proposed metric outperforms other metrics in precise identification of the most influential nodes on λ_2 and λ_N.

V. Conclusions and Future Directions

In this paper, a new node centrality measure based on the local multiplicity concept has been introduced, which can rank nodes of a graph according to their impacts on the spectrum of the network Laplacian matrix. Local multiplicity is a generalization of the network algebraic multiplicity when the network is viewed from a specific node. Nodes can be easily and accurately ranked based on their impacts on any desired eigenvalue of the Laplacian matrix using this local multiplicity-based metric. The proposed metric is computationally effective as it needs only one single eigen-decomposition of the Laplacian matrix and therefore, is advantageous for large-scale networks. Simulations have verified and demonstrated its accurate performances in ranking central nodes in both undirected and directed networks with different scale-free, small-world and random topologies. Following the investigation of this paper, some meaningful research questions, such as 'can this metric give guidelines for adding new nodes to a graph', 'what is the best minimum set of nodes to recover a networked system after a total failure', or 'developing a metric for multiple node removal', will be addressed in the future. In addition, the influence of removing an edge could be similarly evaluated by using the so-called crossed ij-local multiplicities (see [36]–[38]) with i and j being the end-vertices of the edge.

Acknowledgment

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Appendix A
Nomenclature

Symbol	Description
$\boldsymbol{L}$	Laplacian matrix.
$\boldsymbol{\mathcal{L}}$	Normalized Laplacian matrix.
$\boldsymbol{A}$	Adjacency matrix.
λ_i	i^{th} eigenvalue of the Laplacian matrix.
μ_i	i^{th} eigenvalue of the adjacency matrix.
$\mathrm{sp}(\boldsymbol{L})$	Spectrum of the Laplacian matrix $\boldsymbol{L}$.
$\mathcal{E}_i$	Kernel space of $\lambda_i \boldsymbol{I} - \boldsymbol{L}$.
$\boldsymbol{U}_i$	Matrix with columns forming an orthonormal basis of $\mathcal{E}_i$.
m_i	Multiplicity of the eigenvalue λ_i of the Laplacian matrix.
m_{ui}	Local multiplicity of λ_i at node u.
$\boldsymbol{E}_i$	The orthogonal projection onto $\mathcal{E}_i$.
$d(i)$	Degree of node i of the graph.
$d^+(i)$	Outdegree of node i of the graph.
$\boldsymbol{x}_i$	Eigenvector associated with eigenvalue λ_i.
$\boldsymbol{1}$	The all-1 vector.
δ_{ij}	The Kronecker delta.
$\boldsymbol{e}_k$	The k^{th} canonical basis vector of $\mathbb{R}^N$.
$E_L(G)$	Laplacian energy of the graph G.
$\overline{E}(G)$	An estimate of the Laplacian energy.