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

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Abstract

Double orthogonality in the set of eigenvectors of any symmetric graph matrix is exploited to propose a set of nodal centrality metrics, that is “ideal” in the sense of being complete, uncorrelated and mathematically precisely defined and computable. Moreover, we show that, for each node \( m \), such a nodal eigenvector centrality metric reflects the impact of the removal of node \( m \) from the graph at a different eigenfrequency of that graph matrix. Fundamental weights, related to graph angles, are argued to be as important as the eigenvalues of the graph matrix.

While the mathematical foundations of eigenvectors are crystal clear emphasizing its potential as an ideal set of nodal centrality metrics, the “physical” meaning of its application to graphs, the topological structure of a network, seems surprisingly opaque and, hence, constitutes a challenging question with fundamental significance for network science.

1 Introduction

This article focuses on a rare case where mathematics is further developed than physics, in the sense that complete mathematical truth exists, while we fail to grasp its physical meaning. In particular, we discuss the relation between the eigenstructure of graph matrices and their meaning for complex networks.

Apart from the goal of advancing science by increasing our understanding of the eigenstructure, a more practical motivation concerns centrality metrics in complex networks. Generally, nodal centrality metrics quantify the “importance” of a node in a network or how “central” a node is in the graph. Many quantifiers of nodal “importance” have been proposed. 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?” 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, of the graph is needed. Nodal “importance” often depends on the

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1The 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].
process on the network, which then further specifies the precise meaning of importance with respect to that process. For example, in epidemics on networks, nodal importance (here vulnerability) can be defined as the long-run probability that a node is infected.

While obviously the most important property of a metric is its precise definition and meaning, a number of other issues appear as elaborated in [6]: How many metrics are needed? 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 but one neighbor have degree 1, is vulnerable to be disconnected and also may be relatively unimportant with respect to betweenness, 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 removed since they all reflect the same type of “importance” as illustrated in [7].

Here, we take a different view. We present a set of centrality metrics with intriguing mathematical properties and ask what type of properties in the network they may characterize or quantify. In Section 2 we review the mathematical background on the eigenstructure of a symmetric matrix and present a set of nodal centrality metrics, derived from orthogonality properties of the eigenvector matrix. Section 2 determines the $m$-th component of the $k$-th eigenvector $(x_k)_m$ in terms of determinants, culminating in the nice expression (16), that suggests us to propose a complete set of eigenvector centrality metrics for each node. Moreover, (16) expresses $(x_k)_m^2$ as the impact of the removal of node $m$ from $G$ at eigenfrequency $\lambda_k$ of a symmetric graph matrix (such as the adjacency matrix). The appendix A presents other representations and approximations for $(x_k)_m^2$. As a by product of the analysis in Section 3, we present fundamental weights of a graph in Section 4 which are shown to be of a same importance as eigenvalues. Finally, Section 5 concludes, but poses again the question about the meaning of the set of all eigenvector components of a graph related matrix of the graph $G$.

2 A complete set of centrality metrics

2.1 Linear Algebra

Following the notation of [1], we denote by $x_k$ the eigenvector of the symmetric matrix $A$ belonging to the eigenvalue $\lambda_k$. 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 $x_j$,

$$X = \begin{bmatrix} (x_1)_1 & (x_2)_1 & (x_3)_1 & \cdots & (x_N)_1 \\ (x_1)_2 & (x_2)_2 & (x_3)_2 & \cdots & (x_N)_2 \\ (x_1)_3 & (x_2)_3 & (x_3)_3 & \cdots & (x_N)_3 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ (x_1)_N & (x_2)_N & (x_3)_N & \cdots & (x_N)_N \end{bmatrix}$$
The eigenvalue equation $A x_k = \lambda_k x_k$ translates to the matrix equation $A = X \Lambda X^T$, where $\Lambda = \text{diag}(\lambda_k)$.

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

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

stating that the eigenvector $x_k$ belonging to eigenvalue $\lambda_k$ 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

$$y_m = ((x_1)_m, (x_2)_m, \ldots, (x_N)_m)$$

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

$$y_k^T y_m = \sum_{j=1}^{N} (x_j)_k (x_j)_m = \delta_{km}$$

The sum over $j$ in (3) can be interpreted as the sum over all eigenvalues. Indeed, the eigenvalue equation is

$$A x(\lambda) = \lambda x(\lambda)$$

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

$$\sum_{j=1}^{N} (x_j)_m (x_j)_k = \sum_{\lambda \in \{\lambda_1, \lambda_2, \ldots, \lambda_N\}} (x(\lambda))_m (x(\lambda))_k$$

$$= \sum_{j=1}^{N} \int_{-\infty}^{\infty} \delta(\lambda - \lambda_j) (x(\lambda))_m (x(\lambda))_k d\lambda$$

Using the non-negative weight function

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

shows that

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

The right-hand side in (4) is the continuous variant of (3) that expresses orthogonality between functions with respect to the weight function $w$ (see e.g. [1] p. 313). Specifically, the orthogonality property (3) shows that the set \{$(x(\lambda))_m$\}$_{1 \leq m \leq N}$ is a set of $N$ orthogonal polynomials in $\lambda$.

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2The eigendecomposition of a general tri-diagonal stochastic matrix in [8, Appendix] exemplifies how orthogonal polynomials as a function of $\lambda$ enter.
2.2 Graph theory

The topology of a network can be represented by a graph $G$, consisting of a set of nodes connected by a set of links. Many matrices can be associated to a graph, such as the adjacency, Laplacian, signless and normalized Laplacian, modularity, incidence and distance matrix, etc.. We confine ourselves here to a simple, undirected graph $G$ and to its corresponding symmetric adjacency matrix $A$.

Surprisingly little is known \[1\] Chapter 1 about the “physical” meaning of the eigenvalue $\lambda_k$ and its corresponding eigenvector $x_k$ (for each $1 \leq k \leq N$) of the adjacency matrix $A$. One of the best interpretations follows from the probabilistic matrix, $P = \Delta^{-1}A$, where $\Delta = \text{diag}(d_j)$ and the degree of node $j$ is $d_j = \sum_{k=1}^{N} a_{kj}$. The largest eigenvector component $(x_1(P))_j$ of $P$, normalized as $u^T x_1 (P) = 1$, where $u$ is the all one vector, reflects the probability that a random walk on the graph $G$ visits node $j$ in the long run. Theorem 2.2.4 in the book by Cvetković et al. \[9\] provides the explicit relation between the number $N_k(j)$ of walks of length $k$ starting at node $j$ and the corresponding eigenvector component $(x_1)_j$ as

$$\lim_{k\to\infty} \frac{N_k(j)}{\sum_{j=1}^{N} N_k(j)} = (x_1)_j$$

The case of $k = 1$ is studied most and the principal eigenvector $x_1$ corresponding to the spectral radius $\lambda_1$ can be regarded as a “dynamic” degree vector (see Appendix \[13\]), where each component $(x_1)_j$ reflects all possible walks passing through node $j$. Most insight and most relations in graph theory (see e.g. \[1\]) are based on the set $\{x_k\}_{1 \leq k \leq N}$ of eigenvectors. When studying spectral clustering, Von Luxburg et al. \[10\] show figures of several eigenvectors of the Laplacian as a function of the nodal components.

The vector $y_m$, defined in \[2\], reflects the role of the node $m$ over all eigenfrequencies or eigenvalues of $A$. From a graph metrics point of view, we may argue that $y_m$ specifies how important or “central” node $m$ is with respect to the important or characteristic frequencies (i.e. the eigenfrequencies) of the graph matrix $A$, that specifies links in $G$. Perhaps, the following geometric interpretation is daring. Imagine that the graph $G$ is embedded in some geometric structure with negligible mass compared to those of the nodes and links. For example, a planar graph on a large flexible sheet that can be brought into vibration by an external force. Thus, the force bends the sheet up and down so that waves travel over the sheet at certain frequency. The vector $y_m$ may be interpreted as the displacements of node $m$ on the sheet at the eigenfrequencies of the adjacency matrix of the graph $G$. Another view on the vector $y_m = (x(\lambda_1)_m, x(\lambda_2)_m, \ldots, x(\lambda_N)_m)$ or, more generally, on the set $\{(x(\lambda))_m\}_{1 \leq m \leq N}$ versus frequency $\lambda$, is inspired by our human vision: we perceive the real-world only via the frequency range of visible light, while we know (for example from Röntgen photographs) that additional information is revealed in other frequency bands of the spectrum.

Another thought is that, if the frequency interpretation of $\lambda$ is correct, then we may use Fourier analysis to rigorously define localization in space or in frequency. For example, if all components of $y_m$ are constant (or more or less of the same magnitude), then the Fourier (or Laplace) transform indicates that node $m$ is very localized in space\[3\]. The opposite is also true, if only a few components of $y_m$ in successive order are significant, hence localized in the frequency domain, then node $m$ is

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\[3\] Recall that $\sin(x) = \frac{e^{ix} - e^{-ix}}{2i}$ (broad in space) has a Fourier transform proportional to $\delta(f - a) - \delta(f + a)$ (peaked in frequency domain).
globally connected in the spacial domain. Again, a precise physical meaning is difficult to offer.

The case \( y_m^T y_m = \sum_{j=1}^{N} (x_j)_m^2 = 1 \) in second orthogonality relation (3) means that, considered over all eigenvalues (eigenfrequencies or eigenmodes) of a graph, each node in \( G \) is equally important. In other words, the often associated importance to high-degree nodes seems only partially true, i.e. only for certain eigenfrequencies and certain types of graphs (the largest eigenvalues graphs with large spectral gap; see Section 3 below).

In summary, these contemplations question the physical meaning of the vector \( y_m \) that characterizes each node \( m \) in the graph \( G \), with respect to the eigenvalues or eigenmodes of \( A \). The analysis in the next Section 3 will show that \( y_m \) reflects the “importance” of node \( m \) over the eigenfrequencies of \( A \), when node \( m \) is removed from the graph.

3 Eigenvector components of the adjacency matrix \( A \)

The eigenvector \( x_k \) belonging to eigenvalue \( \lambda_k \) constitutes the non-zero vector solution of the linear set of \( N \) equations

\[
(A - \lambda_k I) x_k = 0
\]

where the matrix \( A - \lambda_k I \) is singular, i.e. its rank is smaller than \( N \). The eigenvector \( x_k \) is thus orthogonal to any row vector of \( A - \lambda_k I \). For the adjacency matrix \( A \) of undirected graph \( G \), where \( a_{jj} = 0 \) (meaning that there are no self-loops), the \( m \)-th component of the \( r \)-th row vector \( (A - \lambda_k I)_{\text{row } r} \) is \( a_{rm} = a_{mr} \) and only if \( m = r \), then \( (A - \lambda_k I)_{rr} = -\lambda_k \), so that an eigenvalue \( \lambda_k \) can be interpreted as a special node weight equal for each node such that there exists a vector \( x_k \) that is orthogonal to each link connection vector \( A_{\text{row } r} = (a_{r1}, a_{r2}, \ldots, a_{rN}) \) with a self-weight \(-\lambda_k\) at component \( r \). Since \( A^n x_k = \lambda_k^n x_k \) for any integer \( n \geq 1 \), that same eigenvector \( x_k \) is also orthogonal to any row vector of \( A^n - \lambda_k^n I \). We can thus equally well replace \( A \to A^n \) and \( \lambda_k \to \lambda_k^n \) in the determinant expressions below and to compute tighter bounds on the coupling of eigenvalues of a graph \( G \) and its complement \( G^c \) in Appendix C. What does the independence of an eigenvector \( x_k \) on the integer \( n \) mean topologically?

Let us assume that the eigenvalue \( \lambda_k \) is single with multiplicity one, then \( \text{rank}(A - \lambda_k I) = N - 1 \). This means that the set 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: (i) one of the \( N \) equations/rows in \( A - \lambda_k I \) can be replaced by an additional equation as explored in Section 3.1 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). These approaches are similar to, perhaps less elegant and more basic than computing the adjoint matrix \( Q(\lambda) = c_A(\lambda)(\lambda I - A)^{-1} \), whose columns are eigenvectors (see [1] art. 148 on p. 220).

3.1 Adding a new linear equation

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 the real number \( \beta_k = b^T x_k \) is non-zero. In most cases (except for regular graphs where \( u \) is an eigenvector), that additional 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 of \( x_k \), further discussed in Section 4. Another example is the degree vector, \( b = d \), where
$d^T x_k = \lambda_k w_k$ as shown in [29]. 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!

Without loss of generality, we first replace the $N$-th equation and the resulting set of linear equations becomes

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

Cramer’s solution [11, p. 256] yields

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

The determinant in the denominator can be expanded in cofactors of the row $N$,

$$
\det (A - \lambda_k I)_{\text{row } N=b} = \sum_{i=1}^N (-1)^{N+i} b_i \det (A - \lambda_k I)_{\text{row } N \setminus \text{col } i}
$$

Another way is to rewrite that determinant as

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

where $a_N = (a_{1N}, a_{2N}, \ldots, a_{N-1;N})$ is the $(N-1) \times 1$ vector expressing the existence of links from each node $j \neq N$ to node $N$ and $\tilde{b}_m$ equals the $b$-vector without $m$-th component. Invoking Schur’s block determinant relation [11, p. 255] yields

$$
\det \begin{bmatrix}
(A_{G\setminus \{N\}} - \lambda_k I) & a_N
\end{bmatrix}
$$

and we may proceed by evaluating the real number $\tilde{b}_{N} - \overline{b}_{N}^T (A_{G\setminus \{N\}} - \lambda_k I)^{-1} a_N$ using expressions of the resolvent $(A_{G\setminus \{N\}} - \lambda I)^{-1}$ of $A_{G\setminus \{N\}}$. We remark that, in case $b = u$, then

$$
\det (A_{G_{\text{cone}(N)}} - \lambda I) = \det \begin{bmatrix}
(A_{G\setminus \{N\}} - \lambda I) & u
\end{bmatrix}
$$

\footnote{Using [11, p. 244]}

$$
(yI - A)^{-1} = \sum_{j=1}^N \frac{x_jx_j^T}{y - \lambda_j}
$$

yields, with the eigenvector $z_j$ of $A_{G\setminus \{N\}}$ belonging to $\lambda_j (A_{G\setminus \{N\}})$,

$$
b_N - \overline{b}_N^T (A_{G\setminus \{N\}} - \lambda_k I)^{-1} a_N = b_N + \sum_{j=1}^{N-1} \frac{\overline{b}_N^T z_j}{\lambda_k - \lambda_j (A_{G\setminus \{N\}})} z_j^T a_N
$$

(5)
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 no links to all other nodes in $G$. In other words, the node $j$ is the cone of the graph $G \setminus \{j\}$. Thus, even if $a_N = u$, $\det (A - \lambda I)_{row\ N\ =\ u}$ is not equal to $\det \left( A_{G_{\text{cone}(N)}} - \lambda I \right)$, unless $\lambda = -1$.

The $j$-th component of the $k$-th eigenvector $x_k$ can be written as

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

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

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

with

$$ \det (A - \lambda_k I)_{row\ m\ =\ b} = \sum_{i=1}^{N} (-1)^{i+m} b_i \det (A - \lambda_k I)_{row\ m\ \setminus\ col\ i} $$

$$ \quad = \det (A_{G\setminus\{m\}} - \lambda_k I) \left( b_m - \begin{pmatrix} a_m \end{pmatrix} (A_{G\setminus\{m\}} - \lambda_k I)^{-1} a_m \right) $$

where $a_m = (a_{1m}, \ldots, a_{m-1m}, a_{m+1m}, \ldots, a_{Nm})$. Remark that $A_{G\setminus\{row\ m\ \setminus\ col\ i\}}$ 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, $A_{G\setminus\{row\ m\ \setminus\ col\ i\}}$ is not necessarily symmetric and it has two non-zero diagonal elements $a_{i,i+1}$ and $a_{m,m+1}$. We observe that there is a degree of freedom via the choice of $m$. Thus, for $m = j$, we obtain with (7)

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

or, with (9),

$$ (x_k)_j = \frac{\beta_k}{b_j - \begin{pmatrix} a_j \end{pmatrix} (A_{G\setminus\{j\}} - \lambda_k I)^{-1} a_j} $$

which illustrates the dependence of $(x_k)_j$ on the arbitrary vector $b$. After multiplying (10) 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 $\lambda_k$,

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

We now impose the first orthogonality equation (11), $x_k^T x_k = 1$. It follows from (6) that

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

Invoking the identity

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

\footnote{Similarly from (11), we obtain

$$ \sum_{j=1}^{N} \frac{b_j}{b_j - \begin{pmatrix} a_j \end{pmatrix} (A_{G\setminus\{j\}} - \lambda_k I)^{-1} a_j} = 1 $$}
which can be deduced from Jacobi’s famous theorem of 1833 (see e.g. [11, p. 25]), yields
\[
\alpha_m^2 (k) (x_k)^2_j = \lim_{\lambda \to \lambda_k} \det (A_{G\setminus\{m\}} - \lambda I) \det (A_{G\setminus\{j\}} - \lambda I) - \det (A_{G\setminus\{m,j\}} - \lambda I) \det (A_{G} - \lambda I)
\]
\[
= \det (A_{G\setminus\{m\}} - \lambda_k I) \det (A_{G\setminus\{j\}} - \lambda_k I)
\]
(14)
The condition \(x_k^T x_k = \sum_{j=1}^{N} (x_k)^2_j = 1\) specifies \(\alpha_m (k)\) as
\[
\alpha_m^2 (k) = \det (A_{G\setminus\{m\}} - \lambda_k I) \sum_{j=1}^{N} \det (A_{G\setminus\{j\}} - \lambda_k I)
\]
(15)
We observe that the second orthogonality condition \(\sum_{k=1}^{N} (x_k)^2_j = 1\) (due to double orthogonality [3]) does not seem to possess the potential to generate an elegant alternative. The eigenvector component \((x_k)^2_j\) follows from (14) and (15) as
\[
(x_k)^2_j = \frac{\det (A_{G\setminus\{j\}} - \lambda_k I)}{\sum_{n=1}^{N} \det (A_{G\setminus\{n\}} - \lambda_k I)}
\]
(16)
that is independent of the choice of the vector \(b\).

3.2 Deductions

Interpretation. Relation (16) indicates that the sign in numerator and denominator is always the same (unless \((x_k)^2_j = 0\), which is a consequence of the interlacing [11, p. 246] property of the adjacency matrix \(A = A_G\):
\[
\lambda_{k+1} (A_G) \leq \lambda_k (A_{G\setminus\{j\}}) \leq \lambda_k (A_G)
\]
that holds for any node \(j\) in \(G\) and any \(1 \leq k \leq N - 1\). We deduce from (16) that
\[
\frac{(x_k)^2_j}{(x_k)^2_m} = \frac{\det (A_{G\setminus\{j\}} - \lambda_k I)}{\det (A_{G\setminus\{m\}} - \lambda_k I)} = \frac{c_{A_{G\setminus\{j\}}} (\lambda_k)}{c_{A_{G\setminus\{m\}}} (\lambda_k)}
\]
(17)
illustrating that \(\det (A_{G\setminus\{j\}} - \lambda_k I)\) and \(\det (A_{G\setminus\{m\}} - \lambda_k I)\) have the same sign for any pair of nodes \((j,m)\) for a given frequency \(\lambda_k\). Combining (10) and (16) yields
\[
(x_k)_j = \frac{\det (A - \lambda_k I)_{row\ j=b}}{\beta_k c_k}
\]
where \(c_k = \sum_{n=1}^{N} \det (A_{G\setminus\{n\}} - \lambda_k I)\), from which
\[
\frac{(x_k)_j}{(x_k)_m} = \frac{\det (A - \lambda_k I)_{row\ j=b}}{\det (A - \lambda_k I)_{row\ m=b}}
\]
(18)
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 \(\beta_k\), whose general graph interpretation is clearly less transparent than nodal removal as in \(\det (A_{G\setminus\{j\}} - \lambda_k I)\), even if \(b = u\). We remark that the ratios (17) and (18) only hold at eigenfrequencies of \(A\), thus
\[
\frac{\det (A_{G\setminus\{j\}} - \lambda I)}{\det (A_{G\setminus\{m\}} - \lambda I)} = \left(\frac{\det (A - \lambda I)_{row\ j=b}}{\det (A - \lambda I)_{row\ m=b}}\right)^2
\]
is correct only if $\lambda = \lambda_k$ for $1 \leq k \leq N$.

The magnitude of $(x_k)_j^2$ for node $j$ depends on the characteristic polynomial $c_{A_{G\setminus\{j\}}}(\lambda)$ of $G\setminus\{j\}$ at the frequency $\lambda = \lambda_k(A_G)$. Hence, the importance or centrality of node $j$ for property $k$ at eigenfrequency $\lambda_k$ is proportional to the amplitude of the characteristic polynomial at $\lambda_k$ 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 the removal of node $j$ from the graph $G$, determined by the amplitude at frequency $\lambda_k$, is. In network robustness analyses, the removal of links or nodes challenges the functioning of the network, measured via certain network metrics. The relative impact or effect of the removal of a high degree node at the largest eigenfrequency $\lambda_1$ is larger than the removal of a low degree node. However, at other eigenfrequencies, the reverse must hold due to double orthogonality: combining $\sum_{k=1}^N (x_k)_j^2 = 1$ and yields

$$\sum_{k=1}^N \frac{\det (A_{G\setminus\{j\}} - \lambda_k I)}{\sum_{n=1}^N \det (A_{G\setminus\{n\}} - \lambda_k I)} = 1$$

illustrating that the normalized amplitude of node $j$ over all eigenfrequencies sums to unity for each node $j$ in $G$, complementing the unity sum 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 (16), to interpret $(x_k)_j^2$ as centrality metrics. The eigenvector centrality metrics $(x_k)_j^2$ in (16) quantifies the impact of the removal of node $j$ in the graph $G$ at the characteristic frequency $\lambda_k$ corresponding to eigenvector $x_k$. The impact is, of course, associated to the type of graph matrix!

**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 $c_{A_{G\setminus\{j\}}}(\lambda)$ and $c_{A_G}(\lambda)$, as well as its adjacency matrix $A$. At the vertical lines, that reflect the positions of the eigenvalues of $A$, all values $c_{A_{G\setminus\{j\}}}(\lambda_k)$ for $1 \leq j \leq 10$ have a same sign, in agreement with (17). 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

---

6As illustrated in Fig. 1, the characteristic polynomials $c_{A_G}(x)$ 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. Hence, we coin the deviations in $c_{A_{G\setminus\{j\}}}(x)$ from zero at $\lambda_k(G)$ the amplitude.

7The explicit expressions are

$c_{A_G}(x) = -4 + 4x + 27x^2 - 10x^3 - 52x^4 + 8x^5 + 38x^6 - 2x^7 - 11x^8 + x^{10}$
$c_{A_{G\setminus\{1\}}}(x) = -2 - 5x + 6x^2 + 17x^3 - 6x^4 - 19x^5 + 2x^6 + 8x^7 - x^9$
$c_{A_{G\setminus\{2\}}}(x) = -4x + 16x^3 - 19x^5 + 8x^7 - x^9$
$c_{A_{G\setminus\{3\}}}(x) = -8x + 4x^2 + 29x^3 - 6x^4 - 29x^5 + 2x^6 + 10x^7 - x^9$
$c_{A_{G\setminus\{4\}}}(x) = -4x + 14x^3 - 16x^5 + 7x^7 - x^9$
$c_{A_{G\setminus\{5\}}}(x) = -2 - 5x + 8x^2 + 20x^3 - 8x^4 - 23x^5 + 2x^6 + 9x^7 - x^9$
$c_{A_{G\setminus\{6\}}}(x) = 2 - 7x - 4x^2 + 25x^3 + 2x^4 - 25x^5 + 9x^7 - x^9$
$c_{A_{G\setminus\{7\}}}(x) = -2 - 9x + 6x^2 + 30x^3 - 6x^4 - 29x^5 + 2x^6 + 10x^7 - x^9$
$c_{A_{G\setminus\{8\}}}(x) = -4x + 2x^2 + 18x^3 - 4x^4 - 22x^5 + 2x^6 + 9x^7 - x^9$
$c_{A_{G\setminus\{9\}}}(x) = -4x + 4x^2 + 20x^3 - 6x^4 - 23x^5 + 2x^6 + 9x^7 - x^9$
$c_{A_{G\setminus\{10\}}}(x) = -4x + 4x^2 + 19x^3 - 6x^4 - 23x^5 + 2x^6 + 9x^7 - x^9$
frequency \( \lambda_k \). Fig. 2 illustrates that the topological degree vector \( d \) correlates best with the vector \( y_1 \), defined in (2) and with square components of the principal eigenvector \( x_1 \). At other eigenfrequencies, other nodes are “important”.

Figure 1: The characteristic polynomials \( c_{A\{v\}_j} (\lambda) \) for \( 1 \leq i \leq N \) in red and \( c_{AG} (\lambda) \) in black for an Erdős-Rényi graph \( G_{0.2} \). The blue vertical lines denote the eigenvalues of \( AG \) (zeros of \( c_{AG} (\lambda) \)).

**Absence.** The expression (10) for \( (x_k)^2 \) demonstrates that \( (x_k)_j = 0 \) only if \( \lambda_k \) is an eigenvalue of the adjacency matrix of the graph \( G \) and the graph \( G \{ j \} \). The same conclusion also follows from (11). Interlacing shows that \( (x_k)_j = 0 \) when \( \lambda_k = \lambda_{k+1} \), i.e., when \( \lambda_k \) is an eigenvalue of \( G \) with at least multiplicity equal to 2. A zero \( (x_k)_j = 0 \) implies that

\[
(Ax_k)_j = \sum_{q=1}^{N} a_{jq} (x_k)_q = \sum_{q \in \text{neighbors}(j)} (x_k)_q = 0
\]

meaning that the sum of eigenvector components of all direct neighbors of node \( j \) is zero and that the node \( j \) does not influence the eigenvector component of any of its neighbors. With respect to the frequency \( \lambda_k \) (or property \( k \) of the adjacency matrix of \( G \)), the node \( j \) does not play a role and can thus be thought as being removed from the graph. Similarly, we may conclude that \( (x_k)^2_j \to 0 \) when \( \lambda_k (AG) \to \lambda_k (A_{G \{ j \}}) \), i.e., both \( AG \) and \( A_{G \{ j \}} \) contain almost the same eigenfrequency \( \lambda_k \) (or property \( k \)).
Figure 2: The square of the eigenvector components per node $j$ over all eigenvalues $\lambda_k$. The filled back squares represents the normalized degree $d_j^2/d^T d$.

**Perturbation theory.** Any change in a finite graph $G$ has a non-infinitesimal change on the eigenvalues (via interlacing and trace equations). Indeed, $A_G$ is a zero-one matrix and $A_G' - A_G = \pm e_i e_k^T$, equal to the zero matrix except for a one in row $i$ and column $k$, is the smallest possible change in the class of adjacency matrices. All this would imply that eigenvectors of graphs also change discontinuously (just as the eigenvalues due to (16)) when the graph $G$ is modified. Hence, the orthogonal matrix $X$, containing the eigenvectors of $A$ in the columns, will change in a discrete or discontinuous way when the graph $G$ is minimally changed, for instance, by removing, adding or rewiring a link. Hence, matrix perturbation theory is not simply applicable, because it assumes that the transition of a general matrix $B$ to $B + \varepsilon C$ can be made continuously in $\varepsilon$, thus, that $\varepsilon$ can be made arbitrarily small.

4 The fundamental weight $w_k = u^T x_k$

The equations (11) and (13) constitute in total $N^2$ orthogonality conditions associated to the matrix $X$, whose rank is $N$ (since $|\text{det } X| = 1$). Although the $N^2$ elements of $X$ represent a set of independent row and/or column vectors, curiously, an equal number of additional conditions is embedded in them. The latter seems to indicate that considerable information condensation can be attained, raising the question how many bits are minimally needed to reconstruct $X$ exactly. Any orthogonal matrix
describes a rotation of an orthogonal set of basis vectors in the $N$-dimensional space, which suggests that, beside $N$ bits (corresponding to the basis vectors $e_j$), $N$ rotation angles ($N$ real numbers) are needed. Similar considerations have likely led Cvetković et al. to define graph angles. In Section 3.1, when choosing $b = u$, the fundamental weight $w_k = u^T x_k = \sum_{j=1}^{N} (x_k)_j$ was introduced as additional information to determine the eigenvector components, illustrating its important role. The graph angle $\gamma_k$ is related to fundamental weight by $\cos \gamma_k = \frac{w_k}{\sqrt{N}}$. These considerations may hint that only $2N$ real numbers (eigenvectors and fundamental weights or graph angles) are needed to construct the graph $G$ exactly. A rigorous proof of the minimum number of bits needed to construct a graph is currently an open problem.

Observe from the definition $w_k = u^T x_k = \sum_{j=1}^{N} (x_k)_j$ and the first orthogonality conditions, $\sum_{j=1}^{N} (x_k)_j^2 = 1$, that

$$w_k = \frac{\sum_{j=1}^{N} (x_k)_j}{\sqrt{\sum_{j=1}^{N} (x_k)_j^2}}$$

where $j'$ reflects that $(x_k)_j, \neq 0$, because a zero term does not contribute to the sum. The inequality

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

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

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

Since all components of $x_1$ as non-negative on the Perron-Frobenius theorem, the fundamental weight inequality illustrates that $w_1 \geq 1$, a result earlier found in p. 40} with a different method. Any other eigenvector $x_k$ must have at least one negative component to satisfy the orthogonality condition $x_k^T x_1 = 0$. Hence, for $k > 1$, the lower bound in is negative (and smaller than $-1$), while the upper bound is larger than 1, so that nothing can be concluded about the sign of $w_k$.

Further (see e.g. p. 33), we have that

$$N = \sum_{j=1}^{N} (u^T x_j)^2$$

and, in general, the total number of walks with $k$ hops in the graph $G$ equals

$$N_k = \sum_{j=1}^{N} \lambda_j^k (u^T x_j)^2$$

We mention p. 41] that the vector $w = (w_1^2, w_2^2, \ldots, w_N^2)$ satisfies $V_N(\lambda) w = N w$, where $V_N(\lambda)$ is the Vandermonde matrix of the vector with eigenvalues $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_N)$ and where the vector $N = (N_1, N_2, \ldots, N_N)$ has as components the total number of walks with $k$ hops, $N_k = u^T A^k u$. Since $V_N(\lambda)$ can be inverted when all eigenvalues are different, the fundamental weights $w$ can be expressed in terms of the eigenvalues and the number of walks in the graph $G$.

These bounds can also be deduced from,

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

obtained after Abel partial summation and where $(x_k)_{(1)} \geq (x_k)_{(2)} \geq \cdots \geq (x_k)_{(m)} \geq 0 \geq (x_k)_{(m+1)} \geq \cdots \geq (x_k)_{(N)}$ are the ordered components of the eigenvector $x_k$. 


In the remainder, we present other expressions and bounds for \( w_k \). Using \( \sum_{j=1}^N (x_k)_j^2 = 1 \) in combination with (10) yields

\[
\frac{1}{w_k^2} = \sum_{j=1}^N \frac{\det^2 (A_{G \setminus \{j\}} - \lambda_k I)}{\det^2 (A - \lambda_k I)_{\text{row } j=u}}
\]  

(21)

Further, combining (21) with (12) as

\[
w_k^2 = \frac{\sum_{j=1}^N \det (A_{G \setminus \{j\}} - \lambda_k I)}{\sum_{j=1}^N \det^2 (A - \lambda_k I)_{\text{row } j=u}}
\]

and invoking the inequality (19) leads to

\[
\min_{1 \leq j \leq N} \frac{\det (A_{G \setminus \{j\}} - \lambda_k I)}{\det (A - \lambda_k I)_{\text{row } j=u}} \leq w_k^2 \leq \max_{1 \leq j \leq N} \frac{\det (A_{G \setminus \{j\}} - \lambda_k I)}{\det (A - \lambda_k I)_{\text{row } j=u}}
\]

We can further use the different expressions (8) and (10) for \( \det (A - \lambda_k I)_{\text{row } j=u} \). On the other hand, after combining (15) with the definition (7) of \( \alpha_m (k) \), we obtain

\[
w_k^2 = \frac{\det^2 (A - \lambda_k I)_{\text{row } m=u}}{\det (A_{G \setminus \{m\}} - \lambda_k I) \sum_{j=1}^N \det (A_{G \setminus \{j\}} - \lambda_k I)}
\]

(22)

Hence, comparing (21) and (22) yields

\[
\sum_{j=1}^N \frac{\det^2 (A_{G \setminus \{j\}} - \lambda_k I)}{\det^2 (A - \lambda_k I)_{\text{row } j=u}} \leq \frac{\det (A_{G \setminus \{m\}} - \lambda_k I) \sum_{j=1}^N \det (A_{G \setminus \{j\}} - \lambda_k I)}{\det^2 (A - \lambda_k I)_{\text{row } m=u}}
\]

These expressions are awaiting an interpretation!

5 Summary

The key relation \( A = \Lambda \Lambda^T \) shows that all “topological” information about the graph (left-hand side) is contained in the “spectral space” (right-hand side). While linear algebra, in particular eigenvalue decomposition, is a mature branch of mathematics, the physical meaning of its application to networks and graphs remains puzzling. Many articles have been written on graph metrics and many will still appear. Nearly all metrics are correlated and so far there is no generally accepted set that characterizes a graph without losing too much information. The set of orthogonal – thus uncorrelated – vectors \( y_1, y_2, \ldots, y_N \) mathematically reflects the complete information about the importance of each node in \( G \) over all eigenfrequencies \( \lambda_1, \lambda_2, \ldots, \lambda_N \) and can thus be considered as an “ideal” nodal centrality set of metrics. Akin to sensitivity or robustness analyses on graphs, the elegant expression (16) associates \( (x_k)_j^2 \) to the impact of the removal of node \( j \) in the graph \( G \) at the characteristic frequency \( \lambda_k \) corresponding to eigenvector \( x_k \) of a graph matrix.

Unfortunately, this positive view also has darker sides. First, each graph matrix (such as e.g. the Laplacian, adjacency and modularity matrix) possesses such doubly orthogonal eigenvectors so that the \( N \) nodal eigenfrequency centrality metrics for a certain node \( m \), i.e. the components or squared components of \( y_m \), are also dependent on the specific graph matrix. Hence, there does not seem be a
single ideal set of centrality metrics per graph. Still, we are confronted with the choice of the “ideal” centrality metrics over the space of all possible (symmetric) graph matrices. Second and as mentioned several times, the meaning of both the impact (or amplitude) and characteristic frequency are waiting for an explanation useful to networks. Third, from a practical point of view, the vectors $y_1, y_2, \ldots, y_N$, though complete and uncorrelated, require global information, i.e. the full knowledge of the adjacency matrix of $G$. Even if we would understand the meaning of each vector $y_m$ or of its square components $(x_k)^2$, their complete use (i.e. all components over all frequencies $\lambda_k$) as a centrality metrics set is hardly feasible for large networks. Fourth, besides this computationally infeasibility objection, we can equally well question the normalizations $x_k^T x_k = 1$ for each $1 \leq k \leq N$ that consider each eigenvalue as equally important. Indeed, for a positive semi-definite symmetric matrix $A$ (whose eigenvalues are non-negative), we can write the spectral decomposition

$$A = \sum_{k=1}^{N} \lambda_k x_k x_k^T = \sum_{k=1}^{N} \left( \sqrt{\lambda_k} x_k \right) \left( \sqrt{\lambda_k} x_k \right)^T$$

which suggests to scale the importance of an eigenvector as $v_k = \sqrt{|\lambda_k|} x_k$. Clearly, the eigenvectors corresponding to the larger (in absolute value) eigenvalues deserve more weight, as earlier was exploited in graph reconstructability [16] and only a few of the larger ones may be sufficient as centrality metrics. While their physical meaning is unknown, the set of orthogonal vectors $y_1, y_2, \ldots, y_N$ mathematically reflects the complete information about the importance of each node in $G$ over all eigenfrequencies $\lambda_1, \lambda_2, \ldots, \lambda_N$ and, for that reason alone, we believe that it deserves deeper study to unravel its true significance for networks. In the spirit of the great Hilbert: “Wir müssen wissen”.

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A Other expressions for eigenvector components

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

Theorem 1 If all eigenvalues of $A$ are different, then

$$
(x_m)_i (x_m)_j = \frac{1}{\prod_{k=1; k \neq m}^N (\lambda_m - \lambda_k)} \sum_{r=H_{ij}}^{N-1} b_r (m) (A^r)_{ij}
$$

(23)

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

$$
\prod_{j=1; j \neq m}^n (x - x_j) = \sum_{k=0}^{n-1} b_k (m) x^k
$$

Writing (23) in matrix form yields

$$
E_m = x_m x_m^T = \frac{1}{\prod_{k=1; k \neq m}^N (\lambda_m - \lambda_k)} \sum_{r=0}^{N-1} b_r (m) A^r = \frac{\prod_{j=1; j \neq m}^N (A - \lambda_j I)}{\prod_{k=1; k \neq m}^N (\lambda_m - \lambda_k)}
$$

(24)

Clearly, if $i = j$, then $H_{jj} = 0$ and (23) reduces to

$$
(x_m)_j^2 = \frac{1}{\prod_{k=1; k \neq m}^N (\lambda_m - \lambda_k)} \sum_{r=0}^{N-1} (A^r)_{jj} b_r (m)
$$

(25)

It remains to show how (24) is related to (16).

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 \((x_k)^2_i\). Invoking the Cauchy identity [II p. 257] and \(a_{ij} = a_{ij}^2\) yields

\[
\left( \sum_{j=1}^{N} a_{ij}a_{ij}(x_k)_j \right)^2 = \sum_{j=1}^{N} a_{ij}^2 \sum_{j=1}^{N} (a_{ij}(x_k)_j)^2 - \frac{1}{2} \sum_{j=1}^{N} \sum_{l=1}^{N} (a_{ij}a_{il}(x_k)_l - a_{il}a_{ij}(x_k)_j)^2
\]

\[= d_i \sum_{j=1}^{N} a_{ij}(x_k)_j^2 - \frac{1}{2} \sum_{j=1}^{N} a_{ij} \sum_{l=1}^{N} a_{il} ((x_k)_l - (x_k)_j)^2\]

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

\[
\frac{\lambda_i^2(A)}{d_i}(x_k)_i^2 = 1 - (x_k)_i^2 - \sum_{j=1; j \neq i}^{N} (1 - a_{ij})(x_k)_j^2 - \frac{1}{2d_i} \sum_{j=1}^{N} a_{ij} \sum_{l=1}^{N} a_{il} ((x_k)_l - (x_k)_j)^2
\]

which we rewrite as

\[
(x_k)_i^2 = \frac{1 - r_i(k)}{\frac{\lambda_i^2(A)}{d_i}} + 1 \quad (26)
\]

with

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

Since \(1 \geq r_i(k) \geq 0\), we find the upper bound

\[
(x_k)_i^2 \leq \frac{1}{1 + \frac{\lambda_i^2(A)}{d_i}} \quad (27)
\]

We proceed by approximating \(r_i(k)\). We use the second orthogonality expression [3] for the eigenvector components and ignore the dependence of \(r_i(k)\) on \(k\) so that

\[
1 \simeq (1 - r_i(k)) \sum_{k=1}^{N} \frac{1}{\frac{\lambda_k^2(A)}{d_i}} + 1
\]

Solving for \(r_i(k)\) and substituting the result into (26) leads to the approximation\[11\]

\[
(x_k)_i^2 \simeq \frac{1}{1 + \sum_{l=1; l \neq k}^{N} \frac{\lambda_l^2(A)+d_i}{\lambda_l^2(A)+d_i}} \quad (28)
\]

If \(d_i > 0\), we observe that \(\sum_{l=1; l \neq k}^{N} \frac{\lambda_l^2(A)+d_i}{\lambda_l^2(A)+d_i} \) is finite, so that the approximation (28) never returns a zero eigenvector component.

\[11\]The overall quality of the approximation (28) can be assessed, for example, by the error \(\varepsilon\), determined from the first orthogonality condition \(x_k^T x_k = 1\),

\[
\varepsilon = \sum_{i=1}^{N} \frac{1}{1 + \sum_{l=1; l \neq k}^{N} \frac{\lambda_l^2(A)+d_i}{\lambda_l^2(A)+d_i}} - 1
\]
The degree vector $d$

Any vector in the $N$-dimensional space can be written as a linear combination of orthogonal vectors $x_1, x_2, \ldots, x_N$ that span that space. Hence, the degree vector $d = (d_1, d_2, \ldots, d_N)$ of a graph $G$, where $d_j$ denotes the degree of node $j$, can be written as

$$d = \sum_{j=1}^{N} r_j x_j$$

where the scalars $b_j$ are computed using orthogonality of the vectors $x_1, x_2, \ldots, x_N$. Multiplying both sides by $x_m^T$ and using the orthogonality $x_m^T x_j = \delta_{mj}$ yields

$$x_m^T d = r_m$$

Further, $d = Au$ (see e.g. [1, p. 15]), where the vector $u = (1, 1, \ldots, 1)$ is the all-one vector so that

$$x_m^T d = x_m^T Au = (Ax_m)^T u = \lambda_m x_m^T u = \lambda_m w_m$$

(29)

Hence, we find that the spectral decomposition of the degree vector,

$$d = \sum_{j=1}^{N} \lambda_j (u^T x_j) x_j = \sum_{j=1}^{N} \lambda_j w_j x_j$$

(30)

Now, we rewrite (30) as

$$d = \lambda_1 w_1 x_1 + c$$

where the correction vector $c$ equals

$$c = \sum_{j=2}^{N} \lambda_j w_j x_j$$

The correction vector $c = 0$ only for regular graphs, where the principal eigenvalue is $x_1 = \frac{1}{\sqrt{N}} u$ and $u^T x_k = 0$ for each $2 \leq k \leq N$ because eigenvectors are orthogonal. If the correction vector $c$ is negligibly small (e.g. when the spectral gap is large ($\lambda_1 >> \lambda_2$) or for almost regular graphs or in other cases that we still need to investigate), then

$$d \approx \lambda_1 w_1 x_1$$

(31)

In simple dynamic processes on a network, such as SIS epidemics\[13\], the vector $v$ with the nodal infection probabilities is proportional to $x_1$ close to the epidemic phase transition. Only in those graphs obeying (31) where the degree vector $d$ is (approximately) proportional to the principal eigenvector $x_1$, the dynamics (e.g. $v$) is directly proportional to the graph’s topological structure.

---

\[12\] When we write the spectral decomposition (30) of the $k$-th component of the degree vector as

$$d_k = \sum_{j=1}^{N} (d^T x_j) (x_j)_k = \sum_{j=1}^{N} \sum_{m=1}^{N} d_m (x_j)_m (x_j)_k = \sum_{m=1}^{N} d_m \left\{ \sum_{j=1}^{N} (x_j)_m (x_j)_k \right\}$$

Since such a spectral decomposition holds for any $N$-dimensional vector, we naturally find the second type \[13\] of orthogonality.

\[13\] Also Kuramoto synchronization, see e.g. [17].
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]. When symmetric matrices commute, the eigenvectors are the same. Let $y_k$ be the eigenvector of $A^c$ belonging to eigenvalue $\theta_k$, so that $A^c y_k = \theta_k y_k$. Since both $A$ and $A^c$ are symmetric, a complete set of eigenvectors exists, so that

$$ y_k = \sum_{j=1}^{N} (y_k^T x_j) x_j $$

and

$$ x_m = \sum_{j=1}^{N} (x_m^T y_j) y_j $$

Now,

$$ A^c x_m = J x_m - (\lambda_m + 1) x_m $$

$$ = w_m u - (\lambda_m + 1) x_m $$

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

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

and

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

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

$$ x_m^T y_k = \frac{w_m v_k}{\theta_k + \lambda_m + 1} $$

and

$$ y_k = v_k \sum_{j=1}^{N} \frac{w_j}{\theta_k + \lambda_j + 1} x_j $$

and

$$ x_m = w_m \sum_{j=1}^{N} \frac{v_j}{\theta_j + \lambda_m + 1} y_j $$

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, for any $m$,

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

while, in general, $\sum_{j=1}^{N} w_j^2 = N$. Invoking (19) 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 $\theta_k$ of the complementary adjacency matrix $A^c$ can be bounded in terms of eigenvalues $\lambda_j$ 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 (19), but we can use $N_2 = d^T d = \sum_{j=1}^{N} \lambda_j^2 w_j^2$. However, we rather prefer to follow another track by computing $x_m^T (A^c)^n y_k = \theta_k^n x_m y_k$ for any integer $n \geq 1$ as $y_k^T (A^c)^n x_m$ 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 $y_k^T (A^c)^n x_m = x_m^T (A^c)^n y_k$ yields, for any integer $n \geq 1$,

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

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

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

and, vice versa,

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

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

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

Similarly as above, invoking (19) yields, for any $1 \leq k \leq N$ and $n \geq 1$,

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

This inequality can be used to derive bounds for any eigenvalue $\theta_k$ of $A^c$ in terms of eigenvalues $\lambda_j$ of $A$ by optimizing $n$. The presented approach complements the determinant theory of $\det (A^c - \lambda I)$ in [11] p. 42-43].