Graph eigenvectors, fundamental weights and centrality metrics for nodes in networks

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Abstract

Several expressions for the j-th component $(x_k)_j$ of the k-th eigenvector x_k of a symmetric matrix A belonging to eigenvalue λ_k and normalized as $x_k^T x_k = 1$ are presented. In particular, the expression

$$(x_k)_j^2 = -\frac{1}{c'_A(\lambda_k)} \det\left(A_{\setminus\{j\}} - \lambda_k I\right)$$

where $c_A(\lambda) = \det(A - \lambda I)$ is the characteristic polynomial of A, $c'_A(\lambda) = \frac{dc_A(\lambda)}{d\lambda}$ and $A_{\setminus\{j\}}$ is obtained from A by removal of row j and column j, suggests us to consider the square eigenvector component as a graph centrality metric for node j that reflects the impact of the removal of node j from the graph at an eigenfrequency/eigenvalue λ_k of a graph related matrix (such as the adjacency or Laplacian matrix). Removal of nodes in a graph relates to the robustness of a graph. The set of such nodal centrality metrics, the squared eigenvector components $(x_k)_j^2$ of the adjacency matrix over all eigenvalue λ_k for each node j, is "ideal" in the sense of being complete, *almost* uncorrelated and mathematically precisely defined and computable. Fundamental weights (column sum of X) and dual fundamental weights (row sum of X) are introduced as spectral metrics that condense information embedded in the orthogonal eigenvector matrix X, with elements $X_{ij} = (x_j)_i$.

In addition to the criterion "If the algebraic connectivity is positive, then the graph is connected", we found an alternative condition: "If $\min_{1\le k\le N}\left(\lambda_k^2(A)\right) = d_{\min}$, where $d_{\min}$ is the minimum degree in the graph, then the graph is disconnected."

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1 Introduction

Generally, nodal centrality metrics quantify the "importance" of a node[1] in a network or how "central" a node is in the graph. Many quantifiers of nodal "importance" have been proposed, that are reviewed in [2, 3, 4]. Perhaps, the simplest – both in meaning as well as in computation – is the degree of a node defined as the number of direct neighbors of a node in the network. Relevant questions such as "What is the most influential node in a social networks?" [5] and "What is the most vulnerable node when attacked or removed?" are difficult to answer, because a precise translation of "influence" or "vulnerability" in terms of computable quantities, called metrics [6], of the graph is needed. Nodal "importance" often depends on the process on the network, which then further specifies the precise meaning of importance with respect to that process. For example, in epidemics on networks [7], nodal importance (here vulnerability) can be defined as the long-run probability that a node is infected [8], given an effective infection rate τ of the virus. The most "influential" spreader can be defined as the fastest spreader, that, when initially injected with information, reaches in the shortest time the metastable fraction of infected nodes, again given an effective infection rate τ. Both the nodal ranking in vulnerability and the fastest spreader change with effective infection rate τ, clearly illustrating that only topological metrics are inadequate to determine the "most important" node.

Besides the precise definition, meaning and applicability or usefulness of a graph metric, a number of other issues appear as elaborated in [9]: How many metrics are needed to compare graphs? How strongly is a set of two metrics correlated? How difficult is the computation of the metric and how much information of the network is required (only local information as the degree or global information as for the diameter)? In most cases, more than one metric is needed to quantify the desired "importance". For example, a high-degree node of which all neighbors have degree 1 and one neighbor has degree 2, is vulnerable to be disconnected from the remainder of the network, in spite of its high degree. When multiple metrics are chosen, they should be as independent or orthogonal as possible, because strongly correlated metrics can be combined to a single one, since they all reflect the same type of "importance" as illustrated in [10].

Here, we take a different view. We present a complete set of orthogonal centrality metrics and try to interpret what type of properties in the network they may characterize or quantify. As reviewed in Appendix A, a non-zero vector $x(\lambda)$ only satisfies the eigenvalue equation

$$Ax(\lambda) = \lambda\, x(\lambda)$$

if the real number λ, which we can interpret as a "frequency", is an eigenvalue of an $N \times N$ symmetric matrix A such that $x_k = x(\lambda_k)$ is the eigenvector at eigenfrequency $\lambda = \lambda_k$. We normalize x_k so that $x_k^T x_k = 1$, according to the *first* [11] orthogonality equations (64) and denote the j-th eigenvector component by $(x_k)_j$, where the index j refers to nodes and the index k to eigenfrequencies. Two different expressions (3) and (18) for the *square* of the j-th component of the k-th eigenvector $(x_k)_j$ of the adjacency matrix A belonging to eigenvalue λ_k are presented in Section 2. The determinantal expression (3) is derived in Section 2.1, essentially using merely linear algebra. The walk-based expression (18) for $(x_k)_j^2$, as consequence of earlier results, is incorporated for reasons of completeness

[1] The importance of a link in G can be assessed as the importance of a node in the corresponding line graph $l(G)$, defined in [1, p. 17-21].

in Section 2.2 and because it gives another interpretation of $(x_k)_j^2$ in terms of closed walks, starting and ending at node j. Section 2.3 interprets expression (3) for $(x_k)_j^2$ as the *impact of the removal of node j from G at eigenfrequency λ_k* of a symmetric graph matrix (such as the adjacency matrix or the Laplacian). Another, somewhat disconnected approach is based on the eigenvalue equation of the adjacency matrix A in Section 3, that derives another expression (24) for $(x_k)_j^2$. Several bounds are given in Section 3, of which some extend earlier published bounds. The elegance of (3) illustrates that the *square* $(x_k)_j^2$ is likely more suited than $(x_k)_j$ to explain the behavior of the eigenstructure, which reminds us to the basic interpretation of quantum mechanics (see e.g. [12, 13]), where the wave function can be complex, while its modulus is interpreted as a probability. Unfortunately, as shown in Appendix A.4.2 for the adjacency matrix A, the vector $\xi_j = \left((x_1)_j^2, (x_2)_j^2, \ldots, (x_N)_j^2\right)$ of the adjacency centrality metrics $(x_k)_j^2$ at all eigenfrequencies k for node j is not independent (or orthogonal) to ξ_l for node l, which implies that the set of adjacency eigenvector centrality metrics $\{\xi_j\}_{1\leq j\leq N}$ is not complete!

Section 4 introduces the definitions and basic properties of the fundamental weights and the dual fundamental weights of a graph. Fundamental weights and their dual are proposed as possible condensations of the $N \times N$ orthogonal matrix X containing all eigenvectors $\{x_k\}_{1\leq k\leq N}$ in its columns. The aim to find a more economical way (i.e. less than N^2 elements) for X, while not loosing information (i.e. able to reconstruct X), started already with Cvetkovic [14], who introduced "graph angles". For a sufficiently large graph, Van Dam and Haemers [15] have argued that the set of all eigenvalues alone (thus ignoring eigenvectors or X) is a unique fingerprint or signature of the graph. For exact graph reconstruction and storage of networks, the most condensed form (i.e. least number of bits) of X without sacrificing information is still an open problem. We believe that fundamental weights and their dual may add, but do not solve the quest. Section 5 briefly concludes. Appendix A overviews eigenvectors and eigenvalues of a symmetric matrix.

2 Square $(x_k)_j^2$ of the eigenvector components

Various closed-form expressions for $(x_k)_j^2$ are presented.

2.1 Eigenvector components as determinants

We assume that the eigenvalue λ_k is single with multiplicity one, so that $\operatorname{rank}(A - \lambda_k I) = N - 1$. This means that $(A - \lambda_k I)\, x_k = 0$ contains only $N - 1$ linearly independent equations to determine the N unknowns $(x_k)_1, (x_k)_2, \ldots, (x_k)_N$. There are basically two approaches[2] to determine the N unknowns: (i) one of the N equations/rows in $A - \lambda_k I$ can be replaced by an additional equation as explored below and (ii) the set is rewritten in $N - 1$ unknowns in terms of one of them, say $(x_k)_N$, whose analysis is omitted, because the resulting expressions for $(x_k)_j$ are less general as those in (i).

We replace an arbitrary equation or row in the set $(A - \lambda_k I)\, x_k = 0$ by a new linear equation $b^T x_k = \sum_{j=1}^{N} b_j\, (x_k)_j$, where b is a real vector and the real number $\beta_k = b^T x_k$ is non-zero. In most cases (except for regular graphs where the all-one vector $u = (1, 1, \ldots, 1)$ is an eigenvector), that additional

[2] These two approaches are similar to computing the adjoint matrix $Q(\lambda) = c_A(\lambda)\,(\lambda I - A)^{-1}$, whose columns are eigenvectors (see [1, art. 148 on p. 220], [16, Chapter IV]).

equation is a normalization relation for the eigenvector and the simplest linear one is $u^T x_k = w_k$, where $w_k \neq 0$ is a real number and called *the fundamental weight* [11, 17] of x_k, further discussed in Section 4 while formulas for β_k are summarized in Appendix D. Another example is the degree vector, $b = d$, where $d^T x_k = \lambda_k w_k$. The general orthogonality equation $x_k^T x_m = \sum_{j=1}^{N} (x_k)_j (x_m)_j = \delta_{km}$ is another linear equation in the unknown components of the vector x_k, given the components of the vector x_m. However, since in this case $x_k^T x_m = 0$, those linear equations cannot be used!

Theorem 1 *Let A and $A_{G\setminus\{j\}}$ denote the adjacency matrix of the graph G and of the graph $G_{\setminus\{j\}}$ in which node j and all its incident links are removed from G, respectively. For any vector b with $\beta_k = b^T x_k \neq 0$, the j-th component of eigenvector x_k of A belonging to eigenvalue λ_k can be written as*

$$(x_k)_j = \frac{\beta_k \det\left(A_{G\setminus\{j\}} - \lambda_k I\right)}{\det\left(A - \lambda_k I\right)_{\text{row } j=b}} \tag{1}$$

or

$$(x_k)_j = -\frac{\det\left(A - \lambda_k I\right)_{\text{row } j=b}}{\beta_k c_A'(\lambda_k)} \tag{2}$$

where $\det\left(A - \lambda_k I\right)_{\text{row } j=b}$ is the $N \times N$ matrix obtained from $(A - \lambda_k I)$ by replacing row j by the vector b. The square of the j-th component of eigenvector x_k of A belonging to eigenvalue λ_k with multiplicity 1 equals

$$(x_k)_j^2 = -\frac{1}{c_A'(\lambda_k)} \det\left(A_{G\setminus\{j\}} - \lambda_k I\right) \tag{3}$$

where $c_A(\lambda) = \det(A - \lambda I)$ is the characteristic polynomial of A and $c_A'(\lambda) = \frac{dc_A(\lambda)}{d\lambda}$.

Although formulated in terms of the adjacency matrix of a graph, Theorem 1 holds for any symmetric matrix. Recently, a survey of formula (3) has appeared in [18], after a sequence of versions on arxiv1908.03795, in which "our" formula (3) also plays a role in the story and its history[3].

Proof: Without loss of generality, we first replace the N-th equation in $(A - \lambda_k I) x_k = 0$ by $b^T x_k = \beta_k$ and the resulting set of linear equations becomes

$$\begin{bmatrix} (A - \lambda_k I)_{\setminus \text{row } N} \\ b \end{bmatrix} x_k = \begin{bmatrix} 0_{(N-1)\times 1} \\ \beta_k \end{bmatrix}$$

where $(A - \lambda_k I)_{\setminus \text{row } N}$ is the $(N-1) \times N$ matrix obtained from $(A - \lambda_k I)$ by removing row N. Cramer's solution [1, p. 256] yields

$$(x_k)_j = \frac{\left| \begin{matrix} (A - \lambda_k I)_{\setminus \text{row } N} \\ b \end{matrix} \right|_{\text{col } j = \begin{bmatrix} 0_{(N-1)\times 1} \\ \beta_k \end{bmatrix}}}{\left| \begin{matrix} (A - \lambda_k I)_{\setminus \text{row } N} \\ b \end{matrix} \right|} = \frac{(-1)^{N+j} \beta_k \det\left(A - \lambda_k I\right)_{\setminus \text{row } N \setminus \text{col } j}}{\det\left(A - \lambda_k I\right)_{\text{row } N=b}}$$

[3] The story on 14 November 2019 in https://www.quantamagazine.org/neutrinos-lead-to-unexpected-discovery-in-basic-math-20191113

contained a pointer to (3) which is now omitted.

The j-th component of the k-th eigenvector x_k can be written as[4]

$$(x_k)_j = \alpha_m(k)(-1)^j \det(A - \lambda_k I)_{\setminus \text{row } m \setminus \text{col } j} \tag{4}$$

where we have now deleted row $1 \leq m \leq N$, instead of row N as before, and where the scaling factor is

$$\alpha_m(k) = \frac{(-1)^m \beta_k}{\det(A - \lambda_k I)_{\text{row } m=b}} \tag{5}$$

Combining (4) with (5) for $m = j$ leads to (1).

We now impose the orthogonality equation $x_k^T x_k = 1$. It follows from (4) that

$$(x_k)_j^2 = \alpha_m^2(k)\left(\det(A - \lambda_k I)_{\setminus \text{row } m \setminus \text{col } j}\right)^2$$

Invoking the identity

$$\left(\det\left(A_{G\setminus \text{row } m\setminus \text{col } j} - \lambda I\right)\right)^2 = \det\left(A_{G\setminus\{m\}} - \lambda I\right)\det\left(A_{G\setminus\{j\}} - \lambda I\right) - \det\left(A_{G\setminus\{m,j\}} - \lambda I\right)\det\left(A_G - \lambda I\right) \tag{6}$$

which can be deduced from Jacobi's famous theorem of 1833 (see e.g. [19, p. 25]), yields

$$\begin{aligned}\alpha_m^{-2}(k)(x_k)_j^2 &= \lim_{\lambda\to\lambda_k} \det\left(A_{G\setminus\{m\}} - \lambda I\right)\det\left(A_{G\setminus\{j\}} - \lambda I\right) - \det\left(A_{G\setminus\{m,j\}} - \lambda I\right)\det\left(A_G - \lambda I\right) \\ &= \det\left(A_{G\setminus\{m\}} - \lambda_k I\right)\det\left(A_{G\setminus\{j\}} - \lambda_k I\right)\end{aligned} \tag{7}$$

The condition $x_k^T x_k = \sum_{n=1}^N (x_k)_n^2 = 1$ specifies $\alpha_m(k)$ as

$$\alpha_m^{-2}(k) = \det\left(A_{G\setminus\{m\}} - \lambda_k I\right)\sum_{n=1}^N \det\left(A_{G\setminus\{n\}} - \lambda_k I\right) \tag{8}$$

We observe that there is a degree of freedom via the choice of m. Thus, for $m = j$ in (4), we obtain from (7) and (8)

$$(x_k)_j^2 = \frac{\det\left(A_{G\setminus\{j\}} - \lambda_k I\right)}{\sum_{n=1}^N \det\left(A_{G\setminus\{n\}} - \lambda_k I\right)} \tag{9}$$

that is independent of the choice of the vector b. Since [20]

$$\sum_{n=1}^N \det\left(A_{G\setminus\{n\}} - \lambda I\right) = -\frac{d}{d\lambda}\det(A - \lambda I) = -c_A'(\lambda) \tag{10}$$

we arrive at (3). Combining (1) and (3) yields[5] (2). □

Another proof of (3): We start from the resolvent [1, p. 244] of a symmetric matrix A

$$(A - zI)_{jj}^{-1} = \frac{\det\left(A_{\setminus\{j\}} - zI\right)}{\det(A - zI)} = \sum_{m=1}^N \frac{(x_m)_j^2}{\lambda_m - z}$$

[4] Remark that the adjacency matrix $A_{G\setminus \text{row } m\setminus \text{col } i}$ represents a directed graph in which the out-going links of node m and the in-coming links to node i are removed; everywhere else, the in-coming and out-going links are the same (bidirectional). Thus, $A_{G\setminus \text{row } m\setminus \text{col } i}$ is not necessarily symmetric and it has $|m - i|$ non-zero diagonal elements, $a_{k+1,k}$ for $m \leq k < i$.

[5] We remark that taking the derivative of both sides of (2) with respect to b_m results in (1).

from which, using $c_A(\lambda) = \det(A - \lambda I) = \prod_{j=1}^{N}(\lambda_j - \lambda)$,

$$\det\left(A_{\backslash\{j\}} - \lambda_k I\right) = \sum_{m=1}^{N} (x_m)_j^2 \lim_{z\to\lambda_k} \frac{\prod_{j=1}^{N}(\lambda_j - z)}{\lambda_m - z}$$
$$= (x_k)_j^2 \prod_{j=1;j\neq k}^{N} (\lambda_j - \lambda_k)$$

Invoking (17) yields (3). □

The second proof of (3), written as $x_j^2 = \frac{P_{G-j}(\lambda)}{P'_G(\lambda)}$ where $P_G(z) = \det(A - zI)$, has appeared earlier in Cvetcovic *et al.* [21, Theorem 3.1], who referred to Hagos [22], who in turn mentioned that Mukherjee and Datta [23] (using a perturbation technique) and Li and Feng (only for the largest eigenvalue) have preceded him. Hagos [22] mentioned rightly that "Eq. (3) is probably not as well known as it should be", which may justify why we have placed (3) in the abstract as well. In addition, Hagos [22] has shown that (in our notation)

$$\sum_{l=1}^{r_k} (x_l)_j^2 = \frac{r_k}{c'_A(\lambda_k)} \det\left(A_{G\backslash\{j\}} - \lambda_k I\right)$$

where λ_k is an eigenvalue with multiplicity r_k and x_l is one of the r_k orthogonal eigenvectors belonging to eigenvalue λ_k.

Corollary 1 *If λ_k is an eigenvalue of A with multiplicity of two, then*

$$(x_k)_j^2 = \frac{1}{c''_A(\lambda_k)} \sum_{n=1;n\neq j}^{N-1} \det\left(A_{G\backslash\{j,n\}} - \lambda_k I\right) \tag{11}$$

Proof: If λ_k is an eigenvalue of A with multiplicity of two, then it holds that $c_A(\lambda_k) = c'_A(\lambda_k) = 0$. Moreover, (10) and the fact that $\det\left(A_{G\backslash\{m\}} - \lambda_k I\right)$ must have the same sign (see e.g. (21) below), show that all $\det\left(A_{G\backslash\{m\}} - \lambda_k I\right)$ must vanish, implying that λ_k is then also an eigenvalue of all $A_{G\backslash\{m\}}$, for each node m removed from G. This observation agrees with the Interlacing theorem [1] that tells us that all eigenvalues of $A_{G\backslash\{m\}}$ (for each m) are lying in between the eigenvalues of A. If two eigenvalues of A coincide (e.g. $\lambda_k = \lambda_{k+1}$), the corresponding eigenvalue of each $A_{G\backslash\{m\}}$, i.e. $\lambda_k \geq \lambda\left(A_{G\backslash\{m\}}\right) \geq \lambda_{k+1}$, is squeezed to that same value λ_k. Applying de l'Hospital's rule,

$$(x_k)_j^2 = -\lim_{\lambda\to\lambda_k} \frac{\det\left(A_{G\backslash\{j\}} - \lambda I\right)}{c'_A(\lambda)} = -\lim_{\lambda\to\lambda_k} \frac{\frac{d}{d\lambda}\det\left(A_{G\backslash\{j\}} - \lambda I\right)}{c''_A(\lambda)}$$

The derivative (10) yields

$$\sum_{n=1;n\neq j}^{N-1} \det\left(A_{G\backslash\{j,n\}} - \lambda I\right) = -\frac{d}{d\lambda}\det\left(A_{G\backslash\{j\}} - \lambda I\right)$$

Combining these formulas, leads to (11). □

If $c'_A(\lambda_k) = 0$, (11) reflects the effect of removing all pair of nodes containing node j.

Corollary 2 *The product of the j-th and m-th component of eigenvector x_k of A belonging to eigenvalue λ_k with multiplicity 1 equals*

$$(x_k)_j (x_k)_m = \frac{(-1)^{j+m+1}}{c'_A(\lambda_k)} \det\left(A_{\setminus \text{row}\, j \setminus \text{col}\, m} - \lambda_k I\right) \tag{12}$$

Proof: We expand the determinant in (2) in the cofactors of row j and obtain, with $\beta_k = \sum_{m=1}^{N} b_m (x_k)_m$,

$$\sum_{m=1}^{N} b_m (x_k)_m (x_k)_j = -\frac{(-1)^j}{c'_A(\lambda_k)} \sum_{m=1}^{N} (-1)^m b_m \det\left(A_{\setminus \text{row}\, j \setminus \text{col}\, m} - \lambda_k I\right)$$

Since this relation holds for any vector $b = (b_1, b_2, \ldots, b_N)$, equating the corresponding coefficient b_m at both sides yields (12). □

When $m = j$ in (12), we arrive again at (3). Hence, (12) generalizes (3). The second orthogonality relation (66) indicates that

$$(-1)^{j+m+1} \sum_{k=1}^{N} \frac{\det\left(A_{\setminus \text{row}\, j \setminus \text{col}\, m} - \lambda_k I\right)}{c'_A(\lambda_k)} = \delta_{jm}$$

2.2 Walk expansion

The following theorem is a direct consequence of the analysis in [1, p. 228]:

Theorem 2 *If all eigenvalues of A are different, then*

$$(x_k)_i (x_k)_j = \frac{1}{\prod_{l=1;l\neq k}^{N} (\lambda_k - \lambda_l)} \sum_{r=H_{ij}}^{N-1} b_r(k) (A^r)_{ij} \tag{13}$$

where H_{ij} is the hopcount (number of links) of the shortest path between node i and j and where the coefficients $b_r(k)$ obey

$$\prod_{j=1;j\neq k}^{N} (x - \lambda_j) = \sum_{j=0}^{N-1} b_j(k) x^j$$

or

$$b_r(k) = \frac{1}{r!} \frac{d^r}{dx^r} \prod_{j=1;j\neq k}^{N} (x - \lambda_j) \Bigg|_{x=0} \tag{14}$$

Writing (13) in matrix form yields

$$x_k x_k^T = \frac{1}{\prod_{l=1;l\neq k}^{N} (\lambda_k - \lambda_l)} \sum_{r=0}^{N-1} b_r(k) A^r = \frac{\prod_{j=1;j\neq k}^{N} (A - \lambda_j I)}{\prod_{l=1;l\neq k}^{N} (\lambda_k - \lambda_l)} \tag{15}$$

The coefficients $b_r(k)$ defined in (14) in the walk expansion (13) are only function of the eigenvalues $\{\lambda_k\}_{1\leq k\leq N}$ of the symmetric matrix A. Apart from $b_N(m) = 0$, $b_{N-1}(m) = 1$, we have $b_{N-2}(m) = \lambda_m$. More general, we can express $b_r(k)$ in terms of the coefficients c_n of the characteristic polynomial of

the adjacency matrix [1, p. 212], defined as $c_A(x) = \det(A - xI) = (-1)^N \prod_{k=1}^{N} (x - \lambda_k) = \sum_{n=0}^{N} c_n x^n$, as

$$b_k(m) = \frac{(-1)^{N-1}}{\lambda_m^{k+1}} \sum_{n=0}^{k} c_n \lambda_m^n$$

Clearly, if $i = j$, then $H_{jj} = 0$ and (13) reduces to

$$(x_k)_j^2 = \frac{1}{\prod_{l=1;l\neq k}^{N} (\lambda_k - \lambda_l)} \sum_{r=0}^{N-1} b_r(k) (A^r)_{jj} \tag{16}$$

The definition of the characteristic polynomial of matrix A is $c_A(\lambda) = \det(A - \lambda I) = \prod_{j=1}^{N} (\lambda_j - \lambda)$, from which $\log c_A(\lambda) = \sum_{j=1}^{N} \log(\lambda_j - \lambda)$. Differentiation yields

$$c_A'(\lambda) = -c_A(\lambda) \sum_{j=1}^{N} \frac{1}{\lambda_j - \lambda} = -\sum_{j=1}^{N} \frac{\prod_{k=1}^{N} (\lambda_k - \lambda)}{\lambda_j - \lambda} = -\sum_{j=1}^{N} \prod_{k=1;k\neq j}^{N} (\lambda_k - \lambda)$$

from which

$$c_A'(\lambda_m) = -\prod_{k=1;k\neq m}^{N} (\lambda_k - \lambda_m) = (-1)^N \prod_{k=1;k\neq m}^{N} (\lambda_m - \lambda_k) \tag{17}$$

The derivative $c_A'(\lambda_m)$ in (10) and (17) plays the role of a normalization factor so that the squared eigenvector components satisfy $\sum_{j=1}^{N} (x_k)_j^2 = 1$. Thus, we can write (16) as[6]

$$(x_k)_j^2 = \frac{(-1)^N}{c_A'(\lambda_k)} \sum_{r=0}^{N-1} b_r(k) (A^r)_{jj} \tag{18}$$

Theorem 2 expresses the product of two eigenvector components in terms of the eigenvalues only. In particular, (13) equals the sum of the number $(A^r)_{ij}$ of walks, weighted by a function $b_r(m)$ of eigenvalues, over all r hops paths between node i and node j. The longest possible shortest path in a graph contains $N - 1$ hops and $(A^r)_{ij}$ equals the number of *shortest paths* with r hops from node i to node j, provided $(A^m)_{ij} = 0$ for all integers $m < r$. The squared eigenvector component $(x_k)_j^2$ corresponding to node j in (18) sums over the number $(A^r)_{jj}$ of closed walks, starting and ending at node j, of all possible lenghts (expressed in number r of hops or links) up to $N-1$, weighted by $b_r(k)$ that determines how the number of closed walks influences any eigenvector components at frequency λ_k. Thus, the appearence of $(A^r)_{jj}$ reflects the only dependence of $(x_k)_j^2$ on the node j, while $b_r(k)$ and $c_A'(\lambda_k)$ only change with frequence/eigenvalue λ_k.

[6] Invoking the normalization $x_k^T x_k = \sum_{j=1}^{N} (x_k)_j^2 = 1$ and $W_r = \sum_{j=1}^{N} (A^r)_{jj}$, the total number of closed walks of length r (with r hops), we obtain from (18) that

$$c_A'(\lambda_k) = (-1)^N \sum_{r=0}^{N-1} W_r b_r(k)$$

and (18) becomes

$$(x_k)_j^2 = \frac{\sum_{r=0}^{N-1} b_r(k) (A^r)_{jj}}{\sum_{j=1}^{N} \sum_{r=0}^{N-1} b_r(k) (A^r)_{jj}}$$

2.2.1 Example: The hopcount of the shortest path equals $N-1$

When the hopcount of the shortest path in the graph between node i and j equals $H_{ij}=N-1$, (13) directly leads to

$$(x_m)_i (x_m)_j = \frac{\left(A^{N-1}\right)_{ij} (-1)^{m-1}}{\prod_{k=1}^{m-1} (\lambda_k - \lambda_m) \prod_{k=m+1}^{N} (\lambda_m - \lambda_k)} \tag{19}$$

Notice that the product $(x_m)_i (x_m)_j$ in (19) is always positive when m is odd! If the graph is disconnected or there is no path nor walk between node i and j, then $\left(A^{N-1}\right)_{ij}=0$, implying that either $(x_m)_i$ or $(x_m)_j$ are zero, but not both, else all components of all eigenvectors are zero.

As an example of (19), the eigenvector components belonging to $\lambda_1 = 2\cos\frac{\pi}{N+1}$ in the path graph [1, p. 124] are, for $1 \le k \le N$,

$$(x_1)_k = \sqrt{\frac{2}{N+1}} \sin\frac{k\pi}{N+1}$$

and (19), with the longest shortest path between node 1 and N so that $\left(A^{N-1}\right)_{1N}=1$, leads to the (non-trivial) identity,

$$\prod_{k=2}^{N} \left(\cos\frac{\pi}{N+1} - \cos\frac{k\pi}{N+1}\right) = \frac{N+1}{2^N \sin^2\frac{\pi}{N+1}}$$

2.3 Interpretations of the various expressions of $(x_k)_j^2$

Additional deductions from Theorem 1 are presented in Appendix D.

1. *Induced centrality metric.* Everett and Borgatti [24] have defined the induced centrality $C_f(j)$ of node j for the graph invariant f by

$$C_f(j) = f(G) - f\left(G_{\setminus\{j\}}\right) \tag{20}$$

They show that many known metrics can be formulated as induced centralities. For example, if the graph invariant f is the total number of links in the graph, then the induced centrality $C_f(j)$ is simply the degree d_j of node j.

Since the eigenvalue λ_k of the adjacency matrix A is a zero of the characteristic polynomial, $c_A(\lambda_k) = \det(A - \lambda_k I) = 0$, we can rewrite the square of the j-th component of eigenvector x_k of A belonging to eigenvalue λ_k (with multiplicity 1) in (3) as

$$(x_k)_j^2 = \frac{\det(A_G - \lambda_k I) - \det\left(A_{G\setminus\{j\}} - \lambda_k I\right)}{c'_A(\lambda_k)}$$

and the definition (20) illustrates that the square $(x_k)_j^2$ of the component of the eigenvector x_k of the adjacency matrix A corresponding to node j is an induced centrality. This observation again supports that $(x_k)_j^2$ can be considered as a graph metric. Moreover, (74) shows, for any function g (for which $g(\lambda_k)$ is defined for each eigenvalue λ_k with $1 \le k \le N$) of the adjacency matrix A, that $(g(A))_{jj}$ is also an induced centrality. As an example, (82) shows that the degree d_j is, indeed, an induced centrality. More general, the number of closed walks $(A^m)_{jj} = \sum_{k=1}^{N} \lambda_k^m (x_k)_j^2$ of length m at node j (see [1]) is an induced centrality.

The eigenvector component $(x_k)_j$ in either (1) or (2) cannot be written in the form (20) of an induced centrality. The latter observation makes sense, because if $(x_k)_j$ were an induced centrality of the graph, then any possible $N \times 1$ vector would be an induced centrality (since any $N \times 1$ vector can be written as a linear combination of the N orthogonal eigenvectors $x_1, x_2, \ldots, x_N$ of the adjacency matrix A.)

2. *Component ratios.* We deduce from (3) that

$$\frac{(x_k)_j^2}{(x_k)_m^2} = \frac{\det\left(A_{G\setminus\{j\}} - \lambda_k I\right)}{\det\left(A_{G\setminus\{m\}} - \lambda_k I\right)} = \frac{c_{A_{G\setminus\{j\}}}(\lambda_k)}{c_{A_{G\setminus\{m\}}}(\lambda_k)} \tag{21}$$

illustrating that $\det\left(A_{G\setminus\{j\}} - \lambda_k I\right)$ and $\det\left(A_{G\setminus\{m\}} - \lambda_k I\right)$ have the same sign for any pair of nodes (j, m) for a given frequency λ_k, but, by (10), opposite to the sign of $c'_A(\lambda_k)$ (as verified from Fig. 1). Applying (12) to $\frac{(x_k)_j (x_k)_q}{(x_k)_m (x_k)_q}$, we find that, for any $1 \leq q \leq N$,

$$\frac{(x_k)_j}{(x_k)_m} = \frac{\det\left(A_{\setminus \text{row}\, j \setminus \text{col}\, q} - \lambda_k I\right)}{\det\left(A_{\setminus \text{row}\, q \setminus \text{col}\, m} - \lambda_k I\right)}$$

Choosing $q = j$ and combined with (21) results in

$$\left(\det\left(A_{\setminus \text{row}\, j \setminus \text{col}\, m} - \lambda_k I\right)\right)^2 = \det\left(A_{G\setminus\{j\}} - \lambda_k I\right) \det\left(A_{G\setminus\{m\}} - \lambda_k I\right)$$

which is an instance of Jacobi's general formula (6).

It follows from (2) that

$$\frac{(x_k)_j}{(x_k)_m} = \frac{\det\left(A - \lambda_k I\right)_{\text{row}\, j=b}}{\det\left(A - \lambda_k I\right)_{\text{row}\, m=b}} \tag{22}$$

and The sign of $(x_k)_j$ with respect to $(x_k)_m$ is thus determined by a ratio of determinants that seemingly depend on an arbitrary vector b with non-zero $\beta_k = u^T x_k$, whose general graph interpretation is less transparent than nodal removal as in $\det\left(A_{G\setminus\{j\}} - \lambda_k I\right)$, even if $b = u$. If $k = 1$, then $(x_1)_j \geq 0$, so that $\det\left(A - \lambda_1 I\right)_{\text{row}\, j=b}$ and $\det\left(A - \lambda_1 I\right)_{\text{row}\, m=b}$ have the same sign. However, for $k > 1$, it holds that $\min_j (x_k)_j \leq 0 \leq \max_j (x_k)_j$ and, hence (1) shows that $\min_{1\leq j\leq N} \det\left(A - \lambda_k I\right)_{\text{row}\, j=b}$ has a sign opposite to $\max_{1\leq j\leq N} \det\left(A - \lambda_k I\right)_{\text{row}\, j=b}$. We remark that the ratios (21) and (22) only hold at eigenfrequencies of A, thus

$$\frac{\det\left(A_{G\setminus\{j\}} - \lambda I\right)}{\det\left(A_{G\setminus\{m\}} - \lambda I\right)} = \left(\frac{\det\left(A - \lambda I\right)_{\text{row}\, j=b}}{\det\left(A - \lambda I\right)_{\text{row}\, m=b}}\right)^2 \tag{23}$$

is correct only if $\lambda = \lambda_k$ for $1 \leq k \leq N$.

3. *Zero eigenvector component.* If λ_k is a single eigenvalue of A (thus $c'_A(\lambda_k) \neq 0$) and if λ_k is also an eigenvalue of $A_{G\setminus\{j\}}$, then (3) shows that $(x_k)_j = 0$. Not all other eigenvector components $(x_k)_m$ can be zero, because any eigenvector is different from the zero vector. Hence, if λ_k is not an eigenvalue of multiplicity at least two, then λ_k cannot be an eigenvalue of all $A_{G\setminus\{m\}}$ (for $1 \leq m \leq N$). The eigenvalue equation states that

$$\lambda_k (x_k)_j = \sum_{l=1}^{N} a_{jl} (x_k)_l = \sum_{l\in \mathcal{N}_j} (x_k)_l$$

where $\mathcal{N}_j$ represents the set of direct neighbors of node j. A zero eigenvector component, $(x_k)_j = 0$ at eigenvalue λ_k, means that (a) the average of the eigenvector components of the neighbors of node j is zero and (b) that node j does not affect the eigenvector component of any of its neighbors. When $(x_k)_j = 0$, the removal of node j has no effect at frequency $\lambda_k < \lambda_1$. Since $(x_1)_j > 0$ in a connected graph (by the Perron-Frobenius Theorem), the removal of a node j has always an effect at eigenfrequency λ_1. Based on this notion, we may define *the redundancy* $r_j \in [0, N-1]$ of node j as the number of eigenfrequencies at which $(x_k)_j = (x_k)_j^2 = 0$.

4. *Amplitude.* The magnitude of $(x_k)_j^2$ for node j in (3) depends on the characteristic polynomial $c_{A_{G\setminus\{j\}}}(\lambda)$ of $G\setminus\{j\}$ at the frequency $\lambda = \lambda_k$. As illustrated in Fig. 1, the characteristic polynomials $c_A(x)$ and $c_{A_{G\setminus\{j\}}}(x)$ oscillate around zero in the interval $x \in [\lambda_N, \lambda_1]$, that contains all their real zeros. We coin the deviations in $c_{A_{G\setminus\{j\}}}(x)$ from zero at λ_k the amplitude. Just as in quantum mechanics[7] (see e.g. [12, 13]), where the wave function can be complex, while its modulus is interpreted as a probability, we propose to use the eigenvector components $(x_k)_j$ in computations, but we suggest, based on (3), to interpret $(x_k)_j^2$ as centrality metrics. Hence, the importance or centrality of node j for property $\mathcal{P}_k$ at eigenfrequency λ_k is proportional to the amplitude of the characteristic polynomial at λ_k of the graph in which that node j is removed. Thus, the centrality $(x_k)_j^2$ measures a kind of "robustness" or "resilience", in the sense of how important is the removal of node j from the graph G, determined by the amplitude at frequency λ_k. In network robustness analyses, the removal of links or nodes challenges the functioning of the network, measured via certain network metrics [25, 26]. The relative impact or effect of the removal of a high degree node at the largest eigenfrequency λ_1 is larger than the removal of a low degree node [27]. However, at other eigenfrequencies, the reverse must hold due to double orthogonality (66), $\sum_{k=1}^{N} (x_k)_j^2 = 1$.

Example. For a connected Erdős-Rényi graph with link density $p = 0.2$, $N = 10$ nodes and the degree vector $d = (3, 3, 1, 4, 2, 2, 1, 2, 2, 2)$, Fig. 1 shows all 10 characteristic polynomials[8] $c_{A_{G\setminus\{j\}}}(\lambda)$ and $c_A(\lambda)$, as well as its adjacency matrix A. At the vertical lines, that indicate the positions of the eigenvalues of A, all values $c_{A_{G\setminus\{j\}}}(\lambda_k)$ for $1 \le j \le 10$ have a same sign, in agreement with (21).

[7] Perhaps the expression (18) may be related to Feynman diagrams that express all possible interactions of a particle with others in some potential field?

[8] The explicit expressions are

$$
\begin{aligned}
c_A(x) &= -4 + 4x + 27x^2 - 10x^3 - 52x^4 + 8x^5 + 38x^6 - 2x^7 - 11x^8 + x^{10} \\
c_{A_{G\setminus\{1\}}}(x) &= -2 - 5x + 6x^2 + 17x^3 - 6x^4 - 19x^5 + 2x^6 + 8x^7 - x^9 \\
c_{A_{G\setminus\{2\}}}(x) &= -4x + 16x^3 - 19x^5 + 8x^7 - x^9 \\
c_{A_{G\setminus\{3\}}}(x) &= -8x + 4x^2 + 29x^3 - 6x^4 - 29x^5 + 2x^6 + 10x^7 - x^9 \\
c_{A_{G\setminus\{4\}}}(x) &= -4x + 14x^3 - 16x^5 + 7x^7 - x^9 \\
c_{A_{G\setminus\{5\}}}(x) &= -2 - 5x + 8x^2 + 20x^3 - 8x^4 - 23x^5 + 2x^6 + 9x^7 - x^9 \\
c_{A_{G\setminus\{6\}}}(x) &= 2 - 7x - 4x^2 + 25x^3 + 2x^4 - 25x^5 + 9x^7 - x^9 \\
c_{A_{G\setminus\{7\}}}(x) &= -2 - 9x + 6x^2 + 30x^3 - 6x^4 - 29x^5 + 2x^6 + 10x^7 - x^9 \\
c_{A_{G\setminus\{8\}}}(x) &= -4x + 2x^2 + 18x^3 - 4x^4 - 22x^5 + 2x^6 + 9x^7 - x^9 \\
c_{A_{G\setminus\{9\}}}(x) &= -4x + 4x^2 + 20x^3 - 6x^4 - 23x^5 + 2x^6 + 9x^7 - x^9 \\
c_{A_{G\setminus\{10\}}}(x) &= -4x + 4x^2 + 19x^3 - 6x^4 - 23x^5 + 2x^6 + 9x^7 - x^9
\end{aligned}
$$

The amplitude $c_{A_{G\setminus\{j\}}}(\lambda_k)$ is a relative measure for $(x_k)_j^2$ and indicates the importance of node j at frequency λ_k. Fig. 2 illustrates that the topological degree vector d correlates best with the square components of the principal eigenvector x_1. At other eigenfrequencies, other nodes are "important". Fig. 2 also shows that $(x_1)_j^2 = \min_{1\leq k\leq\leq 10}(x_k)_j^2$ for node $j=3$ and $j=7$, both having the minimum degree $d_{\min}=1$.

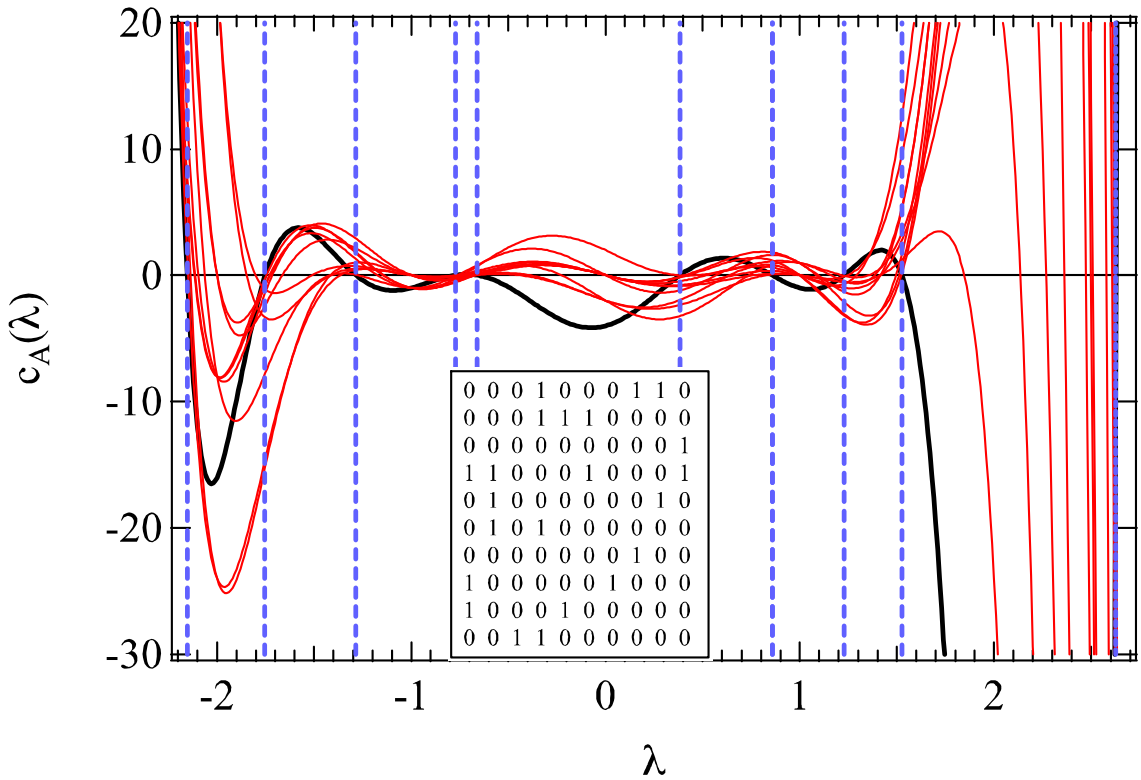

Figure 1: The characteristic polynomials $c_{A_{G\setminus\{n\}}}(\lambda)$ for $1\leq i\leq N$ in red and $c_{A_G}(\lambda)$ in black for an Erdős-Rényi graph $G_{0.2}(10)$, whose adjacency matrix is also shown. The blue vertical lines denote the eigenvalues of A (zeros of $c_A(\lambda)$).

5. *Concern for the adjacency matrix* A: The zero eigenvalue in (83) of Ξ, defined in (76), implies for any adjacency matrix A that $\operatorname{rank}(\Xi) < N$ and that at least one row (or column) is a linear combination of all the other rows (columns). Hence, the set of centrality metrics $\{(\operatorname{row}\Xi)_i\}_{1\leq i\leq N} = \left\{(x_1)_i^2, (x_2)_i^2, \ldots, (x_N)_i^2\right\}_{1\leq i\leq N}$ is *not* independent for the adjacency matrix, indicating that the set of centrality metrics belonging to node j can be written in terms of the centrality metrics of all the others nodes in G.

6. *Link addition/removal to the graph* G. Equation (3) indicates that the addition (or removal) of a link to node j does not change $(x_k)_j$, because $G_{\setminus\{j\}}$ means that, besides the node j itself, also all incident links to node j are removed from the graph. However, a link addition/removal may change the eigenfrequencies $\{\lambda_k\}_{1\leq k\leq N}$. This observation may suggest that, after the addition (or removal) of a link to node i and node j, the nodal eigenvector component $(x_k)_i$ and $(x_k)_j$ change

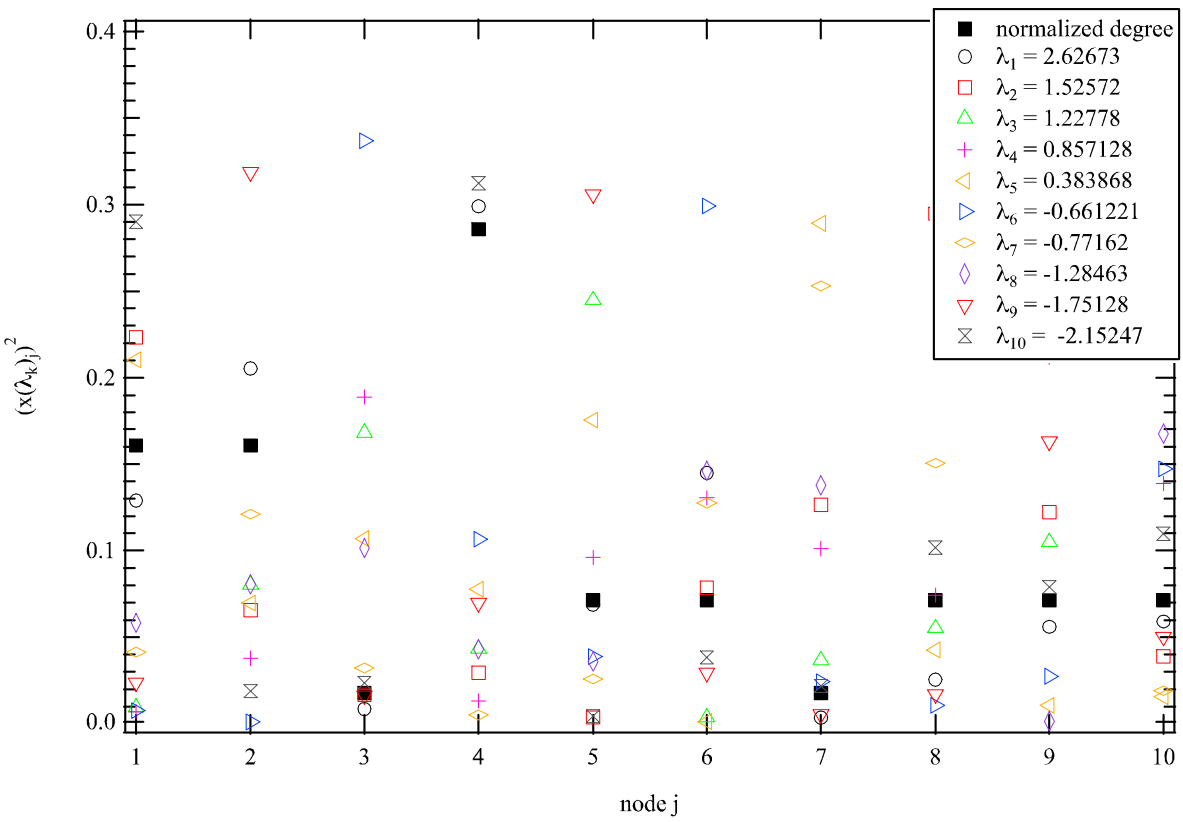

Figure 2: The square of the eigenvector components per node j over all eigenvalues λ_k for the same graph as in Fig. 1. The filled black squares represent the normalized degree $d_j^2/d^T d$.

the least. Simulations do not seem to support this observation, which hints that the effect of link addition/removal on the eigenfrequencies is dominant.

7. *Weighting squared eigenvector components.* Let $f(x) = x^2$ in (73), then

$$A^2 = \sum_{k=1}^{N} \lambda_k^2 x_k x_k^T = \sum_{k=1}^{N} (|\lambda_k| x_k)(|\lambda_k| x_k)^T$$

On the other hand, for the Laplacian $Q = \Delta - A$ whose eigenvalues are non-negative, (73) with $f(x) = x$ becomes

$$Q = \sum_{k=1}^{N} \mu_k z_k z_k^T = \sum_{k=1}^{N} (\sqrt{\mu_k} z_k)(\sqrt{\mu_k} z_k)^T$$

These relations suggest to weight the "importance" of the eigenvectors of A as $v_k = |\lambda_k| x_k$, whereas those of Q as $s_k = \sqrt{\mu_k} z_k$. Moreover, since $\left(A^2\right)_{jj} = Q_{jj} = d_j$ and $\mu_N = 0$, the two expression for the degree

$$d_j = \sum_{k=1}^{N} \lambda_k^2 \left(x_k^2\right)_j = \sum_{k=1}^{N-1} \mu_k \left(z_k^2\right)_j$$

show a weighting of the adjacency eigenvector centralities $\left(x_k^2\right)_j$ by λ_k^2, whereas the Laplacian eigenvector centralities are only weighted proportional with the Laplacian eigenvalue μ_k. Thus, while the

eigenvectors of different graph-related matrices reflect different properties of the graph, although each of them satisfies the first (64) and second (66) orthogonality conditions, the example illustrates that a generally acceptable scaling or weighting does not exist. Clearly, the eigenvectors corresponding to the larger (in absolute value) eigenvalues deserve more weight, as earlier was exploited in graph reconstructability [28] and only a few of the larger ones may be sufficient as centrality metrics.

3 Squared eigenvalue equation

Theorem 3 *The square of the i-th component of the eigenvector x_k of the adjacency matrix A of the graph G belonging to the eigenvalue λ_k equals*

$$(x_k)_i^2 = \frac{1 - r_i(k)}{\frac{\lambda_k^2(A)}{d_i} + 1} \tag{24}$$

where d_i is the degree of node i and

$$r_i(k) = \sum_{j=1;j\neq i}^{N} (1 - a_{ij})(x_k)_j^2 + \frac{1}{2d_i} \sum_{j=1}^{N} a_{ij} \sum_{l=1}^{N} a_{il} \left((x_k)_l - (x_k)_j\right)^2 \tag{25}$$

obeys $0 \leq r_i(k) \leq 1$.

Proof: We start from the squared eigenvalue equation

$$\lambda_k^2(A)(x_k)_i^2 = \left(\sum_{j=1}^{N} a_{ij}(x_k)_j\right)^2$$

to deduce an approximation for $(x_k)_i^2$. Invoking the Cauchy identity [1, p. 257] and $a_{ij} = a_{ij}^2$ yields

$$\begin{aligned}\left(\sum_{j=1}^{N} a_{ij}a_{ij}(x_k)_j\right)^2 &= \sum_{j=1}^{N} a_{ij}^2 \sum_{j=1}^{N} \left(a_{ij}(x_k)_j\right)^2 - \frac{1}{2}\sum_{j=1}^{N}\sum_{l=1}^{N} \left(a_{ij}a_{il}(x_k)_l - a_{il}a_{ij}(x_k)_j\right)^2 \\ &= d_i \sum_{j=1}^{N} a_{ij}(x_k)_j^2 - \frac{1}{2}\sum_{j=1}^{N} a_{ij} \sum_{l=1}^{N} a_{il}\left((x_k)_l - (x_k)_j\right)^2\end{aligned}$$

where the degree $d_i = \sum_{j=1}^{N} a_{ij}$. Further, using the first orthogonality relation (64), $1 = \sum_{j=1}^{N}(x_k)_j^2$, and

$$\sum_{j=1}^{N} a_{ij}(x_k)_j^2 = 1 - (x_k)_i^2 - \sum_{j=1;j\neq i}^{N} (1 - a_{ij})(x_k)_j^2$$

we obtain

$$\frac{\lambda_k^2(A)}{d_i}(x_k)_i^2 = 1 - (x_k)_i^2 - \sum_{j=1;j\neq i}^{N} (1 - a_{ij})(x_k)_j^2 - \frac{1}{2d_i}\sum_{j=1}^{N} a_{ij} \sum_{l=1}^{N} a_{il}\left((x_k)_l - (x_k)_j\right)^2$$

which we rewrite as (24). The definition (25) shows that $r_i(k) \geq 0$, whereas it follows from (24) that $r_i(k) \leq 1$. □

Since $r_i(k) \geq 0$, Theorem 3 directly leads to the upper bound

$$(x_k)_i^2 \leq \frac{1}{1 + \frac{\lambda_k^2(A)}{d_i}} \tag{26}$$

which appeared earlier for $k = 1$ in [29] and [30, p. 29]. Equality in (26) only holds if $r_i(k) = 0$, which is equivalent to both

$$\sum_{j=1;j\neq i}^{N} (1 - a_{ij})(x_k)_j^2 = \sum_{j\notin\mathcal{N}_i}^{N} (x_k)_j^2 = 0$$

where $\mathcal{N}_i$ is the set of all direct neighbors of node i, and $(x_k)_l = (x_k)_j$ for all nodes $l, j \in \mathcal{N}_i$. In conclusion, for any eigenfrequency k, equality in (26) is only possible if $(x_k)_j = 0$ for $j \notin \mathcal{N}_i$ and $(x_k)_l = \frac{\pm 1}{\sqrt{d_i}}$ for $l \in \mathcal{N}_i$. If $k = 1$, equality can only happen in a disconnected graph consisting of a regular graph on d_i nodes (thus the complete graph K_{d_i}) and $N - d_i$ disconnected nodes from node i.

3.1 Bounds for eigenvector components

We present a number of bounds for the minimum and maximum of eigenvector components, either over frequencies k or over nodes j.

We remark as in [30, p. 31] that $\min_{1\le j\le N}(x_k)_j^2$, deduced from (26), can be sharpened.

Corollary 3 *For any graph, it holds that*

$$\min_{1\le j\le N}(x_k)_j^2 \le \frac{1 - \frac{d_{\min}}{2} s_k}{\frac{\lambda_k^2(A)}{d_{\min}} + N - d_{\min}} \tag{27}$$

where $s_k = \min_{l,j}\left((x_k)_l - (x_k)_j\right)^2$ *is the minimal square spacing between eigenvector components of* x_k.

Proof: The definition (25) of $r_i(k)$ reveals that

$$\sum_{j=1;j\neq i}^{N} (1 - a_{ij})\,(x_k)_j^2 \ge (N - 1 - d_i) \min_{1\le j\le N}(x_k)_j^2$$

and

$$\sum_{j=1}^{N} a_{ij} \sum_{l=1}^{N} a_{il}\left((x_k)_l - (x_k)_j\right)^2 \ge d_i^2 \min_{l,j}\left((x_k)_l - (x_k)_j\right)^2 = d_i^2 s_k$$

so that

$$r_i(k) \ge (N - 1 - d_i) \min_{1\le j\le N}(x_k)_j^2 + \frac{d_i}{2} s_k$$

Hence, (24) can be bounded

$$\min_{1\le j\le N}(x_k)_j^2 \le (x_k)_i^2 = \frac{1 - r_i(k)}{\frac{\lambda_k^2(A)}{d_i} + 1} \le \frac{1 - (N - 1 - d_i)\min_{1\le j\le N}(x_k)_j^2 - \frac{d_i}{2} s_k}{\frac{\lambda_k^2(A)}{d_i} + 1}$$

which holds for all nodes i, also for the node with minimum degree, leading to (27). □

Inequality (27) extends the result of Nikiforov [31] (where $k = 1$ and the minimal square spacing $s_k = 0$) to all eigenfrequencies k. The right-hand side of (27) (with $s_k = 0$) is minimized for $k = 1$. Since $\frac{\lambda_k^2(A)}{d_i} + 1$ is maximal if $d_i = d_{\min}$ and $k = 1$, (24) shows that $\min_{1\le k\le N}(x_k)_i^2$ is reached when $k = 1$ at a minimum degree node if $\max_{1\le k\le N} r_i(k) = r_i(1)$. However, the minimum degree node q does not always obey $\min_{1\le k\le N}(x_k)_q^2 = (x_1)_q^2$.

Inspired by Cioabă and Gregory, we extend their Theorem 3.4 in [29]:

Theorem 4 *For any graph G, it holds that*

$$\min_{1\le j\le N}(x_k)_j \le \frac{\lambda_k^m(A) w_k}{N_m} \le \max_{1\le j\le N}(x_k)_j \tag{28}$$

where $w_k = \sum_{j=1}^{N} (x_k)_j$ *is fundamental weight (42) and* $N_m = u^T A^m u = \sum_{i=1}^{N} \sum_{j=1}^{N} (A^m)_{ij}$ *is the total number of walks with* m *hops in the graph* G*. Furthermore, we have*

$$\frac{|\lambda_k^m(A)|}{\sqrt{N_{2m}}} \leq \max_{1\leq j\leq N} (x_k)_j \tag{29}$$

The companion of (28) over frequencies k *is*

$$\min_{1\leq k\leq N} (x_k)_j^2 \leq \frac{(A^m)_{jj}}{W_m} \leq \max_{1\leq k\leq N} (x_k)_j^2 \tag{30}$$

where $W_m = \sum_{l=1}^{N} (A^m)_{ll} = \sum_{k=1}^{N} \lambda_k^m$ *is the total number of closed walks [1] with* m *hops/links.*

Proof: Consider the eigenvalue equation

$$\lambda_k(A^m)(x_k)_i = \sum_{j=1}^{N} (A^m)_{ij} (x_k)_j$$

First, we bound the sum

$$\min_{1\leq j\leq N} (x_k)_j \sum_{j=1}^{N} (A^m)_{ij} \leq \sum_{j=1}^{N} (A^m)_{ij} (x_k)_j \leq \max_{1\leq j\leq N} (x_k)_j \sum_{j=1}^{N} (A^m)_{ij} \tag{31}$$

and after introducing the above eigenvalue equation with $\lambda_k(A^m) = \lambda_k^m(A)$, we sum over all i using the definition (42) of the fundamental weight w_k,

$$\min_{1\leq j\leq N} (x_k)_j \sum_{i=1}^{N} \sum_{j=1}^{N} (A^m)_{ij} \leq \lambda_k^m(A) w_k \leq \max_{1\leq j\leq N} (x_k)_j \sum_{i=1}^{N} \sum_{j=1}^{N} (A^m)_{ij}$$

from which we find (28). Next, we square the inequality (31)

$$\lambda_k^2(A^m)(x_k)_i^2 \leq \left(\max_{1\leq j\leq N} (x_k)_j\right)^2 \sum_{j=1}^{N} \sum_{l=1}^{N} (A^m)_{ij} (A^m)_{il}$$

and then we sum over all i, using $\sum_{i=1}^{N} (x_k)_i^2 = 1$,

$$\lambda_k^2(A^m) \leq \left(\max_{1\leq j\leq N} (x_k)_j\right)^2 \sum_{j=1}^{N} \sum_{l=1}^{N} \left(\sum_{i=1}^{N} (A^m)_{ji} (A^m)_{il}\right) = \left(\max_{1\leq j\leq N} (x_k)_j\right)^2 \sum_{j=1}^{N} \sum_{l=1}^{N} \left(A^{2m}\right)_{jl}$$

which is equivalent to (29).

For any non-negative function f, it follows directly from the general formula (74) that

$$\min_{1\leq k\leq N} (x_k)_j^2 \leq \frac{(f(A))_{jj}}{\sum_{k=1}^{N} f(\lambda_k)} \leq \max_{1\leq k\leq N} (x_k)_j^2$$

where $\sum_{k=1}^{N} f(\lambda_k) = \sum_{l=1}^{N} (f(A))_{ll}$ (obtained by summing (74) over all j and invoking (64)). When choosing $f(x) = x^m$, we obtain (30). □

The bound (30) illustrates that " importance" of node j over all eigenfrequencies k is dictated by the percentage of closed walks $\frac{(A^m)_{jj}}{W_m}$ of any length m from and to that node j, which agrees with the

intuitive notion of importance in a network. For $m = 2$, inequality (30) reduces with $W_2 = 2L = Nd_{av}$, where $d_{av} = \frac{2L}{N}$ is the average degree in the graph G, to

$$\min_{1\leq k\leq N}(x_k)_j^2 \leq \frac{1}{N}\frac{d_j}{d_{av}} \leq \max_{1\leq k\leq N}(x_k)_j^2$$

while the case $m = 0$ yields

$$\min_{1\leq k\leq N}(x_k)_j^2 \leq \frac{1}{N} \leq \max_{1\leq k\leq N}(x_k)_j^2$$

which illustrates that equality in both sides in (30) for irregular graphs is not possible.

It follows from (74) that $(A^m)_{jj} = \sum_{k=1}^N \lambda_k^m (x_k)_j^2$ so that, for large m, $(A^m)_{jj} \sim \lambda_1^m (x_1)_j^2$ and $\sum_{k=1}^N \lambda_k^m \sim \lambda_1^m$, if $\lambda_1 > \max(\lambda_2, |\lambda_N|)$, while $(A^m)_{jj} \sim 2\lambda_1^m (x_1)_j^2$ and $\sum_{k=1}^N \lambda_k^m \sim 2\lambda_1^m$ for complete bipartite graphs. Hence,

$$\lim_{m\to\infty}\frac{(A^m)_{jj}}{\lambda_1^m} = (x_1)_j^2$$

and, for $m \to \infty$, the inequality (30) becomes $\min_{1\leq k\leq N}(x_k)_j^2 \leq (x_1)_j^2 \leq \max_{1\leq k\leq N}(x_k)_j^2$. Thus, the principal eigenvector component can, in absolute value, be the smallest as well as the largest for a node j (see e.g. Fig. 2). Since

$$N_{2n} = \sum_{j=1}^N \lambda_j^{2n}\left(u^T x_j\right)^2 = \lambda_1^{2n}\left(u^T x_1\right)^2\left\{1 + \sum_{j=2}^N\left(\frac{\lambda_j}{\lambda_1}\right)^{2n}\frac{\left(u^T x_j\right)^2}{\left(u^T x_1\right)^2}\right\} \geq \lambda_1^{2n}\left(u^T x_1\right)^2$$

shows that $\frac{N_{2n}}{\lambda_1^{2n}}$ is decreasing in n and $\lim_{n\to\infty}\frac{N_{2n}}{\lambda_1^{2n}} = \left(u^T x_1\right)^2$, inequality (28) for the principal eigenvector $k = 1$ and $m = 2n$ becomes

$$\min_{1\leq q\leq N}(x_1)_q \leq \frac{1}{u^T x_1}\frac{1}{1 + \sum_{j=2}^N\left(\frac{\lambda_j}{\lambda_1}\right)^{2n}\left(\frac{u^T x_j}{u^T x_1}\right)^2} \leq \max_{1\leq q\leq N}(x_1)_q$$

The limit $n \to \infty$ equals

$$\min_{1\leq q\leq N}(x_1)_q \leq \frac{1}{u^T x_1} \leq \max_{1\leq q\leq N}(x_1)_q \tag{32}$$

which results in a sharp upper bound (but less tight lower bound). Equality in the above bounds is reached for regular graphs where $x_1 = \frac{u}{\sqrt{N}}$, $\min_{1\leq q\leq N}(x_1)_q = \max_{1\leq q\leq N}(x_1)_q$ and $u^T x_1 = \sqrt{N}$ such that $E[x_1] = \frac{1}{\sqrt{N}} = \frac{1}{NE[x_1]}$.

Combining (28) and (29) leads to

$$\max\left(\frac{\lambda_k^m(A)w_k}{N_m}, \frac{|\lambda_k^m(A)|}{\sqrt{N_{2m}}}\right) \leq \max_{1\leq j\leq N}(x_k)_j$$

If $\lambda_k(A^m)w_k > 0$, then the inequality $N_m^2 \leq NN_{2m}$ (see e.g. [1, p. 34]) does not allow us to deduce the largest of the two lower bounds.

We now present another lower bound over all eigenfrequencies k.

Corollary 4 *The correction factor $1 - r_i(k)$, defined in (25), obeys*

$$\sum_{k=1}^N (1 - r_i(k)) = 2 \tag{33}$$

Moreover, the maximum eigenvector centrality $(x_k)_i^2$ *of node* i *is never smaller than*

$$\frac{4}{N\left(3+\frac{(A^4)_{ii}}{d_i^2}\right)} \leq \max_{1\leq k\leq N}(x_k)_i^2 \tag{34}$$

Proof: Combining (82) and (24) directly yields[9] (33). Via this method, thus using (24) and (33), the variance of the numbers $\{1-r_i(1),\ldots,(1-r_i(N))\}$ equals

$$\begin{aligned}\mathrm{Var}\left[(1-r_i(k))\right] &= \frac{1}{N}\sum_{k=1}^{N}(1-r_i(k))^2-\left(\frac{1}{N}\sum_{k=1}^{N}(1-r_i(k))\right)^2\\ &= \frac{1}{N}\sum_{k=1}^{N}(x_k)_i^4\left(\frac{\lambda_k^2(A)}{d_i}+1\right)^2-\frac{4}{N^2}\end{aligned}$$

The first term equals

$$\sum_{k=1}^{N}(1-r_i(k))^2=\sum_{k=1}^{N}(x_k)_i^4+\frac{2}{d_i}\sum_{k=1}^{N}(x_k)_i^4\lambda_k^2(A)+\frac{1}{d_i^2}\sum_{k=1}^{N}(x_k)_i^4\lambda_k^4(A)$$

Further, with (82),

$$\sum_{k=1}^{N}(x_k)_i^4\lambda_k^2(A)\leq\max_{1\leq k\leq N}(x_k)_i^2\sum_{k=1}^{N}(x_k)_i^2\lambda_k^2(A)=\max_{1\leq k\leq N}(x_k)_i^2\,d_i$$

and, similarly,

$$\sum_{k=1}^{N}(x_k)_i^4\lambda_k^4(A)\leq\max_{1\leq k\leq N}(x_k)_i^2\sum_{k=1}^{N}(x_k)_i^2\lambda_k^4(A)=\max_{1\leq k\leq N}(x_k)_i^2\left(A^4\right)_{ii}$$

where $\left(A^4\right)_{ii}$ is the number of closed walks with 4 hops starting and ending at node i, results in an upper bound for the variance

$$\mathrm{Var}\left[(1-r_i(k))\right]\leq\frac{1}{N}\left(\max_{1\leq k\leq N}(x_k)_i^2\left(3+\frac{\left(A^4\right)_{ii}}{d_i^2}\right)-\frac{4}{N}\right)$$

Since the variance is non-negative, we find the lower bound (34). □

Equation (33) indicates that the average over the frequencies k is $E_k\left[1-r_i(k)\right]=\frac{1}{N}\sum_{k=1}^{N}(1-r_i(k))=\frac{2}{N}$ so that, approximately, $(x_k)_i^2\approx\frac{1}{N}\frac{2d_i}{\lambda_k^2(A)+d_i}$.

[9] Directly summing the definition (25) gives

$$\begin{aligned}\sum_{k=1}^{N}r_i(k) &= \sum_{j=1;j\neq i}^{N}(1-a_{ij})\sum_{k=1}^{N}(x_k)_j^2+\frac{1}{2d_i}\sum_{j=1}^{N}a_{ij}\sum_{l=1}^{N}a_{il}\sum_{k=1}^{N}((x_k)_l-(x_k)_j)^2\\ &= \sum_{j=1;j\neq i}^{N}(1-a_{ij})+\frac{1}{d_i}\sum_{j=1}^{N}a_{ij}\sum_{l=1}^{N}a_{il}(1-\delta_{lj})\end{aligned}$$

where the second orthogonality relation (66) has been invoked. Further, with $\sum_{j=1;j\neq i}^{N}(1-a_{ij})=(N-1-d_i)$ and

$$\begin{aligned}\frac{1}{d_i}\sum_{j=1}^{N}a_{ij}\sum_{l=1}^{N}a_{il}(1-\delta_{lj}) &= \frac{1}{d_i}\sum_{j=1}^{N}a_{ij}\left\{\sum_{l=1}^{N}a_{il}-a_{ij}\right\}=\frac{1}{d_i}\sum_{j=1}^{N}a_{ij}d_i-\frac{1}{d_i}\sum_{j=1}^{N}a_{ij}^2\\ &= d_i-1\end{aligned}$$

we arrive at (33).

Theorem 5 *For any graph G, it holds that*

$$\min_{1\leq k\leq N}(x_k)_i^2 \leq \frac{1}{N}\frac{\min\left(1+\frac{d_{av}}{d_i},2\right)}{\min_{1\leq k\leq N}\left(\frac{\lambda_k^2(A)}{d_i}+1\right)} \tag{35}$$

and

$$\min_{1\leq i\leq N}(x_k)_i^2 \leq \frac{1}{N}\frac{1+\lambda_k^2(A)E\left[\frac{1}{D}\right]}{1+\frac{\lambda_k^2(A)}{d_{\max}}} \tag{36}$$

where the harmonic mean of the degree[10] *is* $E\left[\frac{1}{D}\right]=\frac{1}{N}\sum_{i=1}^{N}\frac{1}{d_i}$.

Proof: Summing (24) over all k and invoking the second orthogonality relation (66) yields

$$1=\sum_{k=1}^{N}\frac{1-r_i(k)}{\frac{\lambda_k^2(A)}{d_i}+1} \text{ for nodes } 1\leq i\leq N \tag{37}$$

while, similarly, the sum over all i gives

$$1=\sum_{i=1}^{N}\frac{1-r_i(k)}{\frac{\lambda_k^2(A)}{d_i}+1} \text{ for frequency indices } 1\leq k\leq N$$

from which we obtain

$$\min_{1\leq k\leq N}(1-r_i(k)) \leq \left(\sum_{k=1}^{N}\frac{1}{\frac{\lambda_k^2(A)}{d_i}+1}\right)^{-1}$$

and

$$\min_{1\leq i\leq N}(1-r_i(k)) \leq \left(\sum_{i=1}^{N}\frac{1}{\frac{\lambda_k^2(A)}{d_i}+1}\right)^{-1}$$

Invoking the harmonic, geometric and arithmetic mean inequality (for positive, real a_k)

$$\frac{n}{\sum_{k=1}^{n}\frac{1}{a_k}} \leq \sqrt[n]{\prod_{k=1}^{n}a_k} \leq \frac{1}{n}\sum_{k=1}^{n}a_k \tag{38}$$

shows, using $\sum_{k=1}^{N}\left(\frac{\lambda_k^2(A)}{d_i}+1\right)=N+\frac{2L}{d_i}$, that

$$\left(\sum_{k=1}^{N}\frac{1}{\frac{\lambda_k^2(A)}{d_i}+1}\right)^{-1} \leq \frac{1}{N}\left(1+\frac{d_{av}}{d_i}\right)$$

so that

$$\min_{1\leq k\leq N}(1-r_i(k)) \leq \left(\sum_{k=1}^{N}\frac{1}{\frac{\lambda_k^2(A)}{d_i}+1}\right)^{-1} \leq \frac{1}{N}\left(1+\frac{d_{av}}{d_i}\right)$$

which is sharper than $\min_{1\leq k\leq N}(1-r_i(k))\leq\frac{2}{N}$ (deduced from (33)) when $d_{av}\leq d_i$. Hence,

$$\min_{1\leq k\leq N}(1-r_i(k)) \leq \frac{1}{N}\min\left(1+\frac{d_{av}}{d_i},2\right)$$

[10] As in [6], the degree of a randomly chosen node in the graph is denoted by the random variable D.

so that, with $\min_{1\le k\le N}\left\{(x_k)_i^2\left(\frac{\lambda_k^2(A)}{d_i}+1\right)\right\}\ge \min_{1\le k\le N}(x_k)_i^2\min_{1\le k\le N}\left(\frac{\lambda_k^2(A)}{d_i}+1\right)$, we obtain (35). Similarly (for the node index), using $\sum_{i=1}^N\left(\frac{\lambda_k^2(A)}{d_i}+1\right)=N+\lambda_k^2(A)\sum_{i=1}^N\frac{1}{d_i}$, we have

$$\min_{1\le i\le N}\left(1-r_i\left(k\right)\right)\le\frac{1}{N}\left(1+\frac{\lambda_k^2(A)}{N}\sum_{i=1}^N\frac{1}{d_i}\right)$$

and (38) leads to $\frac{1}{d_{av}}\le E\left[\frac{1}{D}\right]=\frac{1}{N}\sum_{i=1}^N\frac{1}{d_i}\le\frac{1}{d_{\min}}$. Invoking

$$\min_{1\le i\le N}\left(1-r_i\left(k\right)\right)=\min_{1\le i\le N}\left\{(x_k)_i^2\left(\frac{\lambda_k^2(A)}{d_i}+1\right)\right\}\ge\min_{1\le i\le N}(x_k)_i^2\left(\frac{\lambda_k^2(A)}{d_{\max}}+1\right)$$

finally yields (36). □

We observe that (36) is better for small $\lambda_k^2(A)$ than (27) ignoring s_k, while the opposite holds for large $\lambda_k^2(A)$.

Further, we bound (37), using (33),

$$\frac{2}{\max_{1\le k\le N}\left(\frac{\lambda_k^2(A)}{d_i}+1\right)}\le\sum_{k=1}^N\frac{1-r_i\left(k\right)}{\frac{\lambda_k^2(A)}{d_i}+1}\le\frac{2}{\min_{1\le k\le N}\left(\frac{\lambda_k^2(A)}{d_i}+1\right)}$$

and find

$$\min_{1\le k\le N}\left(\lambda_k^2(A)\right)\le d_i\le\max_{1\le k\le N}\left(\lambda_k^2(A)\right)=\lambda_1^2(A)$$

Since this inequality holds for each node i, we retrieve the classical bound $\lambda_1(A)\ge\sqrt{d_{\max}}$ (equality holds for the star), but also

$$\min_{1\le k\le N}\left(\lambda_k^2(A)\right)\le d_{\min}$$

which is reminiscent to the inequality $\mu_{N-1}\le d_{\min}$ for the algebraic connectivity[11] (excluding the complete graph) and which we sharpen:

Theorem 6 *In any connected graph, it holds that*

$$\min_{1\le k\le N}\left(\lambda_k^2(A)\right)<d_{\min}\tag{39}$$

Proof: Let us denote the ordering in the eigenvalues as $\lambda_{(1)}^2(A)\ge\lambda_{(2)}^2(A)\ge\ldots\ge\lambda_{(N)}^2(A)$, where $\lambda_{(1)}^2(A)=\lambda_1^2(A)$ and $\lambda_{(N)}^2(A)=\min_{1\le k\le N}\left(\lambda_k^2(A)\right)$ and we write the index k^* being associated with $\lambda_{(k)}^2(A)$, the k-th largest eigenvalue of A^2. After applying Abel summation to (37), we obtain

$$\sum_{k=1}^N\frac{1-r_i\left(k\right)}{\frac{\lambda_k^2(A)}{d_i}+1}=\sum_{k=1}^{N-1}\left\{\sum_{l=1}^k\left(1-r_i\left(l^*\right)\right)\right\}\left(\frac{1}{\frac{\lambda_{(k)}^2(A)}{d_i}+1}-\frac{1}{\frac{\lambda_{(k+1)}^2(A)}{d_i}+1}\right)+\frac{1}{\frac{\lambda_{(N)}^2(A)}{d_i}+1}\sum_{l=1}^N\left(1-r_i\left(l^*\right)\right)$$

Using (33) and (37) yields

$$1=-S_i+\frac{2}{\frac{\lambda_{(N)}^2(A)}{d_i}+1}$$

[11] The algebraic connectivity [32, 1] is the second smallest eigenvalue μ_{N-1} of the Laplacian $Q=\Delta-A$. Both the Laplacian Q and A^2 have the same diagonal elements $Q_{jj}=\left(A^2\right)_{jj}=d_j$.

where

$$S_i = \sum_{k=1}^{N-1} \left\{ \sum_{l=1}^{k} \left(1 - r_i\left(l^*\right)\right) \right\} \left(\frac{1}{\frac{\lambda_{(k+1)}^2(A)}{d_i} + 1} - \frac{1}{\frac{\lambda_{(k)}^2(A)}{d_i} + 1} \right) \tag{40}$$

which is non-negative (because each term in the k-sum is), $S_i \geq 0$. Hence, for each node i, we obtain that

$$\min_{1 \leq k \leq N} \left(\lambda_k^2(A)\right) = d_i \frac{1 - S_i}{1 + S_i} = d_i \left(1 - \frac{2}{\frac{1}{S_i} + 1}\right) \tag{41}$$

Equation (41) shows that $S_i \leq 1$, and thus that $0 \leq S_i \leq 1$ and that $\min_{1 \leq k \leq N} \left(\lambda_k^2(A)\right) = d_i$ if $S_i = 0$. Further, if $d_i > d_j$, then it follows from (41) that $S_i > S_j$ and S_i increases with the degree d_i. Hence, $S_{\min} = \min_{1 \leq i \leq N} S_i$ corresponds to the node with minimum degree.

Since each term in (40) is non-negative, S_i can only be zero if each term in the k-sum is zero,

$$\left\{ \sum_{l=1}^{k} \left(1 - r_i\left(l^*\right)\right) \right\} \left(\frac{1}{\frac{\lambda_{(k+1)}^2(A)}{d_i} + 1} - \frac{1}{\frac{\lambda_{(k)}^2(A)}{d_i} + 1} \right) = 0$$

The first factor $\sum_{l=1}^{k} \left(1 - r_i\left(l^*\right)\right) = \left(1 - r_i\left(1\right)\right) + \sum_{l=2}^{k} \left(1 - r_i\left(l^*\right)\right)$, because $r_i\left(1^*\right) = r_i\left(1\right)$ as $\lambda_{(1)}^2(A) = \lambda_1^2(A)$. In a connected graph, (24) demonstrates that $r_i\left(1\right) < 1$, because each component of the principal eigenvector x_1 is positive (by the Perron-Frobenius Theorem). Hence, for each $1 \leq k \leq N-1$, $\sum_{l=1}^{k} \left(1 - r_i\left(l^*\right)\right) > 0$. The last factor cannot always be zero, because it would require that $\lambda_{(k+1)}^2(A) = \lambda_{(k)}^2(A)$ for all k, which is impossible. Hence, in a connected graph, $S_i > 0$ for each node i. □

A consequence of Theorem 6 is

Corollary 5 *If* $\min_{1 \leq k \leq N} \left(\lambda_k^2(A)\right) = d_{\min}$*, then the graph is disconnected.*

The reverse of the Corollary 5 is not always true[12].

If $\min_{1 \leq k \leq N} \left(\lambda_k^2(A)\right) = 0$, then $S_i = 1$ for each node i. When excluding graphs with isolated nodes (i.e. degree zero nodes), (41) implies that, if $S_i = 1$ for node i, then $\min_{1 \leq k \leq N} \left(\lambda_k^2(A)\right) = 0$ and, thus $S_j = 1$ for each other node j. Hence, in any graph with $d_i > 0$, in order for A to have a zero eigenvalue[13], there must hold that $S_i = 1$ for each node i.

4 The fundamental weight and its dual

When choosing $b = u$ in Section 2.1, the fundamental weight $w_k = u^T x_k = \sum_{j=1}^{N} \left(x_k\right)_j$ was introduced as additional information to determine the eigenvector components. The graph angle γ_k in [14] is related to the fundamental weight by $\cos \gamma_k = \frac{w_k}{\sqrt{N}}$, where the angle θ_{ab} between two vectors a and b obeys $\cos \theta_{ab} = \frac{a^T b}{\|a\|_2 \|b\|_2}$ and $\|a\|_2^2 = a^T a$. Geometrically in $N = 3$ dimensions, the 3 orthogonal axes are completely defined by the knowledge of 3 angles. However, in higher dimensions $N > 3$, all $\binom{N}{2}$ orthogonality relations (64), which directly imply the second set of $\binom{N}{2}$ orthogonality relations (66)

[12] Moreover, simulations on small Erdős-Rényi graphs show that $\xi = d_{\min} - \min_{1 \leq k \leq N} \left(\lambda_k^2(A)\right) - \mu_{N-1}$ is non-negative in most (but not all) cases.

[13] It also follows from (24) that, if $\lambda_{(N)}^2(A) = 0$, then $\left(x_{N^*}\right)_i^2 = 1 - r_i\left(N^*\right)$, where N^* here equals the index k for which $\lambda_k^2(A) = 0$, while summing over all i shows that $\sum_{i=1}^{N} r_i\left(N^*\right) = N - 1$.

due commutativity between X and X^{-1}, are needed to specify the N orthogonal axes ($x_k^T x_m = \cos\theta_{km}$ and θ_{km} is either $\frac{\pi}{2}$ or 0) so that we expect $O\left(N^2\right)$ graph angles rather than $O\left(N\right)$.

Section 4.1 presents alternative definitions of the fundamental and dual fundamental weights, while Section 4.2 derives a first set of their properties. Using fundamental weights, we compute tight bounds on the coupling of eigenvalues of a graph G and its complement G^c in Appendix C.

4.1 Definitions

The dual of the definition

$$w_k = \sum_{j=1}^{N} \left(x_k\right)_j \tag{42}$$

is

$$\varphi_j = \sum_{k=1}^{N} \left(x_k\right)_j \tag{43}$$

which is the sum of the eigenvector components of node j over all eigenfrequencies. The corresponding vectors $w = (w_1, w_2, \ldots, w_N)$ and $\varphi = (\varphi_1, \varphi_2, \ldots, \varphi_N)$ are called the fundamental weight and dual fundamental weight vector of the adjacency matrix A of a graph G, respectively. Those vectors can be written as the row sum and column sum of the orthogonal matrix X in (63),

$$w = X^T u \tag{44}$$

$$\varphi = X u \tag{45}$$

or, in terms of the eigenvectors $\{x_k\}_{1\le k\le N}$ and $\{y_k\}_{1\le k\le N}$, defined in (65),

$$w = \sum_{k=1}^{N} y_k \tag{46}$$

$$\varphi = \sum_{k=1}^{N} x_k \tag{47}$$

Hence, $\frac{1}{N}\varphi$ is the average of all eigenvectors of the adjacency matrix A. The corresponding vector components are, for the fundamental weight,

$$w_k = u^T x_k \tag{48}$$

and for the dual fundamental weight

$$\varphi_j = u^T y_j \tag{49}$$

illustrating that the role in (48) and (49) of the vectors x_k and y_k is reversed with respect to (46) and (47).

Suppose that a node relabeling in the graph G is defined by the permutation matrix P, which is an orthogonal matrix [1, art 11, p. 21]. We denote the relabeled adjacency matrix by $\widetilde{A} = P^T A P$ and its spectral decomposition by $\widetilde{A} = \widetilde{X}\Lambda\widetilde{X}^T$, where $\widetilde{X} = P^T X$. The definition (44) of w shows that $\widetilde{w} = w$, so that w is *invariant* under a relabeling transformation. However, the definition (45) of φ shows that $\widetilde{\varphi} = P^T\varphi$; in other words, the components of $\widetilde{\varphi}$ change position after relabeling.

Theorem 7 *There exist regular graphs for which the adjacency matrix A possesses a symmetric orthogonal matrix $X = X^T$.*

Barik *et al.* [33] have shown that only regular graphs, such as the complete graph K_N, for $N = 4k$ and $k \in \mathbb{N}_0$, and the regular bipartite graph $K_{2k,2k}$, are diagonalizable by a Hadamard matrix. An $n \times n$ Hadamard matrix H_n contains as elements either -1 and 1 and obeys $H_n H_n^T = nI_n$. The normalized matrix $X_n = \frac{1}{\sqrt{n}} H_n$ is an orthogonal matrix, from which it follows that $\det H_n = n^{\frac{n}{2}}$, which is maximal among all $n \times n$ matrices with elements in absolute value less than or equal to 1, which includes all orthogonal matrices. Any relabeling (permutation of rows and columns) of a Hadamard matrix is again a Hadamard matrix; multiplying any row or column by -1 preserves the Hadamard properties.

Sylvester found a construction for *symmetric* Hadamard matrices $H_{2^k} = H_{2^{k-1}} \otimes H_2$, where $\otimes$ is the Kronecker product [1] and $H_2 = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$, that contain the u vector in the first column.

Proof[14]**:** Let $H_n = \left[u | \widetilde{H}\right]$ so that $H_n e_1 = u$. Consider the diagonal matrix $D = I - e_1 e_1^T$, then

$$H_n D H_n^T = H_n H_n^T - H_n e_1 \left(H_n e_1\right)^T = nI_n - u.u^T = nI - J$$

Hence, the Laplacian matrix of the complete graph K_n is $Q_{K_n} = nI - J = H_n D H_n^T$. Since K_n is a regular graph, the eigenvectors of the Laplacian Q and the adjacency matrix A are the same[15]. In conclusion, any Hadamard matrix with $H_n e_1 = u$ provides the orthogonal matrix for the complete graph and the Sylvester construction demonstrates that there exist symmetric such Hadamard matrices for $n = 4k$. □

It will transpire that graphs with a symmetric orthogonal matrix $X = X^T$ possess extremal properties: (44) and (44) show that $w = \varphi$, only if $X = X^T$.

4.2 Properties

The definitions in Section 4.1 lead to a number of immediate consequences.

8. The norms $\|w\|_2$ and $\|\varphi\|_2$ are the same. In particular,

$$w^T w = \varphi^T \varphi = N$$

shows that their norm equals that of the all-one vector u,

$$\|w\|_2 = \|\varphi\|_2 = \|u\|_2 = \sqrt{N}$$

This norm property follows either from (44) as $w^T w = u^T X X^T u = u^T u$, because $XX^T = I$, or from $w^T w = \sum_{k=1}^N \sum_{m=1}^N y_k^T y_m$ and the orthogonality relations (66). Similarly for φ, where a possible node relabeling does not influence the norm: $\widetilde{\varphi}^T \widetilde{\varphi} = \varphi^T P P^T \varphi = \varphi^T \varphi$, because P is an orthogonal matrix.

[14] The proof (only for K_N) is slightly simpler than the one in [33].

[15] Indeed, for a regular graph with degree r, the Laplacian is $Q = (r+1) I - A$. If $Q = ZMZ^T$ and $A = X \Lambda X^T$, we observe that $ZMZ^T = X \left((r+1) I - \Lambda\right) X^T$, implying that $X = Z$.

9. *Bounds of maximum and minimum.* The bound $N = \varphi^T \varphi = \sum_{j=1}^N \varphi_j^2 \leq N \max_{1\leq j\leq N} \varphi_j^2$ illustrates that

$$-\sqrt{N} \leq \min_{1\leq j\leq N} \varphi_j \leq 1 \leq \max_{1\leq j\leq N} \varphi_j \leq \sqrt{N}$$

and similarly for w. In the case of w, a much sharper lower bound for the maximum is known (**art.** 17).

10. Any vector z in an N-dimensional space can be written as a linear combination of a set of N orthogonal vectors that span that space, such as the set $\{x_k\}_{1\leq k\leq N}$ and the set $\{y_k\}_{1\leq k\leq N}$,

$$z = \sum_{k=1}^N \left(z^T y_k\right) y_k = \sum_{k=1}^N \left(z^T x_k\right) x_k$$

For example,

$$u = \sum_{j=1}^N \varphi_j y_j = \sum_{k=1}^N w_k x_k \tag{50}$$

indicating that the coordinate vector of u with respect to the basis $\{x_k\}_{1\leq k\leq N}$ is the w vector and with respect to the basis $\{y_j\}_{1\leq j\leq N}$ is the φ vector. Another example is, using (67),

$$x_k = \sum_{j=1}^N \left(x_k^T y_j\right) y_j = \sum_{j=1}^N \left(X^2\right)_{jk} y_j \text{ and } y_j = \sum_{k=1}^N \left(X^2\right)_{jk} x_k$$

The definitions (46) and (47) express w and φ as such a linear combination, from which it follows, for any integer $1 \leq m \leq N$, that

$$w^T y_m = 1 \tag{51}$$

and[16]

$$\varphi^T x_m = 1 \tag{52}$$

Both scalar products (51) and (52) also follow from the identities $XX^T u = u$ and $X^T X u = u$, respectively. The geometric meaning is that, for any m, the vector w and φ make the same angle $\theta_{y_m w}$ and $\theta_{x_m \varphi}$ with any vector y_m and any eigenvector x_m of A, respectively. Hence, with respect to the orthogonal basis spanned by the eigenvectors $\{x_k\}_{1\leq k\leq N}$, the vector φ plays the same role as the vector u with respect to the "classical" orthogonal basis $\{e_k\}_{1\leq k\leq N}$. The transformation $Xu = \varphi$ rotates the all-one vector u into the vector φ, while the inverse rotation yields $X^{-1}u = X^T u = w$.

11. After left-multiplying the eigenvalue equation $Ax_k = \lambda_k x_k$ by u^T and summing the resulting eigenvalue relation $d^T x_k = \lambda_k w_k$ over all k yields

$$\sum_{k=1}^N \lambda_k w_k = \sum_{k=1}^N \left(\sum_{j=1}^N d_j \left(x_k\right)_j\right) = \sum_{j=1}^N d_j \varphi_j$$

[16] We also mention the dual expressions, derived by invoking (67),

$$\begin{cases} w^T x_m = \left(X^2 u\right)_m \\ \varphi^T y_m = \left(X^2 u\right)_m \end{cases}$$

In other words, we observe that

$$w^T \lambda = \varphi^T d \tag{53}$$

where the eigenvalue vector $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_N)$ is related to the degree vector d via the fundamental weight vector w and its dual vector φ. Further, recall that $\lambda^T \lambda = 2L$ and $d^T u = 2L$, but $d^T d > 2L$. Thus, $w^T \lambda = \varphi^T d$, combined with

$$\left(d^T \varphi\right)^2 \leq \|d\|_2^2 \, \|\varphi\|_2^2 = \|d\|_2^2 \, N$$

and

$$\left(\lambda^T w\right)^2 \leq \|\lambda\|_2^2 \, \|w\|_2^2 = 2LN \leq \|d\|_2^2 \, N$$

means that the angle $\theta_{d\varphi}$ between the vector d and φ is larger than the angle $\theta_{\lambda w}$ between the vector λ and w. Thus, we can say that λ and w are closer correlated than d and φ.

The generalization of (53), based on the eigenvalue equation $A^m x_k = \lambda_k^m x_k$ is

$$w^T \lambda^m = \varphi^T d^{(m)} \tag{54}$$

or

$$\sum_{k=1}^{N} \lambda_k^m w_k = \sum_{j=1}^{N} \left(A^m u\right)_j \varphi_j$$

where the vector $\lambda^m = (\lambda_1^m, \lambda_2^m, \ldots, \lambda_N^m) = \Lambda^m u$ and the vector $d^{(m)} = \left(\left(A^m u\right)_1, \left(A^m u\right)_2, \ldots, \left(A^m u\right)_N\right) = A^m u$, with $d^{(0)} = u$ and $d^{(1)} = d$.

Although the vector d cannot be equal to the vector λ, we cannot conclude from (54) that w cannot be equal to φ. Indeed, suppose that $w = \varphi \neq 0$, then (54) reduces to $w^T \left(\lambda^m - d^{(m)}\right) = 0$, which is equivalent to

$$0 = w^T \left(A^m - \Lambda^m\right) u = w^T \left(X \Lambda^m X^T - \Lambda^m X X^T\right) u = w^T \left(X \Lambda^m - \Lambda^m X\right) w = -w^T \left(X^T \Lambda^m - \Lambda^m X^T\right) w$$

and only possible for all m if $X = X^T$.

12. Since $s_X = u^T X u = \left(X^T u\right)^T u = u^T (X u)$, we have with (44) and (45) that

$$s_X = w^T u = u^T \varphi \tag{55}$$

which also follows from (54) for $m = 0$. The sum of the elements of the orthogonal matrix X thus equals

$$s_X = \sum_{j=1}^{N} \sum_{k=1}^{N} \left(x_k\right)_j = \sum_{j=1}^{N} \varphi_j = \sum_{k=1}^{N} w_k$$

Since $|s_X| = \left|w^T u\right| \leq \sqrt{\|w\|_2^2 \, \|u\|_2^2}$, we find with $\|w\|_2^2 = N$ that $-N \leq s_X \leq N$. Moreover, the sum of the elements of the matrix $w w^T = X^T J X$ and its transpose $\varphi \varphi^T = X J X^T$ (where the all-one matrix is $J = u.u^T$) equals

$$s_X^2 = u^T \left(w w^T\right) u = u^T \left(\varphi \varphi^T\right) u$$

13. Since $X^T = X^{-1}$ is non-singular ($\det X = \pm 1$), it follows from (44) and (45) that the all-one vector can be expressed as

$$u = X w = X^T \varphi$$

Thus, we find from the definition (44) and (45) that

$$\varphi = X^2 w \text{ and } w = \left(X^T\right)^2 \varphi$$

and

$$w^T \varphi = w^T X^2 w = u^T X^2 u$$

so that the sum $s_{X^2} = u^T X^2 u$ of the elements in X^2 equals

$$s_{X^2} = w^T \varphi \tag{56}$$

Since $w^T \varphi = \|w\|_2 \|\varphi\|_2 \cos\theta_{w\varphi} = N \cos\theta_{w\varphi}$, we find that the sum of the elements of X^2 obeys $-N \leq u^T X^2 u \leq N$ and equality in either lower or upper bound only holds if $w = -\varphi$ or $w = \varphi$.

14. Since $u^T \lambda = 0$ due to trace$(A) = 0$, we find

$$\varphi^T A \varphi = 0 \tag{57}$$

Relation (57) holds for any adjacency matrix $A = A^T$. At first glance, the Rayleigh equations may hint that φ is an eigenvector belonging to eigenvalue $\lambda = 0$, which is false, because for any component j, we find

$$(A\varphi)_j = (AXu)_j = (X\Lambda u)_j = (X\lambda)_j = \sum_{k=1}^{N} (x_k)_j \lambda_k$$

while (81) shows that only $\sum_{k=1}^{N} (x_k)_j^2 \lambda_k = 0$. Moreover, (57) demonstrates that not all components of φ can be negative nor all can be positive for a graph (except for the null graph without any links for which $A = 0$). For, otherwise, if $\varphi_j < 0$ or $\varphi_j > 0$ for all j, then $\varphi^T A \varphi = 2 \sum_{i=1}^{N} \sum_{j=i+1}^{N} a_{ij} \varphi_i \varphi_j > 0$ contradicting (57). The vector $\varphi = \sqrt{N} e_j$ (see **art.** 15) does not violate (57) because $a_{jj} = 0$. In general, φ has positive, zero and negative components. It is convenient to order (e.g. by a node relabeling) the dual fundamental weights as

$$\varphi_{(1)} \geq \ldots \geq \varphi_{(q)} \geq 0 \geq \varphi_{(q+1)} \geq \ldots \geq \varphi_{(N)}$$

with $1 \leq q < N$.

A generalization of (57) follows from $A^m = X \Lambda^m X^T$ and $u = X^T \varphi$ as

$$\varphi^T A^m \varphi = \varphi^T X \Lambda^m X^T \varphi = u^T \Lambda^m u = \sum_{j=1}^{N} \lambda_j^m = W_m$$

Hence, the number W_m of closed walks with m hops equals

$$W_m = \varphi^T A^m \varphi = \text{ trace}\left(A^m\right) = \sum_{j=1}^{N} \lambda_j^m \tag{58}$$

whereas the total number N_m of walks with m hops equals

$$N_m = u^T A^m u = w^T \Lambda^m w = \sum_{j=1}^{N} w_j^2 \lambda_j^m \tag{59}$$

15. *Regular graphs.* In any connected regular graph (with degree vector $d = ru$), it holds that $x_1 = \frac{u}{\sqrt{N}}$. Since u is always an eigenvector of the Laplacian matrix Q, this **art.** 15 holds for the Laplacian of any graph as well (with replacement below of e_1 by e_N, because u corresponds to the smallest Laplacian eigenvalue $\mu_N = 0$). If the graph is not connected, a different normalization of u is required.

The definition (48) indicates that $w_1 = u^T x_1 = \sqrt{N}$, while $w_k = 0$ (due to orthogonality (64)), so that the entire $w = \sqrt{N} e_1$ vector is known. Thus, if the graph is regular, then $w = \sqrt{N} e_1$ and the sum (55) of the elements of X equals $s_X = u^T w = \sqrt{N}$, while (56) shows that $s_{X^2} = \varphi_1$, which is clearly not invariant to node relabeling! The converse, "if $s_X = \sqrt{N}$, then the graph is regular", is likely not true[17].

16. *Fundamental weight w_k in terms of ordered eigenvector components.* We order the eigenvector components as

$$\min_{1\le q\le N} (x_k)_q = (x_k)_{(N)} \le (x_k)_{(N-1)} \le \cdots \le (x_k)_{(1)} = \max_{1\le q\le N} (x_k)_q$$

and apply Abel's summation to $1 = x_k^T x_k = \sum_{j=1}^N (x_k)_j^2 = \sum_{j=1}^N (x_k)_{(j)}^2$,

$$1 = \sum_{j=1}^{N-1} \left(\sum_{l=1}^{j} (x_k)_{(j)} \right) \Big((x_k)_{(j)} - (x_k)_{(j+1)} \Big) + (x_k)_{(N)} \sum_{l=1}^{N} (x_k)_{(j)}$$

Further,

$$\begin{aligned}
1 &= \sum_{j=1}^{N-1} \left(u^T x_k - \sum_{l=j+1}^{N} (x_k)_{(j)} \right) \Big((x_k)_{(j)} - (x_k)_{(j+1)} \Big) + (x_k)_{(N)}\, u^T x_k \\
&= u^T x_k \sum_{j=1}^{N-1} \Big((x_k)_{(j)} - (x_k)_{(j+1)} \Big) - \sum_{j=1}^{N-1} \left(\sum_{l=j+1}^{N} (x_k)_{(j)} \right) \Big((x_k)_{(j)} - (x_k)_{(j+1)} \Big) + (x_k)_{(N)}\, u^T x_k \\
&= u^T x_k \max_{1\le q\le N} (x_k)_q - \sum_{j=1}^{N-1} \left(\sum_{l=j+1}^{N} (x_k)_{(j)} \right) \Big((x_k)_{(j)} - (x_k)_{(j+1)} \Big)
\end{aligned}$$

where the (telescopic) sum over the spacings of the ranked eigenvector components

$$\sum_{q=1}^{N-1} \Big((x_k)_{(q)} - (x_k)_{(q+1)} \Big) = \max_{1\le q\le N} (x_k)_q - \min_{1\le q\le N} (x_k)_q$$

has been used. In summary, we obtain

$$1 - w_k \min_{1\le q\le N} (x_k)_q = \sum_{j=1}^{N-1} \left(\sum_{l=1}^{j} (x_k)_{(j)} \right) \Big((x_k)_{(j)} - (x_k)_{(j+1)} \Big)$$

and

$$w_k \max_{1\le q\le N} (x_k)_q - 1 = \sum_{j=1}^{N-1} \left(\sum_{l=j+1}^{N} (x_k)_{(j)} \right) \Big((x_k)_{(j)} - (x_k)_{(j+1)} \Big)$$

[17] A counter example of an irregular graph with $s_X \simeq \sqrt{N}$ (up to 6 digits accurate) has been found by Xiangrong Wang.

For $k = 1$, each term in the right-hand side summations is always non-negative, which establishes again (32).

17. *Bounds.* The definition $w_k = u^T x_k = \sum_{j=1}^{N} (x_k)_j$ and the first orthogonality condition (64) yield

$$w_k = \frac{u^T x_k}{x_k^T x_k} = \frac{\sum_{j'=1}^{N} (x_k)_{j'}}{\sum_{j'=1}^{N} (x_k)_{j'}^2}$$

where j' reflects that $(x_k)_{j'} \neq 0$, because a zero term does not contribute to the sum. The inequality [34]

$$\min_{1\leq j\leq n} \frac{r_j}{b_j} \leq \frac{r_1 + r_2 + \cdots + r_n}{b_1 + b_2 + \cdots + b_n} \leq \max_{1\leq j\leq n} \frac{r_j}{b_j} \tag{60}$$

where $b_1, b_2, \ldots, b_n$ are positive real numbers and $r_1, r_2, \ldots, r_n$ are real numbers, yields

$$\min_{1\leq j'\leq N} \frac{1}{(x_k)_{j'}} \leq w_k \leq \max_{1\leq j'\leq N} \frac{1}{(x_k)_{j'}} \tag{61}$$

and, similarly,

$$\min_{1\leq k'\leq N} \frac{1}{(x_{k'})_j} \leq \varphi_j \leq \max_{1\leq k'\leq N} \frac{1}{(x_{k'})_j}$$

All components of x_1 are non-negative by the Perron-Frobenius theorem, whereas $\min_{1\leq j'\leq N} \frac{1}{(x_k)_{j'}} < -1$ for $k > 1$, because any other eigenvector x_k must have at least one negative component to satisfy the orthogonality condition $x_k^T x_1 = 0$. The upper bounds in (32) and in (61) result in

$$\frac{1}{\max_{1\leq j\leq N} (x_1)_j} \leq w_1 \leq \max_{1\leq j'\leq N} \frac{1}{(x_k)_{j'}}$$

which illustrates, together with the lower bound in (61), that $w_1 \geq 1$, a result earlier found in [1, p. 40] with a different method. A sharper lower bound

$$\sqrt{\frac{\lambda_1}{1 - \frac{1}{\omega}}} \leq w_1 \tag{62}$$

where ω is the clique number of the graph G is proved and evaluated in [17].

18. *Upper bound for the minimal spacing.* We assume that the vector components of φ are ordered as in **art.** 14. The corresponding relabeling[18] of node l is denoted by l^*. Several bounds for the spacings $\varphi_{(j)} - \varphi_{(j+1)}$ will be derived, based on Theorem 9 in Appendix B.

We apply (85) to $c = \varphi - u\varphi_{(N)}$ with $a = e_1$ (telescoping series) and with $a = u$ so that $a^T c = s_X - N\varphi_{(N)}$ in (55). The corresponding fractions f are

$$f_{e_1} = \frac{\varphi_{(1)} - \varphi_{(N)}}{N - 1}$$
$$f_u = \frac{\frac{s_X}{N} - \varphi_{(N)}}{\frac{N-1}{2}}$$

[18] Notice that $d_{(l)}$ denotes the l-th largest degree in the graph, while d_{l^*} is the degree of the node l^*, whose dual fundamental weight component $\varphi_{l^*} = \varphi_{(l)}$ is the l-th largest.

Since $\left|\varphi_{(1)}\right| \leq \sqrt{N}$ and $\left|\varphi_{(N)}\right| \leq \sqrt{N}$ (**art.** 9), we conclude from Theorem 9 that

$$\min_{1\leq j\leq N-1}\left\{\varphi_{(j)}-\varphi_{(j+1)}\right\} \leq O\left(\frac{1}{\sqrt{N}}\right)$$

for large N.

19. *Lower bound for the maximal spacing.* For $a=\varphi$ and $\varphi^T\varphi=N$, the fraction (85) becomes

$$f_\varphi = \frac{N-\varphi_{(N)}s_X}{\sum_{m=1}^{N-1} m\varphi_{(N-m)}}$$

Using the Cauchy-Schwarz inequality [1, p. 257]

$$\sum_{m=1}^{N-1} m\varphi_{(N-m)} \leq \sqrt{\sum_{m=1}^{N-1} m^2 \sum_{m=1}^{N-1}\varphi_{(N-m)}^2} = \sqrt{\frac{(N-1)\,N\,(2N-1)}{6}\left(N-\varphi_{(N)}^2\right)}$$

we arrive at

$$\max_{1\leq j\leq N-1}\left\{\varphi_{(j)}-\varphi_{(j+1)}\right\} \geq \frac{1-\varphi_{(N)}\frac{s_X}{N}}{\sqrt{\frac{(N-1)(2N-1)}{6}\left(1-\frac{\varphi_{(N)}^2}{N}\right)}} \geq O\left(\frac{1}{N}\right)$$

We observe that sharper bounds here and in **art.** 18 are only possible when $\varphi_{(N)}$ is known. After applying Abel summation to (55),

$$\sum_{j=1}^{N-1} j\left\{\varphi_{(j)}-\varphi_{(j+1)}\right\} = s_X - N\varphi_{(N)}$$

we find (since $\varphi_{(j)}-\varphi_{(j+1)}\geq 0$) that $\frac{s_X}{N}\geq\varphi_{(N)}\geq-\sqrt{N}$, where s_X can be negative.

20. *Another type of lower bound for the maximal spacing.* **Art.** 11 demonstrates that $d^T\varphi=\lambda^T w$ and $-\sqrt{2LN}\leq\lambda^T w\leq\sqrt{2LN}$, so that, after Abel summation,

$$-\sqrt{2LN} \leq \sum_{j=1}^{N-1}\left(\sum_{l=1}^{j} d_{l^*}\right)\left\{\varphi_{(j)}-\varphi_{(j+1)}\right\} + 2L\varphi_{(N)} \leq \sqrt{2LN}$$

or

$$-\sqrt{\frac{1}{d_{av}}} - \frac{1}{2L}\sum_{j=1}^{N-1}\left(\sum_{l=1}^{j} d_{l^*}\right)\left\{\varphi_{(j)}-\varphi_{(j+1)}\right\} \leq \varphi_{(N)} \leq \sqrt{\frac{1}{d_{av}}} - \frac{1}{2L}\sum_{j=1}^{N-1}\left(\sum_{l=1}^{j} d_{l^*}\right)\left\{\varphi_{(j)}-\varphi_{(j+1)}\right\}$$

Since $\varphi_{(N)}<0$ (ignoring pathological cases), we find that

$$\sqrt{\frac{1}{d_{av}}} < \frac{1}{2L}\sum_{j=1}^{N-1}\left(\sum_{l=1}^{j} d_{l^*}\right)\left\{\varphi_{(j)}-\varphi_{(j+1)}\right\}$$

Further,

$$\sum_{j=1}^{N-1}\left(\sum_{l=1}^{j} d_{l^*}\right)\left\{\varphi_{(j)}-\varphi_{(j+1)}\right\} \leq \max_{1\leq j\leq N-1}\left\{\varphi_{(j)}-\varphi_{(j+1)}\right\}\sum_{j=1}^{N-1}\left(\sum_{l=1}^{j} d_{l^*}\right)$$

and

$$\sum_{j=1}^{N-1}\sum_{l=1}^{j} d_{l^*} = \sum_{l=1}^{N-1}\sum_{j=l}^{N-1} d_{l^*} = \sum_{l=1}^{N-1}(N-l^*)\,d_{l^*} = \sum_{l=1}^{N}(N-l^*)\,d_{l^*} = 2LN - \sum_{l=1}^{N} l^* d_{l^*}$$

Hence,

$$\max_{1\leq j\leq N-1}\left\{\varphi_{(j)}-\varphi_{(j+1)}\right\} > \frac{\sqrt{\frac{1}{d_{av}}}}{N-\frac{1}{2L}\sum_{l=1}^{N} l^* d_{l^*}} > \frac{\sqrt{\frac{1}{d_{av}}}}{N-\frac{d_{\min}}{d_{av}}\frac{(N+1)}{2}} > \frac{1}{N}\frac{\sqrt{\frac{1}{d_{av}}}}{1-\frac{d_{\min}}{2d_{av}}}$$

which is, unfortunately, more conservative than the lower bound in **art.** 19.

5 Conclusion

Three Theorems 1, 3 and 2 present different expressions for the square of eigenvector components of the adjacency matrix of a graph. Many other formulae and bounds are deduced from those Theorems. Section 2.3 proposes the fundamental expression (3) as a nodal centrality metric and shows its relation to the notion of graph robustness. Section 4 presents the definition and properties of the fundamental weights and the dual fundamental weights.

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A Eigenvectors and eigenvalues: brief review

A.1 Definition

We denote by x_k the eigenvector of the symmetric matrix A belonging to the eigenvalue λ_k, normalized so that $x_k^T x_k = 1$. The eigenvalues of an $N \times N$ symmetric matrix $A = A^T$ are real and can be ordered as $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_N$. Let X be the orthogonal matrix with eigenvectors of A in the columns,

$$X = \begin{bmatrix} x_1 & x_2 & x_3 & \cdots & x_N \end{bmatrix}$$

or explicitly in terms of the m-th component $(x_j)_m$ of eigenvector x_j,

$$X = \begin{bmatrix} (x_1)_1 & (x_2)_1 & (x_3)_1 & \cdots & (x_N)_1 \\ (x_1)_2 & (x_2)_2 & (x_3)_2 & \cdots & (x_N)_2 \\ (x_1)_3 & (x_2)_3 & (x_3)_3 & \cdots & (x_N)_3 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ (x_1)_N & (x_2)_N & (x_3)_N & \cdots & (x_N)_N \end{bmatrix} \tag{63}$$

where the element $X_{ij} = (x_j)_i$. The eigenvalue equation $Ax_k = \lambda_k x_k$ translates to the matrix equation $A = X\Lambda X^T$, where $\Lambda = \mathrm{diag}(\lambda_k)$.

The relation $X^T X = I = XX^T$ (see e.g. [1, p. 223]) expresses, in fact, *double orthogonality.* The first equality $X^T X = I$ translates to the well-known orthogonality relation

$$x_k^T x_m = \sum_{j=1}^{N} (x_k)_j (x_m)_j = \delta_{km} \tag{64}$$

stating that the eigenvector x_k belonging to eigenvalue λ_k is orthogonal to any other eigenvector belonging to a different eigenvalue. The second equality $XX^T = I$, which arises from the commutativity of the inverse matrix $X^{-1} = X^T$ with the matrix X itself, can be written as $\sum_{j=1}^{N} (x_j)_m (x_j)_k = \delta_{mk}$ and suggests us to define the row vector in X as

$$y_m = ((x_1)_m, (x_2)_m, \ldots, (x_N)_m) \tag{65}$$

Then, the second orthogonality condition $XX^T = I$ implies orthogonality of the vectors

$$y_l^T y_j = \sum_{k=1}^{N} (x_k)_l (x_k)_j = \delta_{lj} \tag{66}$$

Beside the first (64) and second (66) orthogonality relations, the third combination equals

$$y_j^T x_k = \sum_{l=1}^{N} (x_l)_j (x_k)_l = \sum_{l=1}^{N} X_{jl} X_{lk} = \left(X^2\right)_{jk} \tag{67}$$

A.2 Frequency interpretation

The sum over j in (66) can be interpreted as the sum over all eigenvalues. Indeed, the eigenvalue equation is

$$Ax(\lambda) = \lambda\, x(\lambda) \tag{68}$$

where a non-zero vector $x(\lambda)$ only satisfies this linear equation if λ is an eigenvalue of A such that $x_j = x(\lambda_j)$. We have made the dependence on the parameter λ explicit and can interpret λ as a frequency that ranges continuously over all real numbers. Invoking the Dirac delta-function $\delta(t)$, we can write

$$\begin{aligned}\sum_{j=1}^{N}(x_j)_m(x_j)_k &= \sum_{\lambda\in\{\lambda_1,\lambda_2,\ldots,\lambda_N\}}^{N}(x(\lambda))_m(x(\lambda))_k \\ &= \sum_{j=1}^{N}\int_{-\infty}^{\infty}\delta(\lambda-\lambda_j)(x(\lambda))_m(x(\lambda))_k\,d\lambda\end{aligned}$$

Using the non-negative weight function

$$w(\lambda) = \sum_{j=1}^{N}\delta(\lambda-\lambda_j) = \delta(\det(A-\lambda I))\left|\frac{d\det(A-xI)}{dx}\bigg|_{x=\lambda}\right|$$

shows that

$$\sum_{j=1}^{N}(x_j)_m(x_j)_k = \int_{-\infty}^{\infty}w(\lambda)(x(\lambda))_m(x(\lambda))_k\,d\lambda = \delta_{mk} \tag{69}$$

The right-hand side in (69) is the continuous variant of (66) that expresses orthogonality between functions with respect to the weight function w (see e.g. [1, p. 313]). Specifically[19], the orthogonality property (69) shows that the set $\{(x(\lambda))_m\}_{1\leq m\leq N}$ is a set of N orthogonal polynomials in λ.

A.3 Calculus for eigenvectors

Another advantage of the parametrized eigenvalue equation (68) is that calculus can be applied. Invoking Leibniz' rule, the n-th derivative of both sides of $Ax(\lambda) = \lambda\, x(\lambda)$ with respect to λ is

$$A\frac{d^n x(\lambda)}{d\lambda^n} = \sum_{k=0}^{n}\binom{n}{k}\frac{d^k}{d\lambda^k}(\lambda)\frac{d^{n-k}}{d\lambda^{n-k}}x(\lambda) = \lambda\frac{d^n x(\lambda)}{d\lambda^n} + n\frac{d^{n-1}x(\lambda)}{d\lambda^{n-1}}$$

so that, for $n \geq 1$,

$$(A-\lambda I)\frac{d^n x(\lambda)}{d\lambda^n} = n\frac{d^{n-1}x(\lambda)}{d\lambda^{n-1}} \tag{70}$$

Explicitly, denoting $x^{(n)}(\lambda) = \frac{d^n x(\lambda)}{d\lambda^n}$, we obtain the sequence

$$\begin{aligned}(A-\lambda I)\,x(\lambda) &= 0\\ (A-\lambda I)\,x^{(1)}(\lambda) &= x(\lambda)\\ (A-\lambda I)\,x^{(2)}(\lambda) &= 2x^{(1)}(\lambda)\\ &\vdots\\ (A-\lambda I)\,x^{(n)}(\lambda) &= nx^{(n-1)}(\lambda)\end{aligned}$$

from which we deduce that

$$(A-\lambda I)^{n+1}x^{(n)}(\lambda) = 0 \tag{71}$$

[19] The eigendecomposition of a general tri-diagonal stochastic matrix in [35, Appendix] exemplifies how orthogonal polynomials as a function of λ enter.

but

$$(A-\lambda I)^n x^{(n)}(\lambda) = n! x(\lambda) \tag{72}$$

If λ is not an eigenvalue so that $A-\lambda I$ is of rank N and invertible, then the above shows that $x(\lambda)=0$ (as well as all higher order derivatives). If λ is an eigenvalue, the vector $x^{(n)}(\lambda)$ can be different from the zero vector and orthogonal to all the row vectors of $(A-\lambda I)^{n+1}$.

Theorem 8 *The set of vectors* $\left\{x(\lambda), x^{(1)}(\lambda), x^{(2)}(\lambda), \ldots, x^{(n)}(\lambda)\right\}$ *is linearly independent.*

Proof: Assume, on the contrary, that these vectors are dependent, then

$$b_0 x(\lambda) + b_1 x^{(1)}(\lambda) + b_2 x^{(2)}(\lambda) + \ldots + b_n x^{(n)}(\lambda) = \sum_{j=0}^{n} b_j x^{(j)}(\lambda) = 0$$

and not all b_j are zero. Left-multiplying both sides with $(A-\lambda I)^n$ and taking into account that $(A-\lambda I)^{m+j} x^{(m)}(\lambda) = 0$ for any $j \geq 1$ leads to

$$b_n (A-\lambda I)^n x^{(n)}(\lambda) = 0$$

and (72) indicates that b_n must be zero. Next, we repeat the argument and left-multiply both sides with $(A-\lambda I)^{n-1}$, which leads us to conclude that $b_{n-1}=0$. Continuing in this way shows that each coefficient $b_j = 0$ for $0 \leq j \leq n$, which proves the Theorem 8. □

Consider for $1 \leq k \leq n$ the vectors

$$y_k = (A-\lambda I)^k x^{(n)}(\lambda)$$

Relation (72) shows that $y_n = n! x(\lambda)$, while applying (70) iteratively m-times yields

$$y_k = \frac{n!}{(n-m)!} (A-\lambda I)^{k-m} x^{(n-m)}(\lambda)$$

from which we find

$$y_m = \frac{n!}{(n-m)!} x^{(n-m)}(\lambda) = (A-\lambda I)^m x^{(n)}(\lambda)$$

Hence, any vector y_m is generated by the vector $x^{(n)}(\lambda)$ and Theorem 8 states that the set $\{y_1, y_2, \ldots, y_n\}$ is linearly independent and thus spans the n-dimensional space. In the classical eigenvalue theory [36, p. 43], the vector z satisfying $(A-\lambda_k I)^{n+1} z = 0$ is called a *principal vector of grade* $n+1$ corresponding to eigenvalue λ_k. Theorem 8 and (71) show that $z = \beta x^{(n)}(\lambda)$, for any non-zero number β.

Left-multiplying (72) by $x^T(\xi)$ yields

$$n! x^T(\xi) x(\lambda) = x^T(\xi) (A-\lambda I)^n x^{(n)}(\lambda)$$

If A is a symmetric matrix and ξ is an eigenvalue of A, then $x^T(\xi)(A-\lambda I)^n = x^T(\xi)(\xi-\lambda)^n$, so that

$$\delta_{\xi\lambda} = x^T(\xi) x(\lambda) = \frac{(\xi-\lambda)^n}{n!} x^T(\xi) x^{(n)}(\lambda)$$

Hence, if the eigenvalue ξ is different from the eigenvalue λ, we find that $x^T(\xi) x^{(n)}(\lambda) = 0$ for all $n \geq 0$. However, when $\xi = \lambda$, an inconsistency appears when $n > 0$, which implies that a *principal*

vector of grade $n+1$ vector $x^{(n)}(\lambda)$ with $n>0$ does not exist for symmetric matrices. Another argument is that, for symmetric matrices, the set of eigenvectors $\{x_m\}_{1\leq m\leq N}$ spans the entire space so that $x^{(n)}(\lambda)=0$ for $n\geq 1$, because a non-zero vector cannot be orthogonal to all eigenvectors. Hence, a *principal vector* $x^{(n)}(\lambda)$ *of grade* $n+1$ with $n>0$ can only exist for asymmetric matrices and may be helpful to construct an orthogonal set of vectors when degeneracy occurs (as in Jordan forms).

A.4 Function of a symmetric matrix and stochastic matrix Ξ

From the general relation for diagonalizable matrices (see e.g. [20, p. 526]),

$$f(A)=\sum_{k=1}^{N} f(\lambda_k)\, x_k x_k^T \tag{73}$$

valid for a function f defined on the eigenvalues $\{\lambda_k\}_{1\leq k\leq N}$ of the $N\times N$ matrix A, the element for node j equals

$$(f(A))_{jj}=\sum_{k=1}^{N} f(\lambda_k)\,(x_k)_j^2 \tag{74}$$

Written in matrix form for all $1\leq j\leq N$ results in

$$\begin{bmatrix} (f(A))_{11} \\ (f(A))_{22} \\ (f(A))_{33} \\ \vdots \\ (f(A))_{NN} \end{bmatrix} = \begin{bmatrix} (x_1)_1^2 & (x_2)_1^2 & (x_3)_1^2 & \cdots & (x_N)_1^2 \\ (x_1)_2^2 & (x_2)_2^2 & (x_3)_2^2 & \cdots & (x_N)_2^2 \\ (x_1)_3^2 & (x_2)_3^2 & (x_3)_3^2 & \cdots & (x_N)_3^2 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ (x_1)_N^2 & (x_2)_N^2 & (x_3)_N^2 & \cdots & (x_N)_N^2 \end{bmatrix} \begin{bmatrix} f(\lambda_1) \\ f(\lambda_2) \\ f(\lambda_3) \\ \vdots \\ f(\lambda_N) \end{bmatrix} \tag{75}$$

which we write in matrix form as $\psi=\Xi\chi$, with

$$\psi=\begin{bmatrix} (f(A))_{11} \\ (f(A))_{22} \\ (f(A))_{33} \\ \vdots \\ (f(A))_{NN} \end{bmatrix} \text{ and } \chi=\begin{bmatrix} f(\lambda_1) \\ f(\lambda_2) \\ f(\lambda_3) \\ \vdots \\ f(\lambda_N) \end{bmatrix}$$

and the $N\times N$ matrix $\Xi=X\circ X$, where $\circ$ denotes the Hadamard product[20],

$$\Xi=\begin{bmatrix} (x_1)_1^2 & (x_2)_1^2 & (x_3)_1^2 & \cdots & (x_N)_1^2 \\ (x_1)_2^2 & (x_2)_2^2 & (x_3)_2^2 & \cdots & (x_N)_2^2 \\ (x_1)_3^2 & (x_2)_3^2 & (x_3)_3^2 & \cdots & (x_N)_3^2 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ (x_1)_N^2 & (x_2)_N^2 & (x_3)_N^2 & \cdots & (x_N)_N^2 \end{bmatrix} \tag{76}$$

Since $\Xi u=u$ and $\Xi^T u=u$, by "double orthogonality" of (64) and (66), and since each element $0\leq (x_k)_j^2\leq 1$, the matrix Ξ with squared eigenvector components of a diagonalizable matrix A is

[20] The Hadamard product (entrywise product) of two matrix is $(A\circ B)_{ij}=A_{ij}B_{ij}$. If A and B are both diagonal matrices, then $A.B=A\circ B$.

doubly[21] stochastic [1] with largest eigenvalue equal to 1. All eigenvalues of the generally asymmetric matrix Ξ lie within the unit circle. If the inverse Ξ^{-1} of Ξ exists, then the inverse of $\psi = \Xi\chi$ is $\chi = \Xi^{-1}\psi$.

Example Let us denote the vector $\lambda^k = \left(\lambda_1^k, \lambda_2^k, \ldots, \lambda_N^k\right)$ so that, for $f(z) = z^k$ in (75), we have

$$\operatorname{diag}\left(\left(A^k\right)_{jj}\right) u = \Xi\lambda^k \tag{77}$$

From (77) and $u^T\Xi = u^T$, we find the well-known trace relation, namely that $u^T\operatorname{diag}\left(\left(A^k\right)_{jj}\right) u = \operatorname{trace}\left(A^k\right) = u^T\lambda^k = \sum_{j=1}^N \lambda_j^k$. If the inverse Ξ^{-1} of Ξ exists, then it holds, for any integer k, that

$$\lambda^k = \Xi^{-1}\operatorname{diag}\left(\left(A^k\right)_{jj}\right) u \tag{78}$$

or, the eigenvalue λ_m of a symmetric matrix A (to any integer power k) can be written as a linear combination of the diagonal elements of A^k,

$$\lambda_m^k = \sum_{i=1}^N \left(\Xi^{-1}\right)_{mi} \left(A^k\right)_{ii}$$

whereas $\Lambda^k = X^T A^k X$ shows that

$$\lambda_m^k = \sum_{i=1}^N \sum_{j=1}^N \left(A^k\right)_{ij} (x_m)_i (x_m)_j \tag{79}$$

We can proceed one step further by applying the above to a set $f_1, f_2, \ldots, f_N$ of N functions and obtain the matrix equation

$$F = \Xi G$$

where the $N \times N$ matrix F is

$$F = \begin{bmatrix} (f_1(A))_{11} & (f_2(A))_{11} & (f_3(A))_{11} & \cdots & (f_N(A))_{11} \\ (f_1(A))_{22} & (f_2(A))_{22} & (f_3(A))_{22} & \cdots & (f_N(A))_{22} \\ (f_1(A))_{33} & (f_2(A))_{33} & (f_3(A))_{33} & \cdots & (f_N(A))_{33} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ (f_1(A))_{NN} & (f_2(A))_{NN} & (f_3(A))_{NN} & \cdots & (f_N(A))_{NN} \end{bmatrix}$$

and the $N \times N$ matrix G is

$$G = \begin{bmatrix} f_1(\lambda_1) & f_2(\lambda_1) & f_3(\lambda_1) & \cdots & f_N(\lambda_1) \\ f_1(\lambda_2) & f_2(\lambda_2) & f_3(\lambda_2) & \cdots & f_N(\lambda_2) \\ f_1(\lambda_3) & f_2(\lambda_3) & f_3(\lambda_3) & \cdots & f_N(\lambda_3) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ f_1(\lambda_N) & f_2(\lambda_N) & f_3(\lambda_N) & \cdots & f_N(\lambda_N) \end{bmatrix}$$

If G is invertible (i.e. $\det G \neq 0$), which requires that all eigenvalues are distinct, then we can construct $\Xi = FG^{-1}$ from which we deduce that $\det\Xi = \frac{\det F}{\det G}$. A straightforward choice are the functions $f_n(z) = z^{n-1}$, so that G reduces to a Vandermonde matrix, in which case, $\Xi = FG^{-1}$ leads to the results in Theorem 2.

[21] *Sinkhorn's theorem* (1964) states that any matrix with strictly positive entries can be made doubly stochastic by pre- and post-multiplication by diagonal matrices.

A.4.1 A slightly different approach

The (transpose) of the eigenvalue equation for any real, symmetric matrix A, is

$$X^T A = \Lambda X^T$$

We right-multiply both sides with the vector q,

$$X^T A q = \Lambda X^T q$$

Let $X^T q = v$ and $Aq = r$; both are a $N \times 1$ vectors. Since $\Lambda = \mathrm{diag}(\lambda)$, we can write $\Lambda X^T q = \mathrm{diag}(\lambda)\, v = \mathrm{diag}(v)\, \lambda$ and obtain

$$X^T r = \mathrm{diag}\,(v)\, \lambda$$

Finally, assuming that $\mathrm{diag}(v)$ is invertible, we arrive at

$$\mathrm{diag}\left(\frac{1}{v}\right) X^T r = \lambda \tag{80}$$

which is a companion of (78) for $k = 1$.

If the vector $q = x_k$ equals the k-th eigenvector of A, then $X^T q = e_k$ and the above formal manipulations reduce to $Ax_k = \lambda_k x_k$.

A.4.2 Application to the adjacency matrix

When applying the general theory in Section A.4 to the adjacency matrix A, (74) illustrates that the *squares* of the eigenvector component arise as weights for $f(\lambda_k)$ to specify a function of the adjacency matrix A at node j. In particular, the general formula (77) for powers $f(z) = z^n$ leads to nice formulae: for $n = 0$, we find from (73) the *second* [11] orthogonality relation (66); for $n = 1$ (since $A_{jj} = 0$, from which $\mathrm{trace}(A) = \sum_{k=1}^{N} \lambda_k = 0$)

$$0 = \sum_{k=1}^{N} \lambda_k \left(x_k\right)_j^2 \text{ and } 0 = \Xi\lambda \tag{81}$$

while for $n = 2$ (since $\left(A^2\right)_{jj} = d_j$)

$$d_j = \sum_{k=1}^{N} \lambda_k^2 \left(x_k\right)_j^2 \text{ and } d = \Xi\lambda^2 \tag{82}$$

For any adjacency matrix A, (81) shows [1, p. 229] that

$$\Xi\lambda = 0 \tag{83}$$

so that $\det\Xi = 0$ and that the vector $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_N)$ is the eigenvector of Ξ corresponding to eigenvalue zero. Relation (83) implies that the vector $\xi_j = \left((x_1)_j^2, (x_2)_j^2, \ldots, (x_N)_j^2\right)$ is not independent from ξ_l, and, hence $\xi_j^T \xi_l = \sum_{k=1}^{N} (x_k)_j^2 (x_k)_l^2 \neq \delta_{lj}$. In other words, at least one vector ξ_k can be written as a linear combination of all the other nodal centrality vectors $\{\xi_j\}_{1 \leq j \neq k \leq N}$ and the set $\{\xi_j\}_{1 \leq j \leq N}$ is not complete, in the sense that it does not span the entire N-dimensional space.

The fact that $\det \Xi = \det \Xi^T$, implies that the (left)-eigenvector q of Ξ^T belonging to the zero eigenvalue obeys, for each $1 \leq k \leq N$,

$$0 = \sum_{j=1}^{N} q_j \, (x_k)_j^2$$

which is the companion of (81) over the node labels j.

On the other hand, if we choose $q = u$ in (80), then $Aq = Au = d$, the degree vector, while $X^T q = X^T u = w$ by (44) and (80) reduces to

$$\lambda = \mathrm{diag}\left(\frac{1}{w}\right) X^T d$$

which is a generalization of $\lambda_k = \frac{d^T x_k}{u^T x_k} = \sum_{j=1}^{N} d_j \frac{(x_k)_j}{w_k} = \sum_{j=1}^{N} d_j \frac{(x_k)_j}{\sum_{m=1}^{N} (x_k)_m}$, expressing that any eigenvalue of A can be written as a linear combination of the nodal degrees in a graph. Furthermore, using (83) leads to

$$\Xi \mathrm{diag}\left(\frac{1}{w}\right) X^T d = 0$$

which means that the degree vector is an eigenvector of the matrix $\Xi \mathrm{diag}\left(\frac{1}{w}\right) X^T$ belonging to eigenvalue zero.

B Spacings of vector components

We derive bounds for the minimum and maximum spacing in a vector b, whose components are ordered.

Theorem 9 *Let the set of real numbers $\{b_j\}_{1 \leq j \leq n}$ be ordered as $b_1 \geq b_2 \geq \cdots \geq b_n$, then for non-negative real numbers $\{a_j\}_{1 \leq j \leq n}$ with at least one $a_j > 0$, we have that*

$$\min_{1 \leq j \leq n} (b_j - b_{j+1}) \leq \frac{\sum_{k=1}^{n-1} a_k \, (b_k - b_n)}{n \sum_{l=1}^{n} a_l - \sum_{l=1}^{n} l a_l} \leq \max_{1 \leq j \leq n} (b_j - b_{j+1}) \tag{84}$$

with equality only if all spacings are the same.

Proof: We rewrite Abel's summation formula [1, p. 56] as

$$\sum_{k=1}^{n-1} a_k \, (b_k - b_n) = \sum_{k=1}^{n-1} \left(\sum_{l=1}^{k} a_l \right) (b_k - b_{k+1})$$

Since $b_k - b_{k+1} \geq 0$ and $\sum_{l=1}^{k} a_l \geq 0$, we bound the right-hand side as

$$\min_{1 \leq j \leq N} (b_j - b_{j+1}) \sum_{k=1}^{n-1} \left(\sum_{l=1}^{k} a_l \right) \leq \sum_{k=1}^{n-1} \left(\sum_{l=1}^{k} a_l \right) (b_k - b_{k+1}) \leq \max_{1 \leq j \leq N} (b_j - b_{j+1}) \sum_{k=1}^{n-1} \left(\sum_{l=1}^{k} a_l \right)$$

Further,

$$0 \leq \sum_{k=1}^{n-1} \left(\sum_{l=1}^{k} a_l \right) = \sum_{l=1}^{n-1} \sum_{k=l}^{n-1} a_l = \sum_{l=1}^{n-1} (n-l) \, a_l = n \sum_{l=1}^{n-1} a_l - \sum_{l=1}^{n-1} l a_l = n \sum_{l=1}^{n} a_l - \sum_{l=1}^{n} l a_l$$

Combining all leads to (84). □

Theorem 9 illustrates that spacing of the ordered series $\{b_j\}_{1\le j\le n}$ are the same as that of $\{c_j\}_{1\le j\le n}$, where $c_j = b_j - b_n$ and $c_n = 0$. Indeed, $b_k - b_{k+1} = (b_k - b_n) - (b_{k+1} - b_n) = c_k - c_{k+1}$. If we denote the $(n-1)\times 1$ vectors $a = (a_1, a_2, \ldots, a_{n-1})$, $b = (b_1, b_2, \ldots, b_{n-1})$ and $t = (n-1, n-2, n-3, \ldots, 1)$, so that $c = b - (b_n)\, u$, then the fraction in Theorem 9 can be written as

$$f = \frac{\sum_{k=1}^{n-1} a_k\ (b_k - b_n)}{\sum_{l=1}^{n-1} (n-l)\, a_l} = \frac{a^T c}{a^T t} = \frac{\|c\|_2}{\|t\|_2} \frac{\left(\frac{a}{\|a\|_2}\right)^T \frac{c}{\|c\|_2}}{\left(\frac{a}{\|a\|_2}\right)^T \frac{t}{\|t\|_2}} \tag{85}$$

where in the last equality, f is written terms of normalized vectors, where $\|t\|_2^2 = \sum_{l=1}^{n-1} (n-l)^2 = \sum_{k=1}^{n-1} k^2 = \frac{(n-1)n(2n-1)}{6}$. If $a = c$, then

$$f = \frac{\|c\|_2^2}{c^T t} \ge \frac{\|c\|_2}{\|t\|_2}$$

If $a = e_{n-1}$, then

$$f = b_{n-1} - b_n$$

while if $a = e_1$, then $f = \frac{b_1 - b_n}{n-1}$ and (84) reduces to bounds deduced from the telescoping series $\sum_{j=1}^{n-1} (b_j - b_{j+1}) = b_1 - b_n$. If $a = e_1 - e_2$, then $f = b_1 - b_2$. Finally, if $a = u$, then (85) reduces, with $u^T t = \binom{n}{2}$ to

$$f = \frac{u^T c}{\binom{n}{2}} = \frac{2\left(\frac{1}{n}\sum_{k=1}^{n} b_k - b_n\right)}{n-1}$$

Finding the vector a that either maximizes or minimizes f would be useful.

C Eigenvectors of the complementary graph

The adjacency matrix of the complementary graph G^c is $A^c = J - I - A$. In general, A^c does not commute with A, unless the graph is regular [1, p. 44]. The commutator equals $A^c A - A A^c = JA - AJ$. When symmetric matrices commute, the eigenvectors are the same. Let z_k be the eigenvector of A^c belonging to eigenvalue θ_k, so that $A^c z_k = \theta_k z_k$. Since both A and A^c are symmetric, a complete set of eigenvectors exists. We can express the eigenvectors of A in the basis of the eigenvectors of the complement A^c and vice versa,

$$z_k = \sum_{j=1}^{N} \left(z_k^T x_j\right) x_j \text{ and } x_m = \sum_{j=1}^{N} \left(x_m^T z_j\right) z_j \tag{86}$$

Now,

$$\begin{aligned} A^c x_m &= J x_m - (\lambda_m + 1)\, x_m \\ &= w_m u - (\lambda_m + 1)\, x_m \end{aligned}$$

where, $J x_m = u.u^T x_m = w_m u$ and similarly, $J z_k = v_k u$, where $v_k = u^T z_k$ is the fundamental weight of the complementary graph G^c. Left-multiplying $A^c z_k$ by x_m^T and $A^c x_m$ by z_k^T yields

$$x_m^T A^c z_k = \theta_k x_m^T z_k$$

and

$$z_k^T A^c x_m = w_m v_k - (\lambda_m + 1)\, z_k^T x_m$$

Since $z_m^T A^c y_k = z_k^T A^c x_m$ (because it is a scalar), we deduce that

$$x_m^T z_k = \frac{w_m v_k}{\theta_k + \lambda_m + 1} \tag{87}$$

and, introduced into (86),

$$z_k = v_k \sum_{j=1}^{N} \frac{w_j}{\theta_k + \lambda_j + 1} x_j \text{ and } x_m = w_m \sum_{j=1}^{N} \frac{v_j}{\theta_j + \lambda_m + 1} z_j$$

The last, when left-multiplied with u^T yields, for any k,

$$\sum_{j=1}^{N} \frac{w_j^2}{\theta_k + \lambda_j + 1} = 1$$

and similarly[22], for any m,

$$\sum_{j=1}^{N} \frac{v_j^2}{\theta_j + \lambda_m + 1} = 1$$

while, in general, $\sum_{j=1}^{N} w_j^2 = N$. In conclusion, the key relation (87) expresses the sum of eigenvalues, for each $1 \leq k \leq N$ and each $1 \leq m \leq N$, as

$$\lambda_k (A^c) + \lambda_m (A) = \frac{\left(u^T z_k\right)\left(u^T x_m\right)}{z_k^T x_m} - 1$$

and underlines the importance of the fundamental weights $v_k = u^T z_k$, $w_m = u^T x_m$ and the scalar product $z_k^T x_m$ between eigenvectors of A and A^c.

Invoking (60) yields, for any k,

$$\min_{1 \leq j \leq N} (\theta_k + \lambda_j + 1) \leq N \leq \max_{1 \leq j \leq N} (\theta_k + \lambda_j + 1)$$

Thus, any eigenvalue θ_k of the complementary adjacency matrix A^c can be bounded in terms of eigenvalues λ_j of A. For example, for $\theta_1 > 0$,

$$0 \leq N - 1 - \lambda_1 \leq \theta_1 \leq N - 1 - \lambda_N$$

where the upper bound is useless. We cannot use $2L = \sum_{j=1}^{N} \lambda_j w_j^2$ to derive sharper bounds, because all terms must be positive for the denominator of (60), but we can use $N_2 = d^T d = \sum_{j=1}^{N} \lambda_j^2 w_j^2$.

[22] Using the orthogonality relations $z_k^T z_m = \delta_{km}$, these equations are complemented by

$$\sum_{j=1}^{N} \frac{w_j^2}{(\theta_k + \lambda_j + 1)(\theta_m + \lambda_j + 1)} = \frac{\delta_{km}}{v_k v_m}$$

and, similarly,

$$\sum_{j=1}^{N} \frac{v_j^2}{(\theta_k + \lambda_j + 1)(\theta_m + \lambda_j + 1)} = \frac{\delta_{km}}{w_k w_m}$$

However, we rather prefer to follow another track by computing $x_m^T (A^c)^n z_k = \theta_k^n x_m^T z_k$ for any integer $n \geq 1$ as $z_k^T (A^c)^n x_m$ using

$$(A^c)^n x_m = (J - I - A)^n x_m$$

After some tedious computations, we find

$$(J - I - A)^n x_m = x_m (-1)^n (\lambda_m + 1)^n + \frac{w_m u}{N} \{(N - 1 - \lambda_m)^n - (-\lambda_m - 1)^n\}$$

For example, for $n = 1$, we find again the above. Equating $z_k^T (A^c)^n x_m = x_m^T (A^c)^n z_k$ yields, for any integer $n \geq 1$,

$$x_m^T z_k = \frac{w_m v_k}{N} \frac{(N - 1 - \lambda_m)^n - (-1)^n (\lambda_m + 1)^n}{\theta_k^n - (-1)^n (\lambda_m + 1)^n}$$

Finally, we find the generalized expression for the eigenvector z_k of G^c in terms of those of G,

$$z_k = \frac{v_k}{N} \sum_{j=1}^{N} \frac{(N - 1 - \lambda_j)^n - (-1)^n (\lambda_j + 1)^n}{\theta_k^n - (-1)^n (\lambda_j + 1)^n} w_j x_j$$

and, vice versa,

$$x_m = \frac{w_m}{N} \sum_{j=1}^{N} \frac{(N - 1 - \lambda_m)^n - (-1)^n (\lambda_m + 1)^n}{\theta_j^n - (-1)^n (\lambda_m + 1)^n} v_j z_j$$

After multiplying both sides with u^T, it follows that

$$N = \sum_{j=1}^{N} \frac{(N - 1 - \lambda_j)^n - (-1)^n (\lambda_j + 1)^n}{\theta_k^n - (-1)^n (\lambda_j + 1)^n} w_j^2$$

Similarly as above, invoking (60) yields, for any $1 \leq k \leq N$ and $n \geq 1$,

$$\min_{1 \leq j \leq N} \frac{1 - \left(1 - \frac{N}{1+\lambda_j}\right)^n}{1 - \left(-\frac{\theta_k}{1+\lambda_j}\right)^n} \leq 1 \leq \max_{1 \leq j \leq N} \frac{1 - \left(1 - \frac{N}{1+\lambda_j}\right)^n}{1 - \left(-\frac{\theta_k}{1+\lambda_j}\right)^n}$$

This inequality can be used to derive bounds for any eigenvalue θ_k of A^c in terms of eigenvalues λ_j of A by optimizing n. The presented approach complements the determinant theory of $\det(A^c - \lambda I)$ in [1, p. 42-43].

D Additions to Theorem 1

D.1 Introducing the resolvent

Another way to rewrite the determinant in (5) is

$$\det (A - \lambda_k I)_{\text{row } N=b} = \det \begin{bmatrix} \left(A_{G \setminus \{N\}} - \lambda_k I\right) & (a_N)_{\setminus N} \\ b_{\setminus N}^T & b_N \end{bmatrix}$$

where the $(N-1)\times 1$ vector $w_{\backslash m} = (w_1, \ldots, w_{m-1}, w_{m+1}, \ldots, w_N)$ is obtained from the $N \times 1$ vector w after removing the m-th component. Invoking Schur's block determinant relation [1, p. 255] yields[23]

$$\det \begin{bmatrix} \left(A_{G\backslash\{N\}} - \lambda_k I\right) & (a_N)_{\backslash N} \\ b_{\backslash N}^T & b_N \end{bmatrix} = \det\left(A_{G\backslash\{N\}} - \lambda_k I\right)\left(b_N - b_{\backslash N}^T \left(A_{G\backslash\{N\}} - \lambda_k I\right)^{-1} (a_N)_{\backslash N}\right)$$

Instead of row N, we can delete row m so that

$$\det\left(A - \lambda_k I\right)_{\text{row } m=b} = \det\left(A_{G\backslash\{m\}} - \lambda_k I\right)\left(b_m - b_{\backslash m}^T \left(A_{G\backslash\{m\}} - \lambda_k I\right)^{-1} (a_m)_{\backslash m}\right) \tag{88}$$

where $(a_m)_{\backslash m} = (a_{1m}, \ldots, a_{m-1;m}, a_{m+1,m}, \ldots, a_{Nm})$. Using (88) in (5) transforms (4) to

$$(x_k)_j = \frac{\beta_k}{b_j - b_{\backslash j}^T \left(A_{G\backslash\{j\}} - \lambda_k I\right)^{-1} (a_j)_{\backslash j}} \tag{89}$$

which illustrates the seemingly dependence of $(x_k)_j$ on the arbitrary vector b.

If $b = e_m$, the basic vector with all zero components, except that the m-th component is 1, then (89) reduces, for $m \neq j$, to

$$(x_k)_j = -\frac{(x_k)_m}{\left(\left(A_{G\backslash\{j\}} - \lambda_k I\right)^{-1} (a_j)_{\backslash j}\right)_m}$$

else, for $m = j$, we find an identity. Interchanging m and j, the ratio $\frac{(x_k)_j}{(x_k)_m}$, expressed in two ways, leads to

$$\left(\left(A_{G\backslash\{m\}} - \lambda_k I\right)^{-1} (a_j)_{\backslash m}\right)_j = \frac{1}{\left(\left(A_{G\backslash\{j\}} - \lambda_k I\right)^{-1} (a_j)_{\backslash j}\right)_m}$$

When the vector b equals a row vector in A, it can be shown (see e.g. [37]) that

$$(x_k)_j^2 = \frac{1}{1 + (a_j)_{\backslash j}^T \left(A_{G\backslash\{j\}} - \lambda_k I\right)^{-2} (a_j)_{\backslash j}}$$

[23] We remark that, in case $b = u$, then

$$\det\left(A_{G_{\text{cone}(N)}} - \lambda I\right) = \det \begin{bmatrix} \left(A_{G\backslash\{N\}} - \lambda I\right) & u \\ u^T & -\lambda \end{bmatrix}$$

where $G_{\text{cone}(j)}$ is the "cone at node j" of the original graph G, which is the graph where only node j has now links to all other nodes in G. In other words, the node j is the cone of the graph $G\backslash\{j\}$. Thus, even if $a_N = u$, $\det\left(A - \lambda I\right)_{\text{row } N=u}$ is not equal to $\det\left(A_{G_{\text{cone}(N)}} - \lambda I\right)$, unless $\lambda = -1$.

D.2 Expressions for β_k

After multiplying (1) by b_j and summing over all j and using $\beta_k = b^T x_k = \sum_{j=1}^N b_j (x_k)_j$, we obtain a normalization formula for all λ_k,

$$\sum_{j=1}^N \frac{b_j \det\left(A_{G\setminus\{j\}} - \lambda_k I\right)}{\det\left(A - \lambda_k I\right)_{\text{row } j=b}} = 1 \tag{90}$$

Similarly from (89), we obtain

$$\sum_{j=1}^N \frac{b_j}{b_j - b_{\setminus j}^T \left(A_{G\setminus\{j\}} - \lambda_k I\right)^{-1} (a_j)_{\setminus j}} = 1 \tag{91}$$

and[24] from (2),

$$\beta_k^2 = -\frac{1}{c_A'(\lambda_k)} \sum_{j=1}^N b_j \det\left(A - \lambda_k I\right)_{\text{row } j=b} \tag{92}$$

After combining (8) and (10) with the definition (5) of $\alpha_m(k)$, we obtain[25], for any node m,

$$\beta_k^2 = -\frac{\det\left(A - \lambda_k I\right)^2_{\text{row } m=b}}{c_A'(\lambda_k) \det\left(A_{G\setminus\{m\}} - \lambda_k I\right)} \tag{93}$$

Summing (93) over all m, or similarly introducing (2) in the first orthogonality relation $x_k^T x_k = 1$, yields, with (10),

$$\beta_k^2 = \frac{1}{\left(c_A'(\lambda_k)\right)^2} \sum_{j=1}^N \det\left(A - \lambda_k I\right)^2_{\text{row } j=b} \tag{94}$$

Using $\sum_{j=1}^N (x_k)_j^2 = 1$ in combination with (1) yields

$$\frac{1}{\beta_k^2} = \sum_{j=1}^N \frac{\det^2\left(A_{G\setminus\{j\}} - \lambda_k I\right)}{\det^2\left(A - \lambda_k I\right)_{\text{row } j=b}} \tag{95}$$

Finally, it follows from the Cauchy-Schwarz inequality applied to (92) (or to (90)) and with (94) (or with (95)) that $\beta_k^2 \leq \|b\|_2^2$, which leads to the same bound as the 2-norm of a vector $\|y\|_2^2 = y^T y$, namely $\beta_k^2 = \left(b^T x_k\right)^2 \leq \|b\|_2^2 \|x_k\|_2^2 = \|b\|_2^2$.

[24] Substituting (2) into the eigenvalue equation $\sum_{j=1}^N a_{ij} (x_k)_j = \lambda_k (x_k)_i$ gives

$$\det\left(A - \lambda_k I\right)_{\text{row } i=b} = \frac{1}{\lambda_k} \sum_{j=1}^N a_{ij} \det\left(A - \lambda_k I\right)_{\text{row } j=b}$$

[25] If we choose $b = e_m$, then $\beta_k = (x_k)_m$ and $\det\left(A - \lambda_k I\right)_{\text{row } j=e_m} = (-1)^{j+m} \det\left(A_{G\setminus \text{row } j \setminus \text{col } m} - \lambda I\right)$. Invoking Jacobi's formula (6) in (93) leads to (3).

E Determinantal expressions for w_k and φ_j

We present other expressions for w_k and φ_j by applying Theorem 1.

First, summing (1) over all j leads to

$$w_k = \beta_k \sum_{j=1}^{N} \frac{\det\left(A_{G\setminus\{j\}} - \lambda_k I\right)}{\det\left(A - \lambda_k I\right)_{\text{row } j=b}}$$

while summing (4) over all j yields, after invoking the cofactor expansion of $\det\left(A - \lambda_k I\right)_{\text{row } m=u}$ with respect to row m,

$$w_k = \beta_k \frac{\det\left(A - \lambda_k I\right)_{\text{row } m=u}}{\det\left(A - \lambda_k I\right)_{\text{row } m=b}}$$

so that, for any m,

$$\frac{\det\left(A - \lambda_k I\right)_{\text{row } m=u}}{\det\left(A - \lambda_k I\right)_{\text{row } m=b}} = \sum_{j=1}^{N} \frac{\det\left(A_{G\setminus\{j\}} - \lambda_k I\right)}{\det\left(A - \lambda_k I\right)_{\text{row } j=b}}$$

which complements (90). Similarly, summing (2) over all j yields

$$w_k \beta_k = -\frac{1}{c'_A\left(\lambda_k\right)} \sum_{j=1}^{N} \det\left(A - \lambda_k I\right)_{\text{row } j=b}$$

which is slightly more general than (98) below.

It is immediate from (93) and (94) that, for any node m,

$$w_k^2 = -\frac{\det^2\left(A - \lambda_k I\right)_{\text{row } m=u}}{\det\left(A_{G\setminus\{m\}} - \lambda_k I\right) c'_A\left(\lambda_k\right)} \tag{96}$$

and

$$w_k^2 = \frac{1}{\left(c'_A\left(\lambda_k\right)\right)^2} \sum_{m=1}^{N} \left(\det\left(A - \lambda_k I\right)_{\text{row } m=u}\right)^2 \tag{97}$$

while (92) yields

$$w_k^2 = -\frac{1}{c'_A\left(\lambda_k\right)} \sum_{m=1}^{N} \det\left(A - \lambda_k I\right)_{\text{row } m=u} \tag{98}$$

Application of (95) to $b = u$, yields

$$\frac{1}{w_k^2} = \sum_{j=1}^{N} \frac{\det^2\left(A_{G\setminus\{j\}} - \lambda_k I\right)}{\det^2\left(A - \lambda_k I\right)_{\text{row } j=u}} \tag{99}$$

Less transparent connections between components of w and φ arise after summing (1) or (2),

$$\varphi_j = \sum_{k=1}^{N} \frac{w_k \det\left(A_{G\setminus\{j\}} - \lambda_k I\right)}{\det\left(A - \lambda_k I\right)_{\text{row } j=u}} = -\sum_{k=1}^{N} \frac{\det\left(A - \lambda_k I\right)_{\text{row } j=u}}{w_k c'_A\left(\lambda_k\right)}$$

The potential of these formulas needs further exploration.