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Eigenvector components of symmetric, graph-related matrices

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ABSTRACT

Although eigenvectors belong to the core of linear algebra, relatively few closed-form expressions exist, which we bundle and discuss here. A particular goal is their interpretation for graph-related matrices, such as the adjacency matrix of an undirected, possibly weighted graph.

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1. Introduction

The eigenvectors $x_1, x_2, \ldots, x_N$ of an $N \times N$ symmetric matrix A, belonging to the *real* eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_N$ respectively, are orthogonal. The classical proof (see e.g. [1], [2, p. 88-90], [3, art. 237, 247]) is elegant and a pearl in linear algebra. The

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proof relies on the eigenvalue equation $Ax_k = \lambda_k x_k$ and on geometry, in particular, on the notion of independent vectors that span an N-dimensional space. One of the most powerful properties of the set $\{x_k\}_{1\leq k\leq N}$ of eigenvectors is that they form an orthogonal coordinate frame [3, Sec. 1.3, art. 191] that represents any vector into the eigenbasis of the symmetric matrix (operator) A. Orthogonality is a powerful property, that also appears in the theory of functions (e.g. Fourier series and orthogonal polynomials), as overwhelmingly shown in Lanczos's beautiful book [2]. Here in Section 3, we give another demonstration of the orthogonality of eigenvectors, that does not rely on "geometry nor spaces", but only on the Caley-Hamilton theorem, Cramer's method and Taylor's theorem.

A main motivation, that started with [4] almost a decade ago, is to understand what eigenvector components of graph-related matrices, such as the adjacency matrix, mean. The manuscript starts in Section 2 with a couple of representations of the j-th component $(x_k)_j$ of the eigenvector x_k of a symmetric matrix A belonging to eigenvalue λ_k with multiplicity 1. The elegant formula $(x_k)_j^2 = -\frac{\det(A_{\backslash\{j\}}-\lambda_k I)}{c'_A(\lambda_k)}$ for $1 \leq j,k \leq N$ in (6), which was reviewed in [5], is extended in Section 4 to an eigenvalue λ_k with multiplicity $m_k > 1$. The closed-form formulae in Theorem 3 in Section 4 improve Hagos's result [6] and are applied to strongly regular graphs [7]. We proceed in Section 5 with the interpretation of $(x_k)_j^2$ in terms of walks in graphs and concentrate in Section 6 on the stochastic, asymmetric matrix $\Xi = X \circ X$ with elements $(x_k)_j^2$, because Ξ allows us to construct co-eigenvector graphs, as demonstrated in [8], provided rank(Ξ) $< N - 1$. An open question remains the determination of the rank(Ξ) or, equivalently, the multiplicity of the zero eigenvalue of the stochastic matrix Ξ of an adjacency matrix. Alternatively, what are the conditions imposed on the matrix X or Ξ in order to construct from them co-eigenvector graphs? The final Section 7 proposes to consider the squared eigenvector component $(x_k)_j^2$ as a graph metric, but also points to the weakness of the dependence among those graph metrics $(x_k)_j^2$. Section 8 summarizes and poses open questions. Most proofs are deferred to the Appendices.

2. Eigenvector components as determinants

The characteristic polynomial $c_A(\lambda) = \det(A - \lambda I)$ of an $N \times N$ matrix A has, like any polynomial, a product and a series representation [3, art. 235]

$$c_A(\lambda) = \det(A - \lambda I) = \prod_{j=1}^{N} (\lambda_j - \lambda) = \sum_{k=0}^{N} c_k \lambda^k \tag{1}$$

Differentiation of $\log c_A(\lambda) = \sum_{j=1}^{N} \log(\lambda_j - \lambda)$ with respect to λ yields

$$c'_A(\lambda) = -c_A(\lambda) \sum_{j=1}^{N} \frac{1}{\lambda_j - \lambda} = -\sum_{j=1}^{N} \frac{\prod_{k=1}^{N}(\lambda_k - \lambda)}{\lambda_j - \lambda} = -\sum_{j=1}^{N} \prod_{k=1;k\neq j}^{N} (\lambda_k - \lambda) \tag{2}$$

from which

$$c'_A(\lambda_m) = -\prod_{k=1;k\neq m}^{N} (\lambda_k - \lambda_m) = (-1)^N \prod_{k=1;k\neq m}^{N} (\lambda_m - \lambda_k) \tag{3}$$

The derivative $c'_A(\lambda_m)$ will play an important role in our story on eigenvector components, which is a development of [4].

For simplicity and computational elegance, we limit the computation of eigenvector x_k here in Section 2 by assuming that the eigenvalue λ_k of the symmetric matrix A is single, thus with multiplicity one, $m_k = 1$. A multiplicity $m_k > 1$ is considered in Section 4. If the multiplicity m_k of eigenvalue λ_k equals one, then $\text{rank}(A - \lambda_k I) = N - 1$. This means that the eigenvalue equation $(A - \lambda_k I)\, x_k = 0$ 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 to determine the N unknowns: (i) one of the N equations/rows in $A - \lambda_k I$ can be replaced by an additional linear equation as explored in Section 2.1 and (ii) the set is rewritten in $N-1$ unknowns in terms of one of them, whose derivations are in Section 2.2. These two approaches are complemented in Section 2.3 by a third method, based on the adjoint matrix $\text{adj}(A - \lambda I) = c_A(\lambda)(\lambda I - A)^{-1}$, whose columns are eigenvectors.

2.1. Replacement of an arbitrary row in $A - \lambda_k I$ by a new linear equation $b^T x_k$

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. Let $A_{\setminus\{j\}}$ denote the $(N-1) \times (N-1)$ symmetric matrix, deduced from the $N \times N$ symmetric matrix A after removal of row j and column j.

Theorem 1. *Let the eigenvalue λ_k of the $N \times N$ real, symmetric matrix A possess multiplicity 1. 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*

$$(x_k)_j = \frac{\beta_k \det\left(A_{\setminus\{j\}} - \lambda_k I\right)}{\det(A - \lambda_k I)_{\text{row}\, j=b}} \tag{4}$$

or

$$(x_k)_j = -\frac{\det(A - \lambda_k I)_{\text{row}\, j=b}}{\beta_k c'_A(\lambda_k)} \tag{5}$$

where $\det(A - \lambda_k I)_{\text{row}\, j=b}$ 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

$$(x_k)_j^2 = -\frac{1}{c'_A(\lambda_k)} \det\left(A_{\setminus\{j\}} - \lambda_k I\right) = -\frac{c_{A_{\setminus\{j\}}}(\lambda_k)}{c'_A(\lambda_k)} \tag{6}$$

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

The proof of Theorem 1 is presented in Appendix A.1. In particular in graph theory, the symmetric matrix A and $A_{\backslash\{j\}}$ denote the adjacency matrix of undirected graph G and of the graph $G_{\backslash\{j\}}$ in which node j and all its incident links are removed from G, respectively. Theorem 1 also holds for any Hermitian matrix. Recently, a survey of formula (6), written for a Hermitian matrix A as

$$|x_k|_j^2 \prod_{i=1;i\neq k}^{N} (\lambda_k(A) - \lambda_i(A)) = \prod_{i=1}^{N-1} \left(\lambda_k(A) - \lambda_i\left(A_{\backslash\{j\}}\right)\right)$$

has appeared in [5], after a sequence of versions on arXiv:1908.03795, in which "our" formula (6) also plays a role in its history.[1]

The second proof of (6) in Appendix A.2 has appeared earlier in Cvetkovic et al. [9, Theorem 3.1], who referred to Hagos [6], who in turn mentioned that Mukherjee and Datta [10] (using a perturbation technique) and Li and Feng (only for the largest eigenvalue) have preceded him. Hagos [6] mentioned rightly that "Eq. (6) is probably not as well known as it should be", as witnessed by the appearance of the survey [5].

2.2. The set is rewritten in $N-1$ unknowns in terms of one of them

The second approach avoids the addition of a supplementary linear equation $b^T x_k = \sum_{j=1}^N b_j (x_k)_j = \beta_k$.

Theorem 2. *Let the eigenvalue* λ_k *of the* $N \times N$ *real, symmetric matrix* A *possess multiplicity 1. The eigenvector* x_k*, belonging to the eigenvalue* λ_k *and normalized as* $x_k^T x_k = 1$*, contains, for any integer* $1 \leq m \leq N$*, as* j*-th component*

$$(x_k)_j = (-1)^{j-m} \frac{\det\left((A - \lambda_k I)_{\backslash \operatorname{row} m \backslash \operatorname{col} j}\right)}{\sqrt{\sum_{l=1}^N \det^2\left((A - \lambda_k I)_{\backslash \operatorname{row} m \backslash \operatorname{col} l}\right)}} \qquad \text{for } 1 \leq j \leq N \tag{7}$$

which can also be written as

$$(x_k)_j = (-1)^{j-m} \frac{\det\left((A - \lambda_k I)_{\backslash \operatorname{row} m \backslash \operatorname{col} j}\right)}{\sqrt{-c'_A(\lambda_k) \det\left(A_{\backslash\{m\}} - \lambda_k I\right)}} \tag{8}$$

Two proofs of Theorem 2 are given in Appendix A.3. The second proof in Appendix A.3 illustrates that Theorem 1 is more general than Theorem 2. On the other hand, when

[1] The story on 14 November 2019 in https://www.quantamagazine.org/neutrinos-lead-to-unexpected-discovery-in-basic-math-20191113 contained a pointer to (6) in [4] which is now omitted.

the multiplicity $m_k > 1$, then the approach of reducing the number of equations is more straightforward and followed in Appendix C. A slight variation on the second proof in Appendix A.3 leads to[2]

Corollary 1. *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*

$$(x_k)_j (x_k)_m = \frac{(-1)^{j+m+1}}{c'_A(\lambda_k)} \det\left(A_{\backslash \text{row } j \backslash \text{col } m} - \lambda_k I\right) \tag{9}$$

Proof. We expand the determinant in (5) in the cofactors of row j and obtain, with $\beta_k = \sum_{m=1}^{N} b_m (x_k)_m$,

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

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 (9). □

When $m = j$ in (9), we arrive again at (6). Hence, (9) generalizes (6).

In a similar vein, choosing $m = j$ in (8) reduces to

$$(x_k)_j = \frac{\det\left(A_{\backslash\{j\}} - \lambda_k I\right)}{\sqrt{-c'_A(\lambda_k) \det\left(A_{\backslash\{j\}} - \lambda_k I\right)}}$$

indicating that the sign of $(x_k)_j$ is determined by $\det\left(A_{\backslash\{j\}} - \lambda_k I\right)$. We deduce from (6) that

$$\frac{(x_k)_i^2}{(x_k)_j^2} = \frac{\det\left(A_{\backslash\{i\}} - \lambda_k I\right)}{\det\left(A_{\backslash\{j\}} - \lambda_k I\right)} = \frac{c_{A_{\backslash\{i\}}}(\lambda_k)}{c_{A_{\backslash\{j\}}}(\lambda_k)} \tag{10}$$

illustrating that $\det\left(A_{\backslash\{i\}} - \lambda_k I\right)$ and $\det\left(A_{\backslash\{j\}} - \lambda_k I\right)$ have the same sign for *any pair* of nodes (i, j) for a given frequency λ_k, but, by (40), opposite to the sign of $c'_A(\lambda_k)$ (as verified from Fig. 1). Applying (8) illustrates, for any $1 \leq m \leq N$,

$$\frac{(x_k)_i}{(x_k)_j} = (-1)^{i-j} \frac{\det\left(A_{\backslash \text{row } m \backslash \text{col } i} - \lambda_k I\right)}{\det\left(A_{\backslash \text{row } m \backslash \text{col } j} - \lambda_k I\right)}$$

[2] Assuming the appropriate dimensions of the identity matrix I to obtain a square matrix in the brackets, we use both equivalent notations: $\det\left((A - \lambda_k I)_{\backslash \text{row } m \backslash \text{col } j}\right) = \det\left(A_{\backslash \text{row } m \backslash \text{col } j} - \lambda_k I\right)$.

and choosing $m = j$,

$$\frac{(x_k)_i}{(x_k)_j} = (-1)^{i-j} \frac{\det\left(A_{\backslash \text{row } j \backslash \text{col } i} - \lambda_k I\right)}{\det\left(A_{\backslash \{j\}} - \lambda_k I\right)} \tag{11}$$

shows that generally not much about the sign of the determinants can be concluded.

2.3. The adjoint matrix

Let us define

$$\varphi_{km}^{-1} = \sqrt{\sum_{l=1}^{N} \left(\det\left(A_{\backslash \text{row } m \backslash \text{col } l} - \lambda_k I\right)\right)^2} = \sqrt{-c_A'(\lambda_k) \det\left(A_{\backslash \{m\}} - \lambda_k I\right)} \tag{12}$$

Formulae (7) and (8) show that φ_{km} is a non-negative scaling of the eigenvector x_k. With the definition of the adjugate of matrix A in [3, eq. (A.38) on p. 323],

$$(\text{adj}A)_{ij} = (-1)^{i+j} \det\left(A_{\backslash \text{row } j \backslash \text{col } i}\right)$$

the eigenvector component (7), for any integer $1 \leq m \leq N$, becomes

$$(x_k)_j = \varphi_{km} \left(\text{adj}\left(A - \lambda_k I\right)\right)_{jm} \tag{13}$$

We add [3, p. 339] that the adjoint matrix,

$$\text{adj}\left(A - \lambda I\right) = \left(\lambda I - A\right)^{-1} c_A(\lambda)$$

rewritten as $(A - \lambda I)\text{adj}(A - \lambda I) = -c_A(\lambda)$ shows that our starting equation $(A - \lambda_k I)\, x_k = 0$ is indeed satisfied by (13). Incidentally [11, Chapter IV], we have given a third proof of the eigenvector component $(x_k)_j$ in (7) or (13).

We recall formula [3, (A.92) on p. 343] and its combination with (3),

$$x_k x_k^T = \prod_{l=1;l\neq k}^{N} \frac{A - \lambda_l I}{\lambda_k - \lambda_l} = \frac{(-1)^N}{c_A'(\lambda_k)} \prod_{l=1;l\neq k}^{N} \left(A - \lambda_l I\right) = \frac{-1}{c_A'(\lambda_k)} \prod_{l=1;l\neq k}^{N} \left(\lambda_l I - A\right) \tag{14}$$

which is a consequence of the Caley-Hamilton theorem and Taylor's theorem [3, art. 228]. Appendix B provides an operator calculus of the eigenvalue equation and deduces in an entirely algebraic way, without involving the theory of functions and Taylor's theorem, formula (14) in Section B.2. The matrix element in (14), $\left(x_k x_k^T\right)_{jm} = (x_k)_j (x_k)_m = \frac{-1}{c_A'(\lambda_k)} \left(\prod_{l=1;l\neq k}^{N} \left(\lambda_l I - A\right)\right)_{jm}$, compared to (9), leads to

$$(-1)^{j+m} \det\left(A_{\backslash \text{row } j \backslash \text{col } m} - \lambda_k I\right) = (\text{adj}\,(A - \lambda_k I))_{mj} = \left(\prod_{l=1; l\neq k}^{N} (\lambda_l I - A)\right)_{jm} \tag{15}$$

2.4. Consequences of the theory

Since the matrix $A = A^T$ is symmetric, the matrix $(A - \lambda I)_{\backslash \text{row } m \backslash \text{col } l} = (A - \lambda I)^T_{\backslash \text{row } l \backslash \text{col } m} = (A - \lambda I)_{\backslash \text{row } l \backslash \text{col } m}$ is asymmetric and the zeros of the polynomial $\det\left((A - \lambda I)_{\backslash \text{row } m \backslash \text{col } l}\right)$ with real coefficients can be complex conjugate. The polynomials of the set $\left\{\det\left((A - \lambda I)_{\backslash \text{row } m \backslash \text{col } l}\right)\right\}_{1 \leq m, l \leq N}$ with highest degree are those on the diagonal, i.e. when $m = l$ and $\det\left((A - \lambda I)_{\backslash \text{row } m \backslash \text{col } m}\right) = \det\left(A_{\backslash \{m\}} - \lambda I\right)$, because the resulting matrix after the removal of row m and column l contains two λ entries less than the original matrix $A - \lambda I$ if $m \neq l$, whereas only one λ entry less if $m = l$. Moreover, the polynomials $\det\left(A_{\backslash \{m\}} - \lambda I\right)$ have real zeros, because $A_{G \backslash \{m\}} - \lambda I$ is symmetric.

Since the cofactor expansion of the determinant $\det(A - \lambda_k I)$ along row m is

$$\det(A - \lambda_k I) = \sum_{j=1}^{N} (a_{mj} - \lambda_k \delta_{jm}) (-1)^{m-j} \det\left((A - \lambda_k I)_{\backslash \text{row } m \backslash \text{col } j}\right) \tag{16}$$

we find from (8) that

$$\frac{\det(A - \lambda_k I)}{\sqrt{-c'_A(\lambda_k) \det\left(A_{\backslash \{m\}} - \lambda_k I\right)}} = \sum_{j=1}^{N} (a_{mj} - \lambda_k \delta_{jm}) (x_k)_j$$

which is the row m of the eigenvalue equation $Ax_k = \lambda_k x_k$, because $\det(A - \lambda_k I) = c_A(\lambda_k) = 0$. Furthermore, the cofactor expansion (16) expresses, for any $1 \leq m \leq N$, the k-th eigenvalue as

$$\begin{aligned}\lambda_k &= \frac{\sum_{j=1}^{N} a_{mj} (-1)^{m-j} \det\left((A - \lambda_k I)_{\backslash \text{row } m \backslash \text{col } j}\right)}{\det\left(A_{\backslash \{m\}} - \lambda_k I\right)} \\ &= a_{mm} + \sum_{j=1; j\neq m}^{N} a_{mj} (-1)^{m-j} \frac{\det\left((A - \lambda_k I)_{\backslash \text{row } m \backslash \text{col } j}\right)}{\det\left(A_{\backslash \{m\}} - \lambda_k I\right)}\end{aligned}$$

With (11), we find, for any $1 \leq m \leq N$, that $\lambda_k - a_{mm} = \sum_{j=1; j\neq m}^{N} a_{mj} \frac{(x_k)_j}{(x_k)_m}$. Now, we choose m such that $|(x_k)_m| \geq \left|(x_k)_j\right|$ for any $1 \leq j \leq N$. After taking the absolute value, we arrive at $|\lambda_k - a_{mm}| \leq \sum_{j=1; j\neq m}^{N} |a_{mj}|$, which proves Gerschgorin's Theorem [3, art.

245] and, in addition, that there[3] is a value of m for which $\left|\frac{\det\left((A-\lambda_k I)_{\setminus \text{row } m \setminus \text{col } j}\right)}{\det\left(A_{\setminus\{m\}}-\lambda_k I\right)}\right| \leq 1$ for any $1 \leq j \leq N$. Thus, the polynomial $\det\left(A_{\setminus\{m\}} - \lambda I\right)$ with highest degree among the polynomials $\left\{\det\left((A-\lambda I)_{\setminus \text{row } m \setminus \text{col } j}\right)\right\}_{1\leq m,j\leq N}$ also numerically exceeds or equals in absolute value all others (with $1 \leq j \leq N$) for a particular value of m at a zero $\lambda = \lambda_k$ with multiplicity $m_k = 1$ of the polynomial $\det(A - \lambda I)$.

The cofactor expansion of the determinant $\det\left((A-\lambda I)_{\setminus \text{row } m \setminus \text{col } j}\right)$ does not easily lead to an expression for the eigenvectors of the $N \times N$ matrix A in terms of those of an $(N-1) \times (N-1)$ submatrix of A, which would be helpful in graphs, because the addition or removal of a node frequently occurs. Such a recursive relation is derived in [3, art. 259], but it is actually a spectral decomposition.

Another interesting observation from (8) and (15) is that the matrix $X(\lambda)$ with elements

$$(x(\lambda))_{mj} = \frac{(-1)^{j+m}\det\left((A-\lambda I)_{\setminus \text{row } m \setminus \text{col } j}\right)}{\sqrt{-c_A'(\lambda)\det\left(A_{G\setminus\{m\}}-\lambda I\right)}} = \frac{(\operatorname{adj}(A-\lambda I))_{mj}}{\sqrt{-c_A'(\lambda)\det\left(A_{G\setminus\{m\}}-\lambda I\right)}}$$

that are ratio's of polynomials in λ over the squareroot of polynomials in λ have different rows in m. However, if $\lambda = \lambda_k$ is an eigenvalue of A and all eigenvalues are different, then all rows are the same by (8), because $(x(\lambda_k))_{mj} = (x_k)_j$ is independent of m.

Example. For the matrix

$$A = \begin{bmatrix} 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 1 & 0 \end{bmatrix}$$

with eigenvalues $\lambda = \{2.30278, 0.618034, 0., -1.30278, -1.61803\}$, the corresponding matrix $X(\lambda)$ is

$$X(\lambda) = \begin{bmatrix} \lambda^4-4\lambda^2-2\lambda+1 & \lambda+1 & \lambda^2+\lambda-1 & \lambda^3-2\lambda & \lambda^2+\lambda \\ \lambda+1 & \lambda^4-4\lambda^2-2\lambda+1 & \lambda^2+\lambda-1 & \lambda^2+\lambda & \lambda^3-2\lambda \\ \lambda^2+\lambda-1 & \lambda^2+\lambda-1 & \lambda^4-3\lambda^2+1 & \lambda^3+\lambda^2-\lambda & \lambda^3+\lambda^2-\lambda \\ \lambda^3-2\lambda & \lambda^2+\lambda & -\lambda^3-\lambda^2+\lambda & \lambda^4-2\lambda^2 & \lambda^3+\lambda^2 \\ \lambda^2+\lambda & \lambda^3-2\lambda & \lambda^3+\lambda^2-\lambda & \lambda^3+\lambda^2 & \lambda^4-2\lambda^2 \end{bmatrix} \operatorname{diag}(\varphi)$$

where the diagonal elements of $\operatorname{diag}(\varphi)$ are the components of the vector

[3] Numerical checks on the $N \times N$ matrix R with elements $r_{mj} = \frac{\det\left((A-\lambda_k I)_{\setminus \text{row } m \setminus \text{col } j}\right)}{\det\left(A_{\setminus\{m\}}-\lambda_k I\right)}$ show that there is only one value of m for which $|r_{mj}| \leq 1$ for $1 \leq j \leq N$, but different eigenvalues λ_k and λ_l may possess that same value m.

$$\varphi = \begin{bmatrix} \frac{1}{\sqrt{(\lambda^4-4\lambda^2-2\lambda+1)(5\lambda^4-15\lambda^2-4\lambda+3)}} \\ \frac{1}{\sqrt{(\lambda^4-4\lambda^2-2\lambda+1)(5\lambda^4-15\lambda^2-4\lambda+3)}} \\ \frac{1}{\sqrt{(\lambda^4-3\lambda^2+1)(5\lambda^4-15\lambda^2-4\lambda+3)}} \\ \frac{1}{\sqrt{(\lambda^4-2\lambda^2)(5\lambda^4-15\lambda^2-4\lambda+3)}} \\ \frac{1}{\sqrt{(\lambda^4-2\lambda^2)(5\lambda^4-15\lambda^2-4\lambda+3)}} \end{bmatrix}$$

Evaluating the above matrix $X(\lambda)$ for $\lambda_1 = 2.30278$ reduces to

$$X(\lambda_1) = \begin{bmatrix} 0.245399 & 0.245399 & 0.490799 & 0.5651 & 0.5651 \\ 0.245399 & 0.245399 & 0.490799 & 0.5651 & 0.5651 \\ 0.245399 & 0.245399 & 0.490799 & 0.5651 & 0.5651 \\ 0.245399 & 0.245399 & 0.490799 & 0.5651 & 0.5651 \\ 0.245399 & 0.245399 & 0.490799 & 0.5651 & 0.5651 \end{bmatrix}$$

with the eigenvector x_1 in each row.

3. Orthogonal eigenvector matrix X

The $N \times N$ orthogonal eigenvector matrix X with the eigenvectors $x_1, x_2, \ldots, x_N$ in the columns follows from (13) as

$$X = \begin{bmatrix} (\text{adj}(A-\lambda_1 I))_{1m_1} & (\text{adj}(A-\lambda_2 I))_{1m_2} & \cdots & (\text{adj}(A-\lambda_N I))_{1m_N} \\ (\text{adj}(A-\lambda_1 I))_{2m_1} & (\text{adj}(A-\lambda_2 I))_{2m_2} & \cdots & (\text{adj}(A-\lambda_N I))_{2m_N} \\ \vdots & \vdots & \ddots & \vdots \\ (\text{adj}(A-\lambda_1 I))_{Nm_1} & (\text{adj}(A-\lambda_2 I))_{Nm_2} & \cdots & (\text{adj}(A-\lambda_N I))_{Nm_N} \end{bmatrix} \text{diag}(\varphi)$$

where the vector $\varphi = (\varphi_{1m_1}, \varphi_{2m_2}, \ldots, \varphi_{Nm_N})$. In fact, we observe that X is a part of a three-dimensional matrix (or tensor) with elements $(\text{adj}(A-\lambda_k I))_{lm}$ in the integers k, l and m. However, m can be chosen at will and X is thus everywhere the same in the third m dimension.

In the sequel, we will show that double orthogonality [3, art. 248] arises as a consequence of the Caley-Hamilton theorem, Cramer's method and Taylor's theorem. Clearly, the particular scaling of eigenvector x_k by φ_{km} in (12) plays an essential role in the orthogonality relations. Admittedly, the proof is more complex than the classical, geometric proof.

3.1. *The first orthogonality relation* $x_k^T x_l = \sum_{j=1}^N (x_k)_j (x_l)_j = \delta_{kl}$

With $(x_k)_j = \varphi_{km} (-1)^{j+m} \det\left((A-\lambda_k I)_{\backslash \text{row } m \backslash \text{col } j}\right)$ in (13), the first orthogonality relation $x_k^T x_l = \sum_{j=1}^N (x_k)_j (x_l)_j = \delta_{kl}$ translates to

$$\delta_{kl} = (-1)^{m_k+m_l} \varphi_{km_k}\varphi_{lm_l} \sum_{j=1}^{N} \det\left((A-\lambda_k I)_{\backslash \text{row } m_k \backslash \text{col } j}\right) \det\left((A-\lambda_l I)_{\backslash \text{row } m_l \backslash \text{col } j}\right)$$

where the sum is a non-trivial determinantal property that vanishes if $k \neq l$. Substitution of (15) gives

$$\delta_{kl} = \varphi_{km_k}\varphi_{lm_l} \sum_{j=1}^{N} \left(\prod_{n=1;n\neq k}^{N} (\lambda_n I - A)\right)_{m_k j} \left(\prod_{q=1;q\neq l}^{N} (\lambda_q I - A)\right)_{m_l j}$$

Invoking symmetry and matrix multiplication yields

$$\begin{aligned} \delta_{kl} &= \varphi_{km_k}\varphi_{lm_l} \sum_{j=1}^{N} \left(\prod_{n=1;n\neq k}^{N} (\lambda_n I - A)\right)_{m_k j} \left(\prod_{q=1;q\neq l}^{N} (\lambda_q I - A)\right)_{j m_l} \\ &= \varphi_{km_k}\varphi_{lm_l} \left(\prod_{n=1;n\neq k}^{N} (\lambda_n I - A) \prod_{q=1;q\neq l}^{N} (\lambda_q I - A)\right)_{m_k m_l} \end{aligned} \tag{17}$$

The Taylor series $f(A) = \sum_{k=1}^{N} f(\lambda_k) x_k x_k^T$ in [3, (A.88) on p. 342], applied to $f(x) = \frac{c_A^2(x)}{(x-\lambda_k)(x-\lambda_l)}$ indicates that $\prod_{n=1;n\neq k}^{N} (\lambda_n I - A) \prod_{q=1;q\neq l}^{N} (\lambda_q I - A) = 0$ if $k \neq l$, because $f(\lambda_k) = \lim_{x\to\lambda_k} \frac{c_A^2(x)}{(x-\lambda_k)(x-\lambda_l)} = 0$. For $k = l$, the right-hand side bracket of (17) becomes

$$\left(\prod_{n=1;n\neq k}^{N} (\lambda_n I - A) \prod_{q=1;q\neq l}^{N} (\lambda_q I - A)\right)_{m_k m_l} = \left(\prod_{n=1;n\neq k}^{N} (\lambda_n I - A)^2\right)_{m_k m_k}$$

The general polynomial formula $f(A) = \sum_{k=1}^{N} f(\lambda_k) \prod_{n=1;n\neq k}^{N} \frac{(A-\lambda_n I)}{(\lambda_k-\lambda_n)}$ in [3, (A.90) on p. 342] indicates with $f(x) = \left(\frac{c_A(x)}{x-\lambda_k}\right)^2$ that

$$\prod_{n=1;n\neq k}^{N} (\lambda_n I - A)^2 = \left(c_A'(\lambda_k)\right)^2 \prod_{n=1;n\neq k}^{N} \frac{(A-\lambda_n I)}{(\lambda_k-\lambda_n)} = -c_A'(\lambda_k) \prod_{n=1;n\neq k}^{N} (\lambda_n I - A)$$

Hence, with (15),

$$\begin{aligned} \left(\prod_{n=1;n\neq k}^{N} (\lambda_n I - A)^2\right)_{m_k m_l} &= -c_A'(\lambda_k) \left(\prod_{n=1;n\neq k}^{N} (\lambda_n I - A)\right)_{m_k m_l} \\ &= (-1)^{m_k+m_l+1} c_A'(\lambda_k) \det\left(A_{\backslash \text{row } m_k \backslash \text{col } m_l} - \lambda_k I\right) \end{aligned}$$

the Kronecker delta in (17) becomes with the definition (12) of φ_{km}, for $k = l$,

$$\varphi_{km_k}\varphi_{km_l}\left(\prod_{n=1;n\neq k}^{N}(\lambda_n I-A)^2\right)_{m_k m_l}$$
$$=\varphi_{km_k}\varphi_{km_l}(-1)^{m_k+m_l+1}c_A'(\lambda_k)\det\left(A_{\backslash\,\mathrm{row}\,m_k\backslash\,\mathrm{col}\,m_l}-\lambda_k I\right)$$
$$=\frac{(-1)^{m_k+m_l+1}c_A'(\lambda_k)\det\left(A_{\backslash\,\mathrm{row}\,m_k\backslash\,\mathrm{col}\,m_l}-\lambda_k I\right)}{-c_A'(\lambda_k)\sqrt{\det\left(A_{\backslash\{m_k\}}-\lambda_k I\right)\det\left(A_{\backslash\{m_l\}}-\lambda_k I\right)}}$$

which is indeed equal to 1 if we choose $m_k = m_l = m$.

3.2. The second orthogonality relation $\sum_{k=1}^{N}(x_k)_i (x_k)_j = \delta_{ij}$

Formula (9) in Corollary 1 indicates that the second orthogonality relation $\sum_{k=1}^{N}(x_k)_i (x_k)_j = \delta_{ij}$ is

$$(-1)^{j+m+1}\sum_{k=1}^{N}\frac{\det\left(A_{\backslash\,\mathrm{row}\,j\backslash\,\mathrm{col}\,m}-\lambda_k I\right)}{c_A'(\lambda_k)}=\delta_{jm} \tag{18}$$

Substitution of (15) into (18) yields

$$\delta_{jm}=\left(\sum_{k=1}^{N}\frac{1}{c_A'(\lambda_k)}\prod_{l=1;l\neq k}^{N}(\lambda_l I-A)\right)_{jm}=\left(\sum_{k=1}^{N}\prod_{l=1;l\neq k}^{N}\frac{(A-\lambda_l I)}{(\lambda_k-\lambda_l)}\right)_{jm}$$

The general polynomial formula $f(A)=\sum_{k=1}^{N}f(\lambda_k)\prod_{l=1;l\neq k}^{N}\frac{(A-\lambda_l I)}{(\lambda_k-\lambda_l)}$ in [3, (A.90) on p. 342] indicates for the above that $f(x)=1=x^0$, which indeed demonstrates the second orthogonality relation (18).

Using $(x_k)_j=\varphi_{km}(-1)^{j+m}\det\left((A-\lambda_k I)_{\backslash\,\mathrm{row}\,m\backslash\,\mathrm{col}\,j}\right)$ in (13) results in the more complicated variant of the second orthogonality relation

$$\delta_{ij}=\sum_{k=1}^{N}\varphi_{km}(-1)^{j+m}\det\left((A-\lambda_k I)_{\backslash\,\mathrm{row}\,m\backslash\,\mathrm{col}\,j}\right)(-1)^{i+m}\varphi_{km}\det\left((A-\lambda_k I)_{\backslash\,\mathrm{row}\,m\backslash\,\mathrm{col}\,i}\right)$$
$$=(-1)^{i+j+1}\sum_{k=1}^{N}\frac{\det\left((A-\lambda_k I)_{\backslash\,\mathrm{row}\,m\backslash\,\mathrm{col}\,j}\right)\det\left((A-\lambda_k I)_{\backslash\,\mathrm{row}\,m\backslash\,\mathrm{col}\,i}\right)}{c_A'(\lambda_k)\det\left(A_{\backslash\{m\}}-\lambda_k I\right)}$$

But, since we can choose m at will, the choice $i = m$ leads again to (18), because A is symmetric.

4. Eigenvalue λ_k has multiplicity $m_k > 1$

Appendix C extends the first proof of Theorem 2 to an eigenvalue λ_k with multiplicity $m_k = 2$. Although computations with higher-order multiplicities are known to be more involved, especially in the computations of residues of a complex function, Appendix C illustrates that the increase in complexity is considerable. Hence, closed formulae for eigenvector components belonging to an eigenvalue λ_k of multiplicity $m_k > 1$ are rare and, perhaps, undesirable as they lack insight as well as mathematical beauty. For the square of the eigenvector components, on the other hand, the situation is different. Hagos [6, Theorem 4.1] has attempted to extend formula (6) and proposed (in our notation) that

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

where λ_k is an eigenvalue with multiplicity m_k and x_l is one of the m_k orthogonal eigenvectors belonging to eigenvalue λ_k. However, the above result of Hagos is only partially correct, because both $\det\left(A_{\backslash\{j\}} - \lambda_k I\right) = c'_A(\lambda_k) = 0$ if $m_k > 1$, resulting in an undefined right-hand side. Here in Theorem 3, we extend the theory on eigenvector components in Section 2 to eigenvalues with multiplicity higher than one and give in (23) the exact, closed formula of Hagos' result.

4.1. Preliminary consideration

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, the derivative $\frac{d}{d\lambda}\det(A - \lambda I) = -\sum_{n=1}^{N}\det\left(A_{\backslash\{n\}} - \lambda I\right)$ in (40) and the fact that $\det\left(A_{\backslash\{n\}} - \lambda_k I\right)$ must have the same sign due to (6) shows that all $\det\left(A_{G\backslash\{n\}} - \lambda_k I\right)$ must vanish, implying that λ_k is then also an eigenvalue of all $A_{\backslash\{n\}}$, i.e. for each node n removed from the graph G. This observation agrees with the Interlacing Theorem [3, art. 263] that tells us that all eigenvalues of $A_{\backslash\{n\}}$ for each $1 \le n \le N$ 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 $A_{\backslash\{n\}}$, i.e. $\lambda_k \ge \lambda\left(A_{\backslash\{n\}}\right) \ge \lambda_{k+1}$, is squeezed to that same value λ_k. Appendix C shows for an eigenvalue λ_k with multiplicity $m_k = 2$ that we can always find two orthogonal eigenvectors x_k and x_{k+1} belonging to eigenvalue λ_k, where at least one eigenvector has at least one zero component, for example, $(x_k)_m = 0$.

If eigenvalue λ_k has multiplicity $m_k = 1$, then it is possible that $\det\left(A_{\backslash\{n\}} - \lambda_k I\right) = 0$ for a single n, which implies that $(x_k)_n = 0$ by (39). The eigenvalue equation $Ax_k = \lambda_k x_k$ reduces then for row n to $(Ax_k)_n = \sum_{j=1}^{N} a_{nj}(x_k)_j = 0$, i.e. the n-th row a_n or n-th column a_n^T of the symmetric matrix A is orthogonal the eigenvector, thus $a_n^T x_k = 0$. If A is the adjacency matrix of a graph G, then $(Ax_k)_n = \sum_{j\in\mathcal{N}_n}(x_k)_j = 0$, where $\mathcal{N}_n$ is the set of direct neighbors of node n, means that the sum of the eigenvector components of x_k over all neighbors of node n vanishes. The Perron-Frobenius theorem [12, Chapter XIII] for a reducible non-negative matrix A states that the principal eigenvector x_1 belonging to the largest eigenvalue λ_1 has non-negative components, implying that $\sum_{j\in\mathcal{N}_n}(x_1)_j = 0$ is possible only if all $(x_k)_j = 0$. Hence, if $\sum_{j\in\mathcal{N}_n}(x_1)_j = 0$, then all nodes of a disconnected subgraph containing node n possess a zero eigenvector component $(x_k)_j = 0$, but there must be subgraphs of G whose nodes have positive eigenvector components $(x_k)_l > 0$, because the zero vector is never an eigenvector.

4.2. Eigenvector components belonging to an eigenvalue with multiplicity exceeding 1

Theorem 3. *Let the eigenvalue λ_k of the $N \times N$ real, symmetric matrix A possess multiplicity $m_k > 1$, so that $\lambda_k = \lambda_{k+1} = \cdots = \lambda_{k+m_k-1}$. The sum of the squared j-th component of all eigenvector x_κ of A belonging to eigenvalue λ_k with $\kappa = k, k+1, \ldots, k+m_k-1$ equals*

$$\sum_{\kappa=k}^{k+m_k-1} (x_\kappa)_j^2 = \frac{(-1)^N (m_k)!}{\left.\frac{d^{m_k} c_A(\lambda)}{d\lambda^{m_k}}\right|_{\lambda=\lambda_k}} \left(\prod_{l=1;l\neq\{k,k+1,\ldots,k+m_k-1\}}^N (A - \lambda_l I)\right)_{jj} \tag{19}$$

or

$$\begin{aligned}\sum_{\kappa=k}^{k+m_k-1} (x_\kappa)_j^2 &= \frac{\left(\prod_{l=1;l\neq\{k,k+1,\ldots,k+m_k-1\}}^N (A - \lambda_l I)\right)_{jj}}{\prod_{j=1;j\neq\{k,k+1,\ldots,k+m_k-1\}}^N (\lambda_k - \lambda_j)} \\ &= \left(\prod_{l=1;l\neq\{k,k+1,\ldots,k+m_k-1\}}^N \frac{A - \lambda_l I}{\lambda_k - \lambda_l}\right)_{jj}\end{aligned} \tag{20}$$

where

$$\left.\frac{d^{m_k} c_A(\lambda)}{d\lambda^{m_k}}\right|_{\lambda=\lambda_k} = (-1)^N (m_k)! \prod_{j=1;j\neq\{k,k+1,\ldots,k+m_k-1\}}^N (\lambda_k - \lambda_j) \tag{21}$$

Alternative forms are

$$\sum_{\kappa=k}^{k+m_k-1} (x_\kappa)_j^2 = \frac{(-1)^{m_k-1} \sum_{n_1=1}^{N-1} \sum_{n_2=1}^{N-2} \cdots \sum_{n_{m_k-1}=1}^{N-m_k-1} \det\left(A_{\backslash\{j,n_1,n_2,\ldots,n_{m_k-1}\}} - \lambda_k I\right)}{(m_k-1)! \prod_{j=1;j\neq\{k,k+1,\ldots,k+m_k-1\}}^N (\lambda_j - \lambda_k)} \tag{22}$$

and

$$\sum_{\kappa=k}^{k+m_k-1} (x_\kappa)_j^2 = -\frac{m_k}{\left.\frac{d^{m_k} c_A(\lambda)}{d\lambda^{m_k}}\right|_{\lambda=\lambda_k}} \sum_{n_1=1}^{N-1} \sum_{n_2=1}^{N-2} \cdots \sum_{n_{m_k-1}=1}^{N-m_k-1} \det\left(A_{\backslash\{j,n_1,n_2,\ldots,n_{m_k-1}\}} - \lambda_k I\right) \tag{23}$$

Formulae (19)-(21) in Theorem 3 are proved in Appendix B.3, formulae (22) and (23) are proved in Appendix B.4. If matrix A is the adjacency matrix of a graph G, then $A_{\backslash\{j,n_1,n_2,\ldots,n_{m_k-1}\}}$ is the adjacency matrix of the graph obtained from the graph G, by first deleting the node j (and all its incident links) to create the graph $G_{\backslash\{j\}}$ and subsequently in $G_{\backslash\{j\}}$ any possible combination of set of $m_k - 1$ nodes is removed. Instead of specifying a single eigenvector component $(x_\kappa)_j^2$, Theorem 3 only allows us to compute the average $\frac{1}{m_k}\sum_{\kappa=k}^{k+m_k-1}(x_\kappa)_j^2$ over all m_k squared eigenvector components belonging to the same eigenvalue λ_k.

For example, if $m_k = 2$ and $c''_A(\lambda_k) = \left.\frac{d^2 c_A(\lambda)}{d\lambda^2}\right|_{\lambda=\lambda_k}$, then (23) reduces to

$$\frac{(x_k)_j^2 + (x_{k+1})_j^2}{2} = \frac{1}{c''_A(\lambda_k)} \sum_{n=1;n\neq j}^{N-1} \det\left(A_{\backslash\{j,n\}} - \lambda_k I\right) \tag{24}$$

while (19) returns

$$\frac{(x_k)_j^2 + (x_{k+1})_j^2}{2} = \frac{1}{c''_A(\lambda_k)} \left(\prod_{l=1;l\neq\{k,k+1\}}^{N} (\lambda_l I - A)\right)_{jj} \tag{25}$$

The right-hand side of (24) sums over all the characteristic polynomials $\det\left(A_{\backslash\{j,n\}} - \lambda_k I\right)$ of graphs $G_{\backslash\{j,n\}}$ obtained from the original graph G where first node j is removed and in the resulting graph $G_{\backslash\{j\}}$, subsequently every node is removed.

4.3. Strongly regular graphs

In this subsection, we apply Theorem 3 to strongly regular graphs. A strongly regular graph [3, art. 56] is a regular graph (where all nodes have the same degree r), whose adjacency matrix has three distinct eigenvalues, $\lambda_1 = r$, λ_2 with multiplicity m_2 and λ_3 with multiplicity m_3. The largest eigenvalue λ_1 of the adjacency matrix A of a connected graph has multiplicity $m_1 = 1$ by the Perron-Frobenius Theorem [3, art. 269]. Hence, following the recent book [7] of Brouwer and Van Maldeghem, it holds that $1 + m_2 + m_3 = N$ and, from the property $\text{trace}(A) = \sum_{j=1}^{N}\lambda_j = 0$ for any adjacency matrix A, it follows that $r + m_2\lambda_2 + m_3\lambda_3 = 0$. Solving the positive integers m_2 and m_3 from these two linear equations yields

$$m_2 = -\frac{(N-1)\lambda_3 + r}{\lambda_2 - \lambda_3} \quad \text{and} \quad m_3 = \frac{(N-1)\lambda_2 + r}{\lambda_2 - \lambda_3}$$

If $m_2 \neq m_3$, then Theorem 10 in [3, art. 269] states that the number of common neighbors of adjacent nodes equals $n_1 = r + \lambda_2 + \lambda_3 + \lambda_2\lambda_3$, while $n_2 = r + \lambda_2\lambda_3$ is the number of common neighbors of non-adjacent nodes. Hence, $n_1 - n_2 = \lambda_2 + \lambda_3$ and, combined with $r + m_2\lambda_2 + m_3\lambda_3 = 0$ from $\text{trace}(A) = 0$ allows us to solve the eigenvalue λ_2 and λ_3 as

$$\lambda_2 = \frac{(n_1 - n_2)m_3 + r}{m_3 - m_2} \quad \text{and} \quad \lambda_3 = -\frac{(n_1 - n_2)m_2 + r}{m_3 - m_2}$$

Since eigenvalues of the adjacency matrix are either integer or irrational [3, art. 45], we conclude that *all adjacency matrix eigenvalues of strongly regular graphs are integers*, provided the multiplicity $m_2 \neq m_3$. If $m_2 = m_3 = \frac{N-1}{2}$, then we arrive at the so-called "half case" [7, p. 3], where $\lambda_2 = \frac{\sqrt{N}-1}{2}$ and $\lambda_3 = \frac{-1-\sqrt{N}}{2}$.

We rewrite (20) for strongly regular graphs, by denoting $\overline{k} = 2$ if $k = 3$ and $\overline{k} = 3$ if $k = 2$,

$$\left(\prod_{l=1;l\neq\{k,k+1,\dots,k+m_k-1\}}^{N} \frac{A-\lambda_l I}{\lambda_k - \lambda_l}\right)_{jj} = \left(\frac{A-\lambda_1 I}{\lambda_k-\lambda_1}\left(\frac{A-\lambda_{\overline{k}} I}{\lambda_k-\lambda_{\overline{k}}}\right)^{m_{\overline{k}}}\right)_{jj}$$

Since the matrices $(A - \lambda_l I)$ and $(A - \lambda_m I)$ commute (as explained in Appendix B) and $\lambda_1 = r$, we find

$$\begin{aligned}
&\frac{A-\lambda_1 I}{\lambda_k-\lambda_1}\left(\frac{A-\lambda_{\overline{k}} I}{\lambda_k-\lambda_{\overline{k}}}\right)^{m_{\overline{k}}} \\
&\quad = \frac{(A-rI)\sum_{l=0}^{m_{\overline{k}}}\binom{m_{\overline{k}}}{l}A^l\left(-\lambda_{\overline{k}}\right)^{m_{\overline{k}}-l}}{(\lambda_k-r)\left(\lambda_k-\lambda_{\overline{k}}\right)^{m_k}} \\
&\quad = \frac{A^{1+m_{\overline{k}}}+\sum_{l=1}^{m_{\overline{k}}}\left\{\binom{m_{\overline{k}}}{l-1}\left(-\lambda_{\overline{k}}\right)^{1+m_{\overline{k}}-l}-r\binom{m_{\overline{k}}}{l}\left(-\lambda_{\overline{k}}\right)^{m_{\overline{k}}-l}\right\}A^l-rI\left(-\lambda_{\overline{k}}\right)^{m_{\overline{k}}}}{(\lambda_k-r)\left(\lambda_k-\lambda_{\overline{k}}\right)^{m_k}}
\end{aligned}$$

which leads, for the j-th eigenvector components belonging to eigenvalue λ_k with multiplicity m_k, to

$$\sum_{\kappa=k}^{k+m_k-1}(x_\kappa)_j^2 = \frac{A_{jj}^{1+m_{\overline{k}}}-\sum_{l=1}^{m_{\overline{k}}}\binom{m_{\overline{k}}}{l}\left(-\lambda_{\overline{k}}\right)^{m_{\overline{k}}-l}\left\{\frac{(m_{\overline{k}}+1)r-(r-\lambda_{\overline{k}})l}{m_{\overline{k}}+1-l}\right\}\left(A^l\right)_{jj}-r\left(-\lambda_{\overline{k}}\right)^{m_{\overline{k}}}}{(\lambda_k-r)\left(\lambda_k-\lambda_{\overline{k}}\right)^{m_k}}$$

where $\left(A^l\right)_{jj}$ are the number of closed walks with l hops starting and ending at node j.

An example of a strongly regular graph with $m_2 = N - 2$ and $m_3 = 1$ are regular bipartite graphs with $N = 2m$ nodes, where $\lambda_1 = m = -\lambda_3$ and $\lambda_2 = 0$, so that (20) for $k = 2$ simplifies, with $\left(A^2\right)_{jj} = r$ and $(A)_{jj} = 0$, to

$$\begin{aligned}
\sum_{\kappa=k}^{k+N-3}(x_\kappa)_j^2 &= \frac{\left((A-\lambda_1 I)\left(A-\lambda_{\overline{k}} I\right)\right)_{jj}}{(\lambda_k-\lambda_1)\left(\lambda_k-\lambda_{\overline{k}}\right)} = \frac{\left(A^2-\left(\lambda_1+\lambda_{\overline{k}}\right)A+\lambda_1\lambda_{\overline{k}} I\right)_{jj}}{(\lambda_k-\lambda_1)\left(\lambda_k-\lambda_{\overline{k}}\right)} \\
&= \frac{r+r\lambda_{\overline{k}}}{(\lambda_k-r)\left(\lambda_k-\lambda_{\overline{k}}\right)}
\end{aligned}$$

After evaluation, we find $\sum_{\kappa=2}^{N-1}(x_\kappa)_j^2 = 1 - \frac{1}{m} = 1 - \frac{2}{N}$, which is independent of j. Symmetry and $\sum_{k=1}^{N}(x_k)_i^2 = 1$ suggest that $(x_1)_j^2 = (x_N)_j^2 = \frac{1}{N}$, which indeed is correct [3, (6.28) on p. 213].

5. Walk expansion

We apply the theory, developed in the previous sections, to graphs and deduce a so-called walk expansion in Theorem 4:

Theorem 4. *If all eigenvalues of the adjacency matrix A are different, then the polynomial form of (14) is*

$$(x_k)_i (x_k)_j = \frac{1}{\prod_{l=1;l\neq k}^{N} (\lambda_k - \lambda_l)} \sum_{r=H_{ij}}^{N-1} b_r (k) (A^r)_{ij} \tag{26}$$

where H_{ij} is the hopcount (number of links) of the shortest path between node i and j and where the coefficient $b_r (k)$ obeys $\prod_{j=1;j\neq k}^{N} (x - \lambda_j) = \sum_{j=0}^{N-1} b_j (k) x^j$ and equals

$$b_r (k) = \frac{1}{r!} \frac{d^r}{dx^r} \prod_{j=1;j\neq k}^{N} (x - \lambda_j) \Bigg|_{x=0} \tag{27}$$

Proof. The Taylor series [3, (A.91)] of a function $f(z)$ is a polynomial of degree $n-1$ for any $n \times n$ matrix A,

$$f(A) = \sum_{k=0}^{n-1} c_k [f] A^k \tag{28}$$

where the coefficient $c_k [f]$, which depends on the function f and on the eigenvalues of A, is

$$c_k [f] = \frac{1}{k!} \sum_{m=1}^{n} \frac{f(\lambda_m)}{\prod_{j=1;j\neq m}^{n} (\lambda_m - \lambda_j)} \frac{d^k}{dx^k} \prod_{j=1;j\neq m}^{n} (x - \lambda_j) \Bigg|_{x=0}$$

Applying (28) to the function $f(z) = \frac{(-1)^N c_A(z)}{(z-\lambda_q)} = \prod_{l=1;l\neq q}^{N} (z - \lambda_l)$ and the $N \times N$ adjacency matrix A of a graph G, the Taylor coefficient is

$$\begin{aligned} c_k [f] &= \frac{1}{k!} \sum_{m=1}^{N} \frac{\lim_{x\to\lambda_m} \frac{c_A(x)}{(x-\lambda_q)}}{\prod_{j=1;j\neq m}^{N} (\lambda_m - \lambda_j)} \frac{d^k}{dx^k} \prod_{j=1;j\neq m}^{N} (x - \lambda_j) \Bigg|_{x=0} \\ &= \frac{1}{k!} \frac{\lim_{x\to\lambda_q} \frac{c_A(x)}{(x-\lambda_q)}}{\prod_{j=1;j\neq q}^{N} (\lambda_q - \lambda_j)} \frac{d^k}{dx^k} \prod_{j=1;j\neq q}^{N} (x - \lambda_j) \Bigg|_{x=0} \\ &= \frac{1}{k!} \frac{\prod_{j=1;j\neq q}^{N} (\lambda_q - \lambda_j)}{\prod_{j=1;j\neq q}^{N} (\lambda_q - \lambda_j)} \frac{d^k}{dx^k} \prod_{j=1;j\neq q}^{N} (x - \lambda_j) \Bigg|_{x=0} \end{aligned}$$

Since $f(A) = \prod_{l=1;l\neq q}^{N}(A - \lambda_l I)$, its Taylor expansion (28) is

$$\prod_{l=1;l\neq q}^{N}(A - \lambda_l I) = \sum_{r=0}^{N-1} \frac{1}{r!} \frac{d^r}{dx^r} \prod_{j=1;j\neq q}^{N} (x - \lambda_j)\Bigg|_{x=0} A^r$$

Formula (14) leads to (26) with coefficients $b_r(k)$ in (27). Finally, $(A^r)_{ij} = 0$ if r is smaller than the number H_{ij} of hops in the shortest path between node i and j. □

The coefficients $b_r(k)$ in (27) in the walk expansion (26) 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 (1) of the adjacency matrix as $b_k(m) = \frac{(-1)^{N-1}}{\lambda_m^{k+1}} \sum_{n=0}^{k} c_n \lambda_m^n$.

The derivative $c'_A(\lambda_k)$ in (3) plays the role of a normalization factor so that the squared eigenvector components satisfy $\sum_{j=1}^{N}(x_k)_j^2 = 1$. Clearly, if $i = j$, then $H_{jj} = 0$ and (26) reduces to[4]

$$(x_k)_j^2 = \frac{(-1)^N}{c'_A(\lambda_k)} \sum_{r=0}^{N-1} b_r(k)(A^r)_{jj} \tag{29}$$

but, if $i \neq j$, then the hopcount $H_{ij} > 0$ and (26) contains less terms in the sum than (29).

Theorem 4 expresses the product of two eigenvector components in terms of the eigenvalues and the number $(A^r)_{ij}$ of walks with r hops (or links) between node i and j. The longest possible shortest path in a graph contains $N-1$ hops and $(A^r)_{ij}$ equals [3] 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 (29) sums over the number $(A^r)_{jj}$ of closed walks, starting and ending at node j, of all possible lengths (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

[4] 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 (29) that

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

Thus, (29) becomes

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

at frequency λ_k. Thus, the appearance of $(A^r)_{jj}$ reflects[5] the only dependence of $(x_k)_j^2$ on the node j, while $b_r(k)$ and $c'_A(\lambda_k)$ only change with frequency/eigenvalue λ_k.

Example. When the hopcount of the shortest path in the graph between node i and j equals the maximum possible $H_{ij} = N - 1$, then (26) simplifies to

$$(x_m)_i (x_m)_j = \frac{\left(A^{N-1}\right)_{ij} (-1)^{m-1}}{\prod_{k=1}^{m-1} (\lambda_k - \lambda_m) \prod_{k=m+1}^{N} (\lambda_m - \lambda_k)} \tag{30}$$

The product $(x_m)_i (x_m)_j$ in (30) is always positive (negative) when m is odd (even)! The only possible example of (30) occurs in the path graph. The eigenvalues [3, p. 203] of the path graph P_N on N nodes are $\lambda_m(P_N) = 2\cos\frac{m\pi}{N+1}$ for $1 \leq m \leq N$ and the corresponding eigenvector component for node j is $(x_m)_j = \sqrt{\frac{2}{N+1}} \sin\left(\frac{\pi m j}{N+1}\right)$. The unique longest shortest path is between node 1 and N so that $\left(A^{N-1}\right)_{1N} = 1$ and (30) leads to the (non-trivial) identity for any integer $1 \leq m \leq N$,

$$\begin{aligned} &\frac{(-1)^{m-1}(N+1)}{2^N \sin\left(\frac{\pi m}{N+1}\right) \sin\left(\frac{\pi m N}{N+1}\right)} \\ &\quad = \prod_{k=1}^{m-1} \left(\cos\frac{k\pi}{N+1} - \cos\frac{m\pi}{N+1}\right) \prod_{k=m+1}^{N} \left(\cos\frac{m\pi}{N+1} - \cos\frac{k\pi}{N+1}\right) \end{aligned}$$

6. Stochastic matrix $\Xi = X \circ X$

The stochastic, asymmetric matrix $\Xi = X \circ X$, where $\circ$ denotes the Hadamard product [3, art. 274], consists of the square of the components of the orthogonal matrix X

$$\Xi = \begin{bmatrix} (x_1)_1^2 & (x_2)_1^2 & (x_3)_1^2 & \cdots & (x_n)_1^2 \\ (x_1)_2^2 & (x_2)_2^2 & (x_3)_2^2 & \cdots & (x_n)_2^2 \\ (x_1)_3^2 & (x_2)_3^2 & (x_3)_3^2 & \cdots & (x_n)_3^2 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ (x_1)_N^2 & (x_2)_N^2 & (x_3)_N^2 & \cdots & (x_n)_N^2 \end{bmatrix} \tag{31}$$

and obeys $\Xi u = u$ and $\Xi^T u = u$, where $u = (1, 1, \ldots, 1)$ denotes the all-one vector. With (6), we have

[5] Perhaps the expression (29) may be related to Feynman diagrams that express all possible interactions of a particle with others in some potential field.

$$\Xi = \begin{bmatrix} \det\left(A_{\backslash\{1\}} - \lambda_1 I\right) & \det\left(A_{\backslash\{1\}} - \lambda_2 I\right) & \cdots & \det\left(A_{\backslash\{1\}} - \lambda_N I\right) \\ \det\left(A_{\backslash\{2\}} - \lambda_1 I\right) & \det\left(A_{\backslash\{2\}} - \lambda_2 I\right) & \cdots & \det\left(A_{\backslash\{2\}} - \lambda_N I\right) \\ \vdots & \vdots & \ddots & \vdots \\ \det\left(A_{\backslash\{N\}} - \lambda_1 I\right) & \det\left(A_{\backslash\{N\}} - \lambda_2 I\right) & \cdots & \det\left(A_{\backslash\{N\}} - \lambda_N I\right) \end{bmatrix} \operatorname{diag}(\chi)$$

where the vector $\chi = \left(\frac{-1}{c'_A(\lambda_1)}, \frac{-1}{c'_A(\lambda_2)}, \ldots, \frac{-1}{c'_A(\lambda_N)}\right)$. In the sequel, we confine ourselves to the adjacency matrix A of a simple, unweighted and undirected graph.

Due to $\Xi\lambda = 0$ deduced in [3, art. 96] for an adjacency matrix A of a simple, unweighted and undirected graph, the rank Ξ is at most $N-1$ and thus $\det \Xi = 0$. Equivalently, the stochastic matrix Ξ has (at least) one zero[6] eigenvalue $\xi = 0$. If $\text{rank}(\Xi) = N-1$, then the eigenvalue vector $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_N)$ is the eigenvector belonging to eigenvalue $\xi = 0$. Thus, $\Xi\lambda = 0$ translates, for each $1 \le n \le N$, to

$$\sum_{k=1}^{N} \lambda_k \frac{\det\left(A_{\backslash\{n\}} - \lambda_k I\right)}{c'_A(\lambda_k)} = 0$$

The property $\Xi\lambda = 0$ suffices [8, Theorem 1] for the orthogonal matrix X alone to determine the adjacency matrix A. Indeed, given the orthogonal matrix X, we can compute the matrix $\Xi = X \circ X$. If $\text{rank}(\Xi) = N-1$ or, equivalently, if there is a unique eigenvalue $\xi = 0$, then $\Xi\lambda = 0$ has the eigenvector λ as a unique solution for a zero-one matrix A, from which the diagonal matrix $\Lambda = \text{diag}(\lambda)$ follows. Finally, the spectral decomposition $A = X\Lambda X^T$ allows us to construct the adjacency matrix[7] A of a graph G. The multiplicity of the zero eigenvalue of Ξ is important for the existence of co-eigenvector graphs [8], which are graphs with the same orthogonal eigenvector matrix X but with a different eigenvalue vector $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_N)$. Hence, the orthogonal eigenvector matrix X contains sufficient information to determine a non-empty graph precisely and contains information to find the eigenvalue vector $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_N)$.

[6] In general, a doubly stochastic matrix does not possess a zero eigenvalue. For example, the doubly stochastic matrix

$$\begin{bmatrix} 0.337 & 0.41375 & 0.24925 \\ 0.350787 & 0.318911 & 0.330301 \\ 0.312212 & 0.267339 & 0.420448 \end{bmatrix}$$

has eigenvalues $1., 0.114516, -0.0381555$, while

$$\begin{bmatrix} 0.46459 & 0.396328 & 0.139082 \\ 0.0875058 & 0.327341 & 0.585153 \\ 0.447904 & 0.276331 & 0.275765 \end{bmatrix}$$

has eigenvalues $1., 0.0338478 + 0.207248i, 0.0338478 - 0.207248i$.

[7] An eigenvector can be scaled by any non-zero number [3]. The proper scaling of the eigenvector λ of the matrix Ξ (belonging to the zero eigenvalue) is found to produce zero-one elements of the adjacency matrix A.

Since the eigenvalues of diag(χ), i.e. its diagonal elements, can never be zero for finite N (because $c'_A(\lambda_j)$ is always finite), the only zero eigenvalue – given that eigenvalues of A are simple – originates from the matrix

$$\Xi' = \begin{bmatrix} \det\left(A_{\setminus\{1\}} - \lambda_1 I\right) & \det\left(A_{\setminus\{1\}} - \lambda_2 I\right) & \cdots & \det\left(A_{\setminus\{1\}} - \lambda_N I\right) \\ \det\left(A_{\setminus\{2\}} - \lambda_1 I\right) & \det\left(A_{\setminus\{2\}} - \lambda_2 I\right) & \cdots & \det\left(A_{\setminus\{2\}} - \lambda_N I\right) \\ \vdots & \vdots & \ddots & \vdots \\ \det\left(A_{\setminus\{N\}} - \lambda_1 I\right) & \det\left(A_{\setminus\{N\}} - \lambda_2 I\right) & \cdots & \det\left(A_{\setminus\{N\}} - \lambda_N I\right) \end{bmatrix} \tag{32}$$

Theorem 5. *If eigenvalues of a symmetric matrix A are simple and the set of polynomials $\left\{c_{A_{\setminus\{n\}}}(\lambda)\right\}_{1\leq n\leq N}$ is linearly dependent, then the determinant $\det\Xi$ is zero.*

Proof. A determinant is zero if a row (column) is a linear combination of some other rows (columns). Row n in the matrix Ξ' in (32) consists of N sampling points $\left\{\lambda_k, \det\left(A_{\setminus\{n\}} - \lambda_k I\right)\right\}_{1\leq k\leq N}$ of the polynomial $\det\left(A_{\setminus\{n\}} - \lambda I\right)$ at $\lambda = \{\lambda_1, \lambda_2, \ldots \lambda_N\}$. Since the polynomial $\det\left(A_{\setminus\{n\}} - \lambda I\right)$ is at most of order $N-1$, the interpolating Lagrange polynomial through these N points completely [3, art. 303] specifies $\det\left(A_{\setminus\{n\}} - \lambda I\right) = c_{A_{\setminus\{n\}}}(\lambda)$, which is the characteristic polynomial of the graph $G_{\setminus\{n\}}$ obtained from the original, undirected, possibly weighted graph G without self-loops after removing node n and all its incident links. Finally, if $\det\Xi' = 0$, then it holds hold that $\det\Xi = \det\Xi' \det(\text{diag}(\chi)) = 0$. □

Appendix E reformulates $\det\Xi'$, unfortunately, without further insight.

7. The squared eigenvector component $(x_k)_j^2$ as a graph metric

1. *Induced centrality metric.* Everett and Borgatti [13] have defined the induced centrality $C_f(j)$ of node j for a graph function f, which is also called the vitality index in [14, Definition 3.6.1], by

$$C_f(j) = f(G) - f\left(G_{\setminus\{j\}}\right) \tag{33}$$

Many known metrics can be formulated as induced centralities. For example, if the graph function 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 (6) as

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

Choosing $f(G) = \det(A_G - \lambda_k I)$, the definition (33) hints that $c'_A(\lambda_k)(x_k)_j^2$ is an induced centrality, but the eigenvalue $\lambda_k = \lambda_k(A_G)$ belongs to the graph G, but not necessarily to $G_{\setminus\{j\}}$.

If we extend the definition (33) towards the λ-induced centrality metric,

$$\mathcal{C}_f(j;\lambda) = f(G;\lambda) - f\left(G_{\setminus\{j\}};\lambda\right)$$

where $\lambda \in \mathbb{C}$ is a complex parameter, then the choice $f(G;\lambda) = \det(A_G - \lambda I)$ produces the λ-induced centrality metric

$$\mathcal{C}_{\det(A_G-\lambda I)}(j;\lambda) = \det(A_G - \lambda I) - \det\left(A_{G\setminus\{j\}} - \lambda I\right) = \xi(j;\lambda)\frac{d}{d\lambda}\det(A_G - \lambda I)$$

If the parameter λ tends to the k-th eigenvalue λ_k of the adjacency matrix of the graph G (with multiplicity 1), then

$$\lim_{\lambda\to\lambda_k}\mathcal{C}_{\det(A_G-\lambda I)}(j;\lambda) = -\det\left(A_{G\setminus\{j\}} - \lambda_k I\right) = \xi(j;\lambda_k)\,c'_A(\lambda_k)$$

and (6) shows that $\xi(j;\lambda_k) = (x_k)_j^2$. Hence, the square of the j-th component of eigenvector x_k of A belonging to eigenvalue λ_k with multiplicity $m_k = 1$ can be regarded as a centrality metric for node j,

$$(x_k)_j^2 = \frac{\mathcal{C}_{\det(A_G-\lambda_k I)}(j;\lambda_k)}{c'_A(\lambda_k)}$$

The eigenvector component $(x_k)_j$ in either (4), (5) or (8) cannot be written in the form (33) of an induced centrality. The latter observation makes sense, because if $(x_k)_j$ were an induced centrality of the node j, then any possible $N \times 1$ vector would be an induced centrality, because 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 a symmetric matrix A.

2. *Amplitude.* The magnitude of $(x_k)_j^2$ for node j in (6) depends on the characteristic polynomial $c_{A_{\setminus\{j\}}}(\lambda)$ of the symmetric matrix $A_{\setminus\{j\}}$ at the frequency $\lambda = \lambda_k$. As illustrated in Fig. 1, the characteristic polynomials $c_A(x)$ and $c_{A_{\setminus\{j\}}}(x)$ oscillate around zero in the interval $x \in [\lambda_N, \lambda_1]$, that contains all their real zeros. We coin the deviations in $c_{A_{\setminus\{j\}}}(x)$ from zero at λ_k the *amplitude.* Just as in quantum mechanics (see e.g. [15,16]), where the wave function can be complex, while its modulus is interpreted as a probability, the eigenvector components $(x_k)_j$ should be used in computations, but we suggest, based on (6), to interpret $(x_k)_j^2$ as centrality metrics in a graph. Hence, for a graph G, the importance or centrality of node j for property $\mathcal{P}_k$ embedded in the adjacency matrix A 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 [17,18]. 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 [19]. However, at other eigenfrequencies, the reverse must hold due to double orthogonality $\sum_{k=1}^{N} (x_k)_j^2 = 1$.

Equation (6) 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 $\{\lambda_k\}_{1\leq k\leq N}$.

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] $c_{A_{\setminus\{j\}}}(\lambda)$ 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 $c_{A_{\setminus\{j\}}}(\lambda_k)$ for $1 \leq j \leq 10$ have a same sign, in agreement with (10). The amplitude $c_{A_{\setminus\{j\}}}(\lambda_k)$ is a relative measure for $(x_k)_j^2$ and indicates the importance of node j at frequency λ_k.

3. *An ideal set of graph or centrality metrics.* There exists a large number of proposed graph metrics (see e.g. [20], [21, Section 15.6]). Nearly all graph metrics are non-negative real numbers that allow to normalize them into the interval $[0, 1]$. Graph metrics that specify a property of a node are called centrality metrics (e.g. the degree d_i of node i), while non-centrality metrics measure a global property (e.g. connectivity or path lengths of a graph G). However, many graph metrics are strongly correlated, which has

[8] The explicit expressions are

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

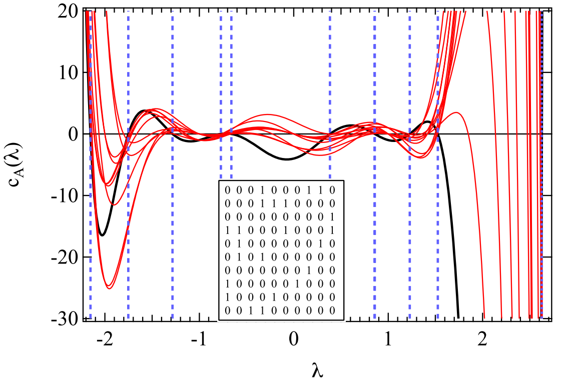

Fig. 1. The characteristic polynomials $c_{A_{\setminus\{n\}}}(\lambda)$ for $1 \leq n \leq N$ in red and $c_A(\lambda)$ in black for an Erdős-Rényi graph $G_{0.2}(10)$, whose adjacency matrix is also shown. The blue vertical lines denote the eigenvalues of A (zeros of $c_A(\lambda)$). All characteristic polynomials $c_{A_{\setminus\{n\}}}(\lambda)$ have the same sign at a zero of $c_A(\lambda)$, as follows from (10). (For interpretation of the colors in the figure(s), the reader is referred to the web version of this article.)

led to an effort to cluster and combine correlated graph metrics [22,23]. In practice, it is desirable to have a set of m graph or centrality metrics that are as uncorrelated as possible, while their number m is sufficient to characterize the graph well enough. Such a close-to-ideal set would enable to compare graphs and to construct design rules for networks that possess the desired properties, given by minimum or maximum values of the m graph metrics. For example, we can still not design "robust/resilient" networks in mathematically precise way, mainly because "robust/resilient" is hard to map to a set of m graph metrics.

Since both row vectors and column vectors (i.e. eigenvectors of the adjacency matrix A) of the orthogonal matrix X are orthogonal (thus independent), and span the N-dimensional space (thus are complete), one would expect that either the rows or columns of the matrix $\Xi = X \circ X$ forms an ideal set of centrality metrics. We have shown that $(x_k)_j^2$ can be regarded as a centrality metric. Section 6 indicates that the stochastic matrix Ξ of the adjacency matrix A of an undirected, possibly weighted graph possesses a zero eigenvalue, which implies for any adjacency matrix A that $\text{rank}(\Xi) < N$ and that at least one row (or column) in Ξ is a linear combination of all the other rows (columns). Hence, the set of centrality metrics $\{(\text{row}\,\Xi)_i\}_{1\leq i\leq N} = \left\{(x_1)_i^2, (x_2)_i^2, \ldots, (x_N)_i^2\right\}_{1\leq i\leq N}$ for each node i is *not* independent for the adjacency matrix, indicating that the set of centrality metrics belonging to node i can be written in terms of the centrality metrics of some other nodes in G. There are only $r_\Xi = \text{rank}(\Xi) \leq N-1$ independent row vectors, implying that only r_Ξ centrality vectors of nodes in the graph G have independent characteristics or properties. If $r_\Xi = N - j$ and if there exist $k \leq j$ different graphs with a different eigenvalue vector, but same orthogonal matrix X, then those k co-eigenvector graphs [8] would have precisely the same sets centrality metrics. Moreover, we know that the $\text{rank}(\Xi)$ can be small and that a graph can have several different orthogonal matrices X with different $\text{rank}(\Xi)$, e.g. in the complete graph as shown in [8]. These considerations question whether $\{(\text{row}\,\Xi)_i\}_{1\leq i\leq N}$ can be regarded as a close-to-ideal set of centrality metrics.

8. Summary

Several computations of eigenvector components $(x_k)_j$ of a symmetric matrix have been derived and compared. The elegant formula (6) for $(x_k)_j^2$, extended to higher multiplicity eigenvalues in Section 4, motivates to regard the set $\left\{(x_1)_j^2, (x_2)_j^2, \ldots, (x_N)_j^2\right\}$ as centrality metrics for node j. We have interpreted $(x_k)_j^2$ as an amplitude of a graph property of node j at eigenfrequency λ_k, which is still unsatisfactory, because graph property here is vague and humans desire a precise or physical meaning. So far, the challenge to understand the meaning of $(x_k)_j^2$ or $(x_k)_j$ for any graph has defeated us. Therefore, we would like to place that challenge on the agenda for further study. However, even if $(x_k)_j^2$ were physically understood, the study of the matrix $\Xi = X \circ X$, revealing that a graph G has only $r_\Xi = \text{rank}(\Xi) \leq N-1$ independent sets $\{(\text{row}\,\Xi)_i\}_{1\leq i\leq r_\Xi}$, questions whether the set $\left\{(x_1)_j^2, (x_2)_j^2, \ldots, (x_N)_j^2\right\}$ is suitable as a set of centrality metrics.

In summary, the challenge to find a “best possible” set of non-negative centrality or graph metrics is still an unsolved mathematical problem.

Declaration of competing interest

No conflict.

Data availability

No data was used for the research described in the article.

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Appendix A. Proofs of theorems

A.1. Proof of Theorem 1

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

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

where $(A-\lambda_k I)_{\backslash \text{ row } N}$ is the $(N-1)\times N$ matrix obtained from $(A-\lambda_k I)$ by removing row N. Cramer's solution [3, art. 220] yields

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

The j-th component of the k-th eigenvector x_k can be written as[9]

$$(x_k)_j = \alpha_m (k) (-1)^j \det (A-\lambda_k I)_{\backslash \text{ row } m \backslash \text{ col } j} \tag{34}$$

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

$$\alpha_m (k) = \frac{(-1)^m \beta_k}{\det (A-\lambda_k I)_{\text{row } m = b}} \tag{35}$$

Combining (34) with (35) for $m = j$ leads to (4).

We now impose the orthogonality equation $x_k^T x_k = 1$. It follows from (34) that

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

Invoking the identity

$$\begin{aligned} \left(\det \left(A_{\backslash \text{ row } m \backslash \text{ col } j} - \lambda I \right) \right)^2 &= \det \left(A_{\backslash \{m\}} - \lambda I \right) \det \left(A_{\backslash \{j\}} - \lambda I \right) \\ &\quad - \det \left(A_{\backslash \{m,j\}} - \lambda I \right) \det (A - \lambda I) \end{aligned} \tag{36}$$

which can be deduced from Jacobi's famous theorem of 1833 (see e.g. [24, p. 25]), yields

$$\begin{aligned} \alpha_m^{-2} (k) (x_k)_j^2 &= \lim_{\lambda \to \lambda_k} \det \left(A_{\backslash \{m\}} - \lambda I \right) \det \left(A_{\backslash \{j\}} - \lambda I \right) \\ &\quad - \det \left(A_{\backslash \{m,j\}} - \lambda I \right) \det (A - \lambda I) \\ &= \det \left(A_{\backslash \{m\}} - \lambda_k I \right) \det \left(A_{\backslash \{j\}} - \lambda_k I \right) \end{aligned} \tag{37}$$

[9] Remark that the adjacency matrix $A_{G\backslash \text{ row } m \backslash \text{ col } i}$ 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, $A_{G\backslash \text{ row } m \backslash \text{ col } i}$ is not necessarily symmetric and it has $|m-i|$ non-zero diagonal elements, $a_{k+1,k}$ for $m \leq k < i$.

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

$$\alpha_m^{-2}(k) = \det\left(A_{\setminus\{m\}} - \lambda_k I\right) \sum_{n=1}^{N} \det\left(A_{\setminus\{n\}} - \lambda_k I\right) \tag{38}$$

We observe that there is a degree of freedom via the choice of m. Thus, for $m = j$ in (34), we obtain from (37) and (38)

$$(x_k)_j^2 = \frac{\det\left(A_{\setminus\{j\}} - \lambda_k I\right)}{\sum_{n=1}^{N} \det\left(A_{\setminus\{n\}} - \lambda_k I\right)} \tag{39}$$

that is independent of the choice of the vector b. Since [25], [3, art. 213],

$$\sum_{n=1}^{N} \det\left(A_{\setminus\{n\}} - \lambda I\right) = -\frac{d}{d\lambda} \det(A - \lambda I) = -c'_A(\lambda) \tag{40}$$

we arrive at (6). Combining (4) and (6) yields[10] (5). □

A.2. Second proof of (6)

We start from the resolvent [3, art. 215, 262] of a symmetric matrix A

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

from which, using $c_A(\lambda) = \det(A - \lambda I) = \prod_{j=1}^{N} (\lambda_j - \lambda)$ and assuming that λ_k is simple,

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

Invoking (3) yields (6). □

A.3. Two proofs of Theorem 2

First Proof: The eigenvalue equation $Ax_k = \lambda_k x_k$ is equivalent to $(A - \lambda_k I) x_k = 0$, which is explicitly written as a set of linear equations

$$\sum_{j=1}^{N} (a_{rj} - \lambda_k \delta_{rj}) (x_k)_j = 0 \qquad \text{for } 1 \leq r \leq N$$

[10] We remark that taking the derivative of both sides of (5) with respect to b_m results in (4).

Since $\text{rank}(A - \lambda_k I) = N - 1$, we can delete an arbitrary equation or row, say i, in and obtain $(A - \lambda_k I)_{\backslash \text{row } i}\, x_k = 0$. The set $(A - \lambda_k I)_{\backslash \text{row } i}\, x_k = 0$, consisting of $N - 1$ linear equations in N unknowns, can be rewritten in terms of one unknown, the component $(x_k)_m = \eta$,

$$\sum_{j=1;j\neq m}^{N} (a_{rj} - \lambda_k \delta_{rj})\,(x_k)_j = -\,(a_{rm} - \lambda_k \delta_{rm})\,(x_k)_m \qquad \text{for } 1 \leq r \leq N \text{ and } r \neq i$$

and in matrix form,

$$(A - \lambda_k I)_{\backslash \text{row } i \backslash \text{col } m}\,(x_k)_{\backslash \text{row } m} = g$$

where the $(N-1) \times 1$ vector

$$g = -\eta \left[\, (a_{1m} - \lambda_k \delta_{1m}) \quad \cdots \quad \left(a_{(i-1)m} - \lambda_k \delta_{(i-1)m}\right) \quad \left(a_{(i+1)m} - \lambda_k \delta_{(i+1)m}\right) \quad \cdots \quad (a_{Nm} - \lambda_k \delta_{Nm}) \,\right]^T$$

The vector g simplifies most if we choose $i = m$, because then the vector g does not depend upon the eigenvalue λ_k anymore. With the choice $i = m$, we arrive at

$$(A - \lambda_k I)_{\backslash\{i\}}\,(x_k)_{\backslash \text{row } i} = -\eta \begin{bmatrix} a_{1i} & \cdots & a_{(i-1)i} & a_{(i+1)i} & \cdots & a_{Ni} \end{bmatrix}^T$$

Cramer's solution [3, art. 220] yields

$$\left((x_k)_{\backslash \text{row } i}\right)_q = \frac{\left|(A - \lambda_k I)_{\backslash\{i\}}\right|_{\text{col } q=g}}{\det\left(A_{\backslash\{i\}} - \lambda_k I\right)}$$

where the determinant $\left|(A - \lambda_k I)_{\backslash\{i\}}\right|_{\text{col } q=g}$ equals, denoting $b_{jj} = a_{jj} - \lambda_k$,

$$\begin{vmatrix}
b_{11} & \cdots & a_{1(i-1)} & a_{1(i+1)} & \cdots & a_{1(q-1)} & -\eta a_{1i} & a_{1(q+1)} & \cdots & a_{1N} \\
\vdots & \ddots & \vdots & \vdots & & \vdots & \vdots & \vdots & & \vdots \\
a_{(i-1)1} & \cdots & b_{(i-1)(i-1)} & \cdots & \cdots & a_{(i-1)(q-1)} & -\eta a_{(i-1)i} & a_{(i-1)(q+1)} & \cdots & a_{(i-1)N} \\
a_{(i+1)1} & \cdots & \cdots & b_{(i+1)(i+1)} & \cdots & a_{(i+1)(q-1)} & -\eta a_{(i+1)i} & a_{(i+1)(q+1)} & \cdots & a_{(i+1)N} \\
\vdots & & \vdots & \vdots & \ddots & \vdots & & \vdots & & \vdots \\
 & & & & \cdots & b_{(q-1)(q-1)} & -\eta a_{(q-1)i} & a_{(q-1)(q+1)} & \cdots & a_{(q-1)N} \\
 & & & & \cdots & a_{q(q-1)} & -\eta a_{qi} & a_{q(q+1)} & \cdots & a_{qN} \\
 & & & & \cdots & a_{(q+1)(q-1)} & -\eta a_{(q+1)i} & b_{(q+1)(q+1)} & \cdots & a_{(q+1)N} \\
 & & & & & \vdots & \vdots & \vdots & \ddots & \vdots \\
a_{N1} & \cdots & a_{N(i-1)} & a_{N(i+1)} & \cdots & a_{N(q-1)} & -\eta a_{Ni} & a_{N(q+1)} & \cdots & b_{NN}
\end{vmatrix}$$

Multiplying a row or column in a determinant by a same scalar is the same as multiplying the determinant by that scalar [3, p. 321] and $\left|(A - \lambda_k I)_{\backslash\{i\}}\right|_{\text{col } q=g} = -\eta \times$

$$\begin{vmatrix}
b_{11} & \cdots & a_{1(i-1)} & a_{1(i+1)} & \cdots & a_{1(q-1)} & a_{1i} & a_{1(q+1)} & \cdots & a_{1N} \\
\vdots & \ddots & \vdots & \vdots & & \vdots & \vdots & \vdots & & \vdots \\
a_{(i-1)1} & \cdots & b_{(i-1)(i-1)} & \cdots & \cdots & a_{(i-1)(q-1)} & a_{(i-1)i} & a_{(i-1)(q+1)} & \cdots & a_{(i-1)N} \\
a_{(i+1)1} & \cdots & \cdots & b_{(i+1)(i+1)} & \cdots & a_{(i+1)(q-1)} & a_{(i+1)i} & a_{(i+1)(q+1)} & \cdots & a_{(i+1)N} \\
\vdots & & \vdots & \vdots & \ddots & \vdots & & \vdots & & \vdots \\
 & & & & \cdots & b_{(q-1)(q-1)} & a_{(q-1)i} & a_{(q-1)(q+1)} & \cdots & a_{(q-1)N} \\
 & & & & \cdots & a_{q(q-1)} & a_{qi} & a_{q(q+1)} & \cdots & a_{qN} \\
 & & & & \cdots & a_{(q+1)(q-1)} & a_{(q+1)i} & b_{(q+1)(q+1)} & \cdots & a_{(q+1)N} \\
 & & & & & \vdots & \vdots & \vdots & \ddots & \vdots \\
a_{N1} & \cdots & a_{N(i-1)} & a_{N(i+1)} & \cdots & a_{N(q-1)} & a_{Ni} & a_{N(q+1)} & \cdots & b_{NN}
\end{vmatrix}$$

Thus, Cramer's solution becomes

$$\left((x_k)_{\setminus \text{row}\, i}\right)_q = -\eta \frac{\left|(A-\lambda_k I)_{\setminus\{i\}}\right|_{\text{col}\, q = \left(A_{\setminus \text{ row}\, i}\right)_{\text{col}\, i}}}{\det\left(A_{\setminus\{i\}} - \lambda_k I\right)}$$

After interchanging column q and column $q-1$, then column $q-1$ and column $q-2$, then column $q-2$ and column $q-3$, and so on until the l-th interchange where $q-l=i$, then column q, that contains the vector $a_i = A_{\text{col}\, i}$, is placed on column i, while column $q-1$ is placed on column q. After $l = q-i$ interchanges of columns, $\left|(A-\lambda_k I)_{\setminus\{i\}}\right|_{\text{col}\, q = \left(A_{\setminus \text{ row}\, i}\right)_{\text{col}\, i}}$ becomes

$$\begin{vmatrix}
b_{11} & \cdots & a_{1(i-1)} & a_{1i} & a_{1(i+1)} & \cdots & a_{1(q-1)} & a_{1(q+1)} & \cdots & a_{1N} \\
\vdots & \ddots & \vdots & \vdots & \vdots & & \vdots & \vdots & & \vdots \\
a_{(i-1)1} & \cdots & b_{(i-1)(i-1)} & a_{(i-1)i} & \cdots & \cdots & a_{(i-1)(q-1)} & a_{(i-1)(q+1)} & \cdots & a_{(i-1)N} \\
a_{(i+1)1} & \cdots & \cdots & a_{(i+1)i} & b_{(i+1)(i+1)} & \cdots & a_{(i+1)(q-1)} & a_{(i+1)(q+1)} & \cdots & a_{(i+1)N} \\
\vdots & & \vdots & & \vdots & \ddots & \vdots & \vdots & & \vdots \\
 & & & a_{(q-1)i} & & \cdots & b_{(q-1)(q-1)} & a_{(q-1)(q+1)} & \cdots & a_{(q-1)N} \\
 & & & a_{qi} & & \cdots & a_{q(q-1)} & a_{q(q+1)} & \cdots & a_{qN} \\
 & & & a_{(q+1)i} & & \cdots & a_{(q+1)(q-1)} & b_{(q+1)(q+1)} & \cdots & a_{(q+1)N} \\
 & & & \vdots & & & \vdots & \vdots & \ddots & \vdots \\
a_{N1} & \cdots & a_{N(i-1)} & a_{Ni} & a_{N(i+1)} & \cdots & a_{N(q-1)} & a_{N(q+1)} & \cdots & b_{NN}
\end{vmatrix}$$

but this determinant is difficult to evaluate, because not all elements $b_{jj} = a_{jj} - \lambda_k$ are on the diagonal. Thus, it is instructive to choose i equal to N. If $i = N$, then we observe that

$$\left|(A-\lambda_k I)_{\setminus\{N\}}\right|_{\text{col}\, q = \left(A_{\setminus \text{ row}\, N}\right)_{\text{col}\, N}} = -\eta\,(-1)^{q-N} \det\left((A-\lambda_k I)_{\setminus \text{ row}\, N \setminus \text{ col}\, q}\right)$$

Hence, Cramer's solution simplifies to

$$\left((x_k)_{\setminus \text{row}\, N}\right)_q = -\eta\,(-1)^{q-N}\, \frac{\det\left((A-\lambda_k I)_{\setminus \text{ row}\, N \setminus \text{ col}\, q}\right)}{\det\left(A_{\setminus\{N\}} - \lambda_k I\right)}$$

Normalization $x_k^T x_k = 1$ then yields

$$1 = \eta^2 + \sum_{q=1}^{N-1} \left((x_k)_{\setminus \text{row } N} \right)_q^2 = \eta^2 \left(1 + \sum_{q=1}^{N-1} \frac{\det^2 \left((A - \lambda_k I)_{\setminus \text{row } N \setminus \text{col } q} \right)}{\det^2 \left(A_{\setminus\{N\}} - \lambda_k I \right)} \right)$$

so that

$$\eta^2 = \frac{\det^2 \left(A_{\setminus\{N\}} - \lambda_k I \right)}{\sum_{q=1}^{N} \det^2 \left((A - \lambda_k I)_{\setminus \text{row } N \setminus \text{col } q} \right)}$$

After choosing the minus sign in $\eta = \frac{-\left(A_{\setminus\{N\}} - \lambda_k I\right)}{\sqrt{\sum_{q=1}^{N} \det^2\left((A-\lambda_k I)_{\setminus \text{row } N \setminus \text{col } q}\right)}}$, the entire eigenvector x_k becomes, for all $1 \leq q \leq N$,

$$(x_k)_q = (-1)^{q-N} \frac{\det \left((A - \lambda_k I)_{\setminus \text{row } N \setminus \text{col } q} \right)}{\sqrt{\sum_{j=1}^{N} \det^2 \left((A - \lambda_k I)_{\setminus \text{row } N \setminus \text{col } j} \right)}}$$

But the choice of N was arbitrary. Hence, the above holds for any node m instead of just node N. After replacing q by j, we arrive at (7).

Jacobi's identity (36) reduces for eigenvalues $\lambda = \lambda_k$ to

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

which we apply the denominator in (7)

$$\sum_{l=1}^{N} \left(\det (A - \lambda_k I)_{\setminus \text{row } m \setminus \text{col } l} \right)^2 = \det \left(A_{\setminus\{m\}} - \lambda_k I \right) \sum_{l=1}^{N} \det \left(A_{\setminus\{l\}} - \lambda_k I \right) \tag{41}$$

With $\sum_{l=1}^{N} \det \left(A_{\setminus\{l\}} - \lambda I \right) = -c_A' (\lambda)$ in (40), we obtain (8). After squaring (8) and again using Jacobi's identity (36) for $\lambda = \lambda_k$, we obtain (6).

Second proof: We derive Theorem 2 from Theorem 1. After expanding $\det(A - \lambda_k I)_{\text{row } j=b}$ along row j,

$$\det (A - \lambda_k I)_{\text{row } j=b} = \sum_{n=1}^{N} b_n (-1)^{j-n} \det (A - \lambda_k I)_{\setminus \text{row } j \setminus \text{col } n} \tag{42}$$

and rewriting (4) with $\beta_k = \sum_{j=1}^{N} b_j (x_k)_j$

$$(x_k)_j \det (A - \lambda_k I)_{\text{row } j=b} = \beta_k \det \left(A_{\setminus\{j\}} - \lambda_k I \right) = \det \left(A_{\setminus\{j\}} - \lambda_k I \right) \sum_{n=1}^{N} b_n (x_k)_n$$

yields

$$(x_k)_j \sum_{n=1}^{N} b_n (-1)^{j-n} \det (A - \lambda_k I)_{\backslash \text{row } j \backslash \text{col } n} = \det \left(A_{\backslash\{j\}} - \lambda_k I\right) \sum_{n=1}^{N} b_n (x_k)_n$$

which holds for any vector b. Equating corresponding components b_n leads, for all $1 \leq n \leq N$, to

$$(x_k)_n = (x_k)_j \frac{(-1)^{j-n} \det (A - \lambda_k I)_{\backslash \text{row } j \backslash \text{col } n}}{\det \left(A_{\backslash\{j\}} - \lambda_k I\right)} \tag{43}$$

Normalization $x_k^T x_k = 1$ shows that

$$1 = \sum_{n=1}^{N} (x_k)_n^2 = \frac{(x_k)_j^2}{\det^2 \left(A_{\backslash\{j\}} - \lambda_k I\right)} \sum_{n=1}^{N} \left(\det (A - \lambda_k I)_{\backslash \text{row } j \backslash \text{col } n}\right)^2$$

and

$$(x_k)_j^2 = \frac{\det^2 \left(A_{\backslash\{j\}} - \lambda_k I\right)}{\sum_{n=1}^{N} \left(\det (A - \lambda_k I)_{\backslash \text{row } j \backslash \text{col } n}\right)^2}$$

which equals (6), after substituting (41). Taking the (positive) squareroot and substituting into (43) results in

$$(x_k)_n = \frac{(-1)^{j-n} \det (A - \lambda_k I)_{\backslash \text{row } j \backslash \text{col } n}}{\sqrt{\sum_{n=1}^{N} \left(\det (A - \lambda_k I)_{\backslash \text{row } j \backslash \text{col } n}\right)^2}}$$

which equals (7) and proves Theorem 2. □

Appendix B. Operator form of the eigenvalue equation

Let x_k be an eigenvector of an $N \times N$ matrix A belonging to the eigenvalue λ_k, then the eigenvalue equation $Ax_k = \lambda_k x_k$ is written as

$$Ax_k = \lambda_j x_k + (\lambda_k - \lambda_j) x_k$$

where the eigenvalue λ_j is possibly another eigenvalue of the matrix A. Clearly, if $\lambda_k = \lambda_j$, then the last term vanishes and we return to the original eigenvalue equation. In summary, it holds for any pair of integers k and j with $1 \leq k, j \leq N$ that

$$(A - \lambda_j I) x_k = (\lambda_k - \lambda_j) x_k \tag{44}$$

Multiplying both sides by $(A - \lambda_m I)$,

$$(A - \lambda_m I)(A - \lambda_j I) x_k = (\lambda_k - \lambda_j)(A - \lambda_m I) x_k$$

invoking (44) at the right-hand side

$$(A - \lambda_m I)(A - \lambda_j I) x_k = (\lambda_k - \lambda_j)(\lambda_k - \lambda_m) x_k$$

yields, after iteration for any positive integer n,

$$\prod_{j=1}^{n} (A - \lambda_j I) x_k = \prod_{j=1}^{n} (\lambda_k - \lambda_j) x_k \tag{45}$$

If $n = N$, the dimension of the matrix A, the index j in the right-hand side product runs of over all eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_N$ of the matrix A and the product thus also contains the factor where $\lambda_j = \lambda_k$ leading to $\prod_{j=1}^{N} (A - \lambda_j I) x_k = 0$. Since any eigenvector must be different from the zero vector, we conclude that the matrix $\prod_{j=1}^{N} (A - \lambda_j I) = c_A(A) = O$, which is nothing else than the famous Caley-Hamilton theorem.

B.1. *The matrix product* $\prod_{j=1}^{n} (A - \lambda_j I)$

The construction that led to (45) indicates that all matrices in the product commute. Commutativity allows us to treat the real matrix A as ordinary real numbers. For example, for $n = 2$ and $n = 3$, we obtain

$$\begin{aligned}
\prod_{j=1}^{2} (A - \lambda_j I) &= (A - \lambda_1 I)(A - \lambda_2 I) = A^2 - (\lambda_1 + \lambda_2) A + \lambda_1 \lambda_2 \\
\prod_{j=1}^{3} (A - \lambda_j I) &= (A - \lambda_3 I) \prod_{j=1}^{2} (A - \lambda_j I) = (A - \lambda_3 I)\left(A^2 - (\lambda_1 + \lambda_2) A + \lambda_1 \lambda_2\right) \\
&= A^3 - (\lambda_1 + \lambda_2 + \lambda_3) A^2 + (\lambda_1\lambda_2 + \lambda_1\lambda_3 + \lambda_2\lambda_3) A - \lambda_1\lambda_2\lambda_3
\end{aligned}$$

Continuing to higher values of n eventually will lead to Vieta's theorem, where the coefficients of powers of A are elementary symmetrical polynomials [3, art. 296-297]. If $n = N$, then the definition of the characteristic polynomial (1) indicates that $\prod_{j=1}^{N} (A - \lambda_j I) = (-1)^N \sum_{k=0}^{N} c_k A^k$, which vanishes as shown above.

Substitution of the eigenvector expansion of the symmetric matrix $A = \sum_{k=0}^{N} \lambda_k x_k x_k^T$,

$$A - \lambda_j I = \sum_{k=1}^{N} \lambda_k x_k x_k^T - \lambda_j \sum_{k=1}^{N} x_k x_k^T = \sum_{k=1;k\neq j}^{N} \lambda_k x_k x_k^T$$

shows that the matrix $A - \lambda_j I$ transforms an $N \times 1$ vector y to the vector $(A - \lambda_j I) y = \sum_{k=1;k\neq j}^{N} \lambda_k \left(x_k^T y\right) x_k$ with zero coordinate along the x_j-vector. In other words, the matrix $\prod_{j=1}^{n} (A - \lambda_j I)$ projects a vector y into the $N - n$-dimensional Euclidean subspace that is orthogonal to the subspace spanned by the eigenvectors

$\{x_1, x_2, \ldots, x_n\}$. In the eigenvector coordinate axis frame, the coordinates of the vector y are $\left(y^T x_1, y^T x_2, \ldots, y^T x_N\right)$, while the coordinates of the vector $\prod_{j=1}^{n} (A - \lambda_j I)\, y$ contain n zeros in the first n positions.

B.2. Eigenvalue λ_k with multiplicity $m_k = 1$

If λ_k is single or simple or an eigenvalue with multiplicity one, then it follows from (45) that

$$\prod_{j=1;j\neq k}^{N} (A - \lambda_j I)\, x_k = \prod_{j=1;j\neq k}^{N} (\lambda_k - \lambda_j)\, x_k$$

which we can write in terms of the characteristic polynomials $c_A(\lambda)$ in (3) as[11]

$$x_k = \frac{(-1)^N}{c_A'(\lambda_k)} \prod_{j=1;j\neq k}^{N} (A - \lambda_j I)\, x_k = \frac{1}{-c_A'(\lambda_k)} \prod_{j=1;j\neq k}^{N} (\lambda_j I - A)\, x_k$$

In order to define an eigenvector uniquely, we impose the normalization condition $x_k^T x_k = 1$. Applied to $x_k = \frac{(-1)^N}{c_A'(\lambda_k)} \prod_{j=1;j\neq k}^{N} (A - \lambda_j I)\, x_k$ and using the symmetry of A yields

$$x_k^T x_k = x_k^T \left(\frac{(-1)^N}{c_A'(\lambda_k)} \prod_{j=1;j\neq k}^{N} (A - \lambda_j I) \right)^2 x_k = 1$$

We define the matrix $U_k = \left(\frac{(-1)^N}{c_A'(\lambda_k)} \prod_{j=1;j\neq k}^{N} (A - \lambda_j I) \right)^2$, written in the eigenspace of the matrix A as $U_k = \sum_{l=1}^{N} \beta_l x_l x_l^T$. The matrix U_k must obey $x_k^T U_k x_k = 1$, implying by the orthogonality of eigenvectors $x_k^T x_m = \delta_{km}$ that $\beta_k = 1$, but all other coefficients β_l can be chosen at will. The simplest choice is $\beta_l = \delta_{lk}$ and $U_k = x_k x_k^T$. Since $U_k^2 = x_k x_k^T x_k x_k^T = U_k$, we find for a simple eigenvalue λ_k that

$$x_k x_k^T = \frac{(-1)^N}{c_A'(\lambda_k)} \prod_{j=1;j\neq k}^{N} (A - \lambda_j I)$$

which equals (14), but differently proved than in [3, art. 234].

B.3. Eigenvalue λ_k with multiplicity $m_k > 1$

The spectral decomposition is generally more complicated if eigenvalues have a multiplicity larger than one. If the eigenvalue λ_k of a symmetric matrix A has multiplicity

[11] Caley-Hamilton's relation $\prod_{j=1}^{N} (A - \lambda_j I)\, x_k = 0$, written as

$$(A - \lambda_k I) \left\{ \prod_{j=1;j\neq k}^{N} (A - \lambda_j I)\, x_k \right\} = 0$$

show, by comparing with (44), that $x_k = \alpha \prod_{j=1;j\neq k}^{N} (A - \lambda_j I)\, x_k$ for each non-zero α.

$m_k > 1$, then more than one eigenvector x_κ with $\kappa = k, k+1, \ldots, k+m_k-1$ is associated to that same eigenvalue λ_k, obeying the eigenvalue equation $Ax_\kappa = \lambda_k x_\kappa$. For example, if $m_k = 2$ and $\lambda_k = \lambda_{k+1}$, then the two orthogonal eigenvectors x_k and x_{k+1} satisfy $Ax_k = \lambda_k x_k$ and $Ax_{k+1} = \lambda_k x_{k+1}$, which implies that any linear combination $y_k = \alpha_1 x_k + \alpha_2 x_{k+1}$ also satisfies the eigenvalue equation $Ay_k = \lambda_k y_k$. Generally, if the eigenvalue λ_k of a symmetric matrix A has multiplicity $m_k > 1$, then any linear combination vector $y_k = \sum_{\kappa=k}^{k+m_k-1} \alpha_\kappa x_\kappa$ is also an eigenvector. Thus, the eigenspace belonging to eigenvalue λ_k has dimension m_k and is spanned by the orthogonal vectors x_κ with $\kappa = k, k+1, \ldots, k+m_k-1$. That ensemble $\{x_\kappa\}_{\kappa=k,k+1,\ldots,k+m_k-1}$ of eigenvectors belonging to the same eigenvalue λ_k acts as a whole and, as we will see, appears together in formulae. Clearly, if the multiplicity is $m_k = 1$, then the eigenspace of dimension one is a line.

If λ_k has multiplicity $m_k > 1$ implying that $\lambda_k = \lambda_{k+1} = \cdots = \lambda_{k+m_k-1}$, then (45) shows that

$$x_\kappa = \frac{\prod_{j=1;j\neq\{k,k+1,\ldots,k+m_k-1\}}^{N} (A - \lambda_j I)\, x_\kappa}{\prod_{j=1;;j\neq\{k,k+1,\ldots,k+m_k-1\}}^{N} (\lambda_k - \lambda_j)} \text{ for } \kappa = k, k+1, \ldots, k+m_k-1$$

where x_κ for $k \leq \kappa \leq k+m_k-1$ is the set of m_k eigenvectors all belonging to the same eigenvalue λ_k. The characteristic polynomial (1) becomes $c_A(\lambda) = (\lambda_k - \lambda)^{m_k} \prod_{j=1;j\neq\{k,k+1,\ldots,k+m_k-1\}}^{N} (\lambda_j - \lambda)$, whose n-th derivative, given by Cauchy's contour integral [26], is

$$\left.\frac{1}{n!} \frac{d^n c_A(\lambda)}{d\lambda^n}\right|_{\lambda=x} = \frac{1}{2\pi i} \int_{C(x)} \frac{c_A(w)}{(w-x)^{n+1}} dw$$

where the closed contour in the complex w-plane encloses the point x. Choosing $x = \lambda_k$,

$$\begin{aligned}\left.\frac{1}{n!} \frac{d^n c_A(\lambda)}{d\lambda^n}\right|_{\lambda=\lambda_k} &= \frac{(-1)^{m_k}}{2\pi i} \int_{C(\lambda_k)} \frac{\prod_{j=1;j\neq\{k,k+1,\ldots,k+m_k-1\}}^{N} (\lambda_j - w)}{(w-\lambda_k)^{n-m_k+1}} dw \\ &= (-1)^{m_k} \frac{1}{(n-m_k)!} \frac{d^{n-m_k}}{d\lambda^{n-m_k}} \left.\prod_{j=1;j\neq\{k,k+1,\ldots,k+m_k-1\}}^{N} (\lambda_j - w)\right|_{\lambda=\lambda_k}\end{aligned}$$

indicates for $n = m_k$ that

$$\prod_{j=1;j\neq\{k,k+1,\ldots,k+m_k-1\}}^{N} (\lambda_k - \lambda_j) = \left.\frac{(-1)^N}{(m_k)!} \frac{d^{m_k} c_A(\lambda)}{d\lambda^{m_k}}\right|_{\lambda=\lambda_k}$$

which is an alternative form of (21). For $n < m_k$, the contour $C(\lambda_k)$ encloses an analytic region of the integrand and Cauchy's integral theorem [26] states that $\left.\frac{1}{n!} \frac{d^n c_A(\lambda)}{d\lambda^n}\right|_{\lambda=\lambda_k} = 0$ for $n < m_k$.

Similarly as in Section B.2, we define the matrix

$$U_\kappa = \left(\frac{(-1)^N (m_k)!}{\left.\frac{d^{m_k} c_A(\lambda)}{d\lambda^{m_k}}\right|_{\lambda=\lambda_k}} \prod_{j=1;j\neq\{k,k+1,\ldots,k+m_k-1\}}^N (A - \lambda_j I) \right)^2$$

and the normalization $x_\kappa^T x_\kappa = 1$, for $\kappa = k, k+1, \ldots, k+m_k-1$, requires that $x_\kappa^T U_\kappa x_\kappa = 1$ for $k, k+1, \ldots, k+m_k-1$, which leads to

$$U_\kappa = \sum_{\kappa=k}^{m_k-1} x_\kappa x_\kappa^T$$

Since $U_\kappa^2 = \sum_{\kappa=k}^{m_k-1} \sum_{l=k}^{m_k-1} x_\kappa \left(x_\kappa^T x_l \right) x_l^T = \sum_{\kappa=k}^{m_k-1} x_\kappa x_\kappa^T = U_\kappa$ by orthogonality $x_\kappa^T x_l = \delta_{\kappa l}$, we arrive at

$$\sum_{\kappa=k}^{m_k-1} x_\kappa x_\kappa^T = \frac{(-1)^N (m_k)!}{\left.\frac{d^{m_k} c_A(\lambda)}{d\lambda^{m_k}}\right|_{\lambda=\lambda_k}} \prod_{j=1;j\neq\{k,k+1,\ldots,k+m_k-1\}}^N (A - \lambda_j I) \tag{46}$$

Taking the j-th diagonal element of (46) leads to (19) in Theorem 3.

B.4. Proof of (22) and (23) in Theorem 3

We extend the proof in Appendix A.2. If the eigenvalue λ_k has multiplicity m_k and $\lambda_k = \lambda_{k+1} = \cdots = \lambda_{k+m_k-1}$, then the resolvent is

$$\frac{\det\left(A_{\backslash\{j\}} - zI\right)}{\det(A - zI)} = \sum_{m=k-1}^{N} \frac{(x_m)_j^2}{\lambda_m - z} + \frac{\sum_{\kappa=k}^{k+m_k-1} (x_\kappa)_j^2}{(\lambda_k - z)} + \sum_{m=k+m_k}^{N} \frac{(x_m)_j^2}{\lambda_m - z}$$

from which we deduce that

$$\sum_{\kappa=k}^{k+m_k-1} (x_\kappa)_j^2 = \lim_{z\to\lambda_k} \frac{(\lambda_k - z)\det\left(A_{\backslash\{j\}} - zI\right)}{\det(A - zI)}$$

With $\det(A - zI) = (\lambda_k - z)^{m_k} \prod_{j=1;j\neq\{k,k+1,\ldots,k+m_k-1\}}^N (\lambda_j - z)$, it holds that

$$\begin{aligned}
\sum_{\kappa=k}^{k+m_k-1} (x_\kappa)_j^2 &= \lim_{z\to\lambda_k} \frac{(\lambda_k - z)^{1-m_k} \det\left(A_{\backslash\{j\}} - zI\right)}{\prod_{j=1;j\neq\{k,k+1,\ldots,k+m_k-1\}}^N (\lambda_j - z)} \\
&= \frac{1}{\prod_{j=1;j\neq\{k,k+1,\ldots,k+m_k-1\}}^N (\lambda_j - \lambda_k)} \lim_{z\to\lambda_k} \frac{\det\left(A_{\backslash\{j\}} - zI\right)}{(\lambda_k - z)^{m_k-1}}
\end{aligned}$$

The Interlacing Theorem [3, art. 263] shows that the polynomial $\det\left(A_{\backslash\{j\}} - zI\right)$ has a zero at λ_k of multiplicity $m_k - 1$, which means, by the de l'Hospital's rule [27, art. 154] that $m_k - 1$ differentiations in numerator and denominator lead to a finite value of the limit. In other words,

$$\lim_{z\to\lambda_k} \frac{\det\left(A_{\backslash\{j\}} - zI\right)}{\left(\lambda_k - z\right)^{m_k-1}} = \lim_{z\to\lambda_k} \frac{\frac{d^{m_k-1}}{dz^{m_k-1}}\det\left(A_{\backslash\{j\}} - zI\right)}{\frac{d^{m_k-1}}{dz^{m_k-1}}\left(\lambda_k - z\right)^{m_k-1}}$$
$$= \frac{1}{(m_k-1)!}\frac{d^{m_k-1}}{dz^{m_k-1}}\det\left(A_{\backslash\{j\}} - zI\right)\Big|_{z=\lambda_k}$$

where $\frac{d^k z^b}{dz^k} = \frac{b!}{(b-k)!}z^{b-k}$, valid for any complex b by replacing $b! = \Gamma(b+1)$, has been used. It remains to iteratively invoke the formula (40) for the derivative of a determinant, $\frac{d}{d\lambda}\det(A - \lambda I) = -\sum_{n=1}^{N}\det\left(A_{\backslash\{n\}} - \lambda I\right)$. We thus find the sequence

$$\frac{d}{dz}\det\left(A_{\backslash\{j\}} - zI\right) = -\sum_{n_1=1}^{N-1}\det\left(A_{\backslash\{j,n_1\}} - zI\right)$$
$$\frac{d^2}{dz^2}\det\left(A_{\backslash\{j\}} - zI\right) = -\sum_{n_1=1}^{N-1}\frac{d}{dz}\det\left(A_{\backslash\{j,n_1\}} - zI\right) = \sum_{n=1}^{N-1}\sum_{n_2=1}^{N-2}\det\left(A_{\backslash\{j,n_1,n_2\}} - zI\right)$$

and, iterating further to an integer m,

$$\frac{d^m}{dz^m}\det\left(A_{\backslash\{j\}} - zI\right) = (-1)^m\sum_{n=1}^{N-1}\sum_{n_2=1}^{N-2}\cdots\sum_{n_m=1}^{N-m}\det\left(A_{\backslash\{j,n_1,n_2,\dots,n_m\}} - zI\right)$$

Applied for $m = m_k - 1$ gives

$$\lim_{z\to\lambda_k}\frac{\det\left(A_{\backslash\{j\}} - zI\right)}{\left(\lambda_k - z\right)^{m_k-1}} = \frac{(-1)^{m_k-1}}{(m_k-1)!}\sum_{n=1}^{N-1}\sum_{n_2=1}^{N-2}\cdots\sum_{n_{m_k-1}=1}^{N-m_k-1}\det\left(A_{\backslash\{j,n_1,n_2,\dots,n_{m_k-1}\}} - \lambda_k I\right)$$

Combining all, finally leads to (22). Substituting (21) in (22) gives (23).

Appendix C. Extension first proof of Theorem 2 to multiplicity $m_k = 2$

The eigenvalue equation $Ax_k = \lambda_k x_k$ is equivalent to $(A - \lambda_k I)x_k = 0$, which is explicitly written as a set of linear equations

$$\sum_{j=1}^{N}\left(a_{rj} - \lambda_k\delta_{rj}\right)\left(x_k\right)_j = 0 \qquad \text{for } 1 \le r \le N$$

If the multiplicity of the eigenvalue λ_k is $m_k = 2$, then $\text{rank}(A - \lambda_k I) = N - 2$, we can delete two arbitrary equations or rows. We choose row $N - 1$ and row N (inspired by the computations in Section A.3). Since there are now two eigenvectors x_k and x_{k+1} belonging to the eigenvalue λ_k, we obtain $(A-\lambda_k I)_{\backslash \text{row } N-1,N}\, y = 0$ satisfied for both eigenvectors $y = x_k$ and $y = x_{k+1}$. The set $(A-\lambda_k I)_{\text{row } N-1,N}\, y = 0$, consisting of $N-2$ linear equations in N unknowns, can be rewritten in terms of two unknowns, the components $y_{N-1} = \eta$ and $y_N = \zeta$,

$$\begin{aligned}
&\sum_{j=1}^{N-2} \left(a_{rj} - \lambda_k \delta_{rj}\right) y_j \\
&\quad = -\left(a_{r,N-1} - \lambda_k \delta_{r,N-1}\right) y_{N-1} - \left(a_{rN} - \lambda_k \delta_{rN}\right) y_N \qquad \text{for } 1 \leq r \leq N-2 \\
&\quad = -a_{r,N-1} y_{N-1} - a_{rN} y_N
\end{aligned}$$

and in matrix form,

$$\left(A_{\backslash\{N-1,N\}} - \lambda_k I\right) y_{\backslash \text{row } N-1,N} = g$$

where the $(N-2)\times 1$ vector

$$g = -\eta \begin{bmatrix} a_{1N-1} & \cdots & a_{N-2,N-1} \end{bmatrix}^T - \zeta \begin{bmatrix} a_{1N} & \cdots & a_{N-2,N} \end{bmatrix}^T$$

Cramer's solution [3, art. 220] yields for $1 \leq q \leq N-2$,

$$y_q = \frac{\left|(A-\lambda_k I)_{\backslash\{N-1,N\}}\right|_{\text{col } q = g}}{\det\left(A_{\backslash\{N-1,N\}} - \lambda_k I\right)}$$

where the determinant $\left|(A-\lambda_k I)_{\backslash\{N-1,N\}}\right|_{\text{col } q=g}$ is split-up into two determinants (similarly to Section A.3). Thus, Cramer's solution becomes

$$\begin{aligned}
y_q = &-\eta \frac{\left|(A-\lambda_k I)_{\backslash\{N-1,N\}}\right|_{\text{col } q = \left(A_{\backslash \text{row}\{N-1,N\}}\right)_{\text{col } N-1}}}{\det\left(A_{\backslash\{N-1,N\}} - \lambda_k I\right)} \\
&- \zeta \frac{\left|(A-\lambda_k I)_{\backslash\{N-1,N\}}\right|_{\text{col } q = \left(A_{\backslash \text{row}\{N-1,N\}}\right)_{\text{col } N}}}{\det\left(A_{\backslash\{N-1,N\}} - \lambda_k I\right)}
\end{aligned}$$

After interchanging column q iteratively (precisely as in Section A.3) to the last column $N-2$, we obtain

$$y_q = -\eta \frac{(-1)^{q-N-1} \det\left((A-\lambda_k I)_{\backslash \text{row } N-1,N \backslash \text{col } q,N}\right)}{\det\left(A_{\backslash\{N-1,N\}} - \lambda_k I\right)}$$

$$
\begin{aligned}
&- \zeta \frac{(-1)^{q-N-1} \det\left((A - \lambda_k I)_{\backslash \text{row } N-1, N \backslash \text{col } q, N-1} \right)}{\det\left(A_{\backslash\{N-1,N\}} - \lambda_k I \right)} \\
&= \eta \frac{(-1)^{q-N} \det\left(\left(A_{\backslash\{N\}} - \lambda_k I \right)_{\backslash \text{row } N-1 \backslash \text{col } q} \right)}{\det\left(A_{\backslash\{N-1,N\}} - \lambda_k I \right)} \\
&+ \zeta \frac{(-1)^{q-N} \det\left(\left(A_{\backslash\{N-1\}} - \lambda_k I \right)_{\backslash \text{row } N \backslash \text{col } q} \right)}{\det\left(A_{\backslash\{N-1,N\}} - \lambda_k I \right)}
\end{aligned}
$$

Hence, for the eigenvector x_k, we find, for $1 \le q \le N-2$

$$
\begin{aligned}
(-1)^{q-N} (x_k)_q = \eta & \frac{\det\left(\left(A_{\backslash\{N\}} - \lambda_k I \right)_{\backslash \text{row } N-1 \backslash \text{col } q} \right)}{\det\left(A_{\backslash\{N-1,N\}} - \lambda_k I \right)} \\
& + \zeta \frac{\det\left(\left(A_{\backslash\{N-1\}} - \lambda_k I \right)_{\backslash \text{row } N \backslash \text{col } q} \right)}{\det\left(A_{\backslash\{N-1,N\}} - \lambda_k I \right)}
\end{aligned}
$$

and, similarly for the eigenvector x_{k+1},

$$
\begin{aligned}
(-1)^{q-N} (x_{k+1})_q = \xi & \frac{\det\left(\left(A_{\backslash\{N\}} - \lambda_k I \right)_{\backslash \text{row } N-1 \backslash \text{col } q} \right)}{\det\left(A_{\backslash\{N-1,N\}} - \lambda_k I \right)} \\
& + \theta \frac{\det\left(\left(A_{\backslash\{N-1\}} - \lambda_k I \right)_{\backslash \text{row } N \backslash \text{col } q} \right)}{\det\left(A_{\backslash\{N-1,N\}} - \lambda_k I \right)}
\end{aligned}
$$

where the unknown eigenvector components $(x_k)_{N-1} = \eta$, $(x_{k+1})_{N-1} = \xi$, $(x_k)_N = \zeta$ and $(x_{k+1})_N = \theta$ are arbitrary real numbers.

C.1. Orthogonalization conditions

The three normalization conditions

$$
x_k^T x_k = 1 \quad x_{k+1}^T x_{k+1} = 1 \quad x_k^T x_{k+1} = 0
$$

will specify three of the unknowns, leaving one of them open to choice. First, $x_k^T x_k = 1$ then yields

$$
\begin{aligned}
1 &= \eta^2 + \zeta^2 + \sum_{q=1}^{N-2} (x_k)_q^2 \\
&= \eta^2 + \zeta^2
\end{aligned}
$$

$$+\sum_{q=1}^{N-2}\frac{\left(\eta\det\left(\left(A_{\backslash\{N\}}-\lambda_k I\right)_{\backslash\text{ row }N-1\backslash\text{ col }q}\right)+\zeta\det\left(\left(A_{\backslash\{N-1\}}-\lambda_k I\right)_{\backslash\text{ row }N\backslash\text{ col }q}\right)\right)^2}{\det^2\left(A_{\backslash\{N-1,N\}}-\lambda_k I\right)}$$

$$=\eta^2+\zeta^2+\eta^2\sum_{q=1}^{N-2}\frac{\det^2\left(\left(A_{\backslash\{N\}}-\lambda_k I\right)_{\backslash\text{ row }N-1\backslash\text{ col }q}\right)}{\det^2\left(A_{\backslash\{N-1,N\}}-\lambda_k I\right)}$$

$$+\zeta^2\sum_{q=1}^{N-1}\frac{\det^2\left(\left(A_{\backslash\{N-1\}}-\lambda_k I\right)_{\backslash\text{ row }N\backslash\text{ col }q}\right)}{\det^2\left(A_{\backslash\{N-1,N\}}-\lambda_k I\right)}$$

$$+2\eta\zeta\sum_{q=1}^{N-1}\frac{\det\left(\left(A_{\backslash\{N\}}-\lambda_k I\right)_{\backslash\text{ row }N-1\backslash\text{ col }q}\right)\det\left(\left(A_{\backslash\{N-1\}}-\lambda_k I\right)_{\backslash\text{ row }N\backslash\text{ col }q}\right)}{\det^2\left(A_{\backslash\{N-1,N\}}-\lambda_k I\right)}$$

With $S=1+\sum_{q=1}^{N-2}\frac{\det^2\left(\left(A_{\backslash\{N\}}-\lambda_k I\right)_{\backslash\text{ row }N-1\backslash\text{ col }q}\right)}{\det^2\left(A_{\backslash\{N-1,N\}}-\lambda_k I\right)}$,
$R=1+\sum_{q=1}^{N-2}\frac{\det^2\left(\left(A_{\backslash\{N-1\}}-\lambda_k I\right)_{\backslash\text{ row }N\backslash\text{ col }q}\right)}{\det^2\left(A_{\backslash\{N-1,N\}}-\lambda_k I\right)}$ and
$V=\sum_{q=1}^{N-2}\frac{\det\left(\left(A_{\backslash\{N\}}-\lambda_k I\right)_{\backslash\text{ row }N-1\backslash\text{ col }q}\right)\det\left(\left(A_{\backslash\{N-1\}}-\lambda_k I\right)_{\backslash\text{ row }N\backslash\text{ col }q}\right)}{\det^2\left(A_{\backslash\{N-1,N\}}-\lambda_k I\right)}$, the condition $x_k^T x_k$ $=1$ becomes

$$1=\eta^2 S+\zeta^2 R+2\eta\zeta V$$

Similarly, the condition $x_{k+1}^T x_{k+1}=1$ leads to

$$1=\xi^2 S+\theta^2 R+2\xi\theta V$$

The final orthogonality condition $x_k^T x_{k+1}$ is

$$0=\sum_{q=1}^{N}\left(x_k\right)_q\left(x_{k+1}\right)_q=\eta\xi+\zeta\theta+\sum_{q=1}^{N-2}\left(x_k\right)_q\left(x_{k+1}\right)_q$$

$$=\eta\xi+\zeta\theta+\sum_{q=1}^{N-2}\left(\eta\frac{\det\left(\left(A_{\backslash\{N\}}-\lambda_k I\right)_{\backslash\text{ row }N-1\backslash\text{ col }q}\right)}{\det\left(A_{\backslash\{N-1,N\}}-\lambda_k I\right)}\right.$$

$$\left.+\zeta\frac{\det\left(\left(A_{\backslash\{N-1\}}-\lambda_k I\right)_{\backslash\text{ row }N\backslash\text{ col }q}\right)}{\det\left(A_{\backslash\{N-1,N\}}-\lambda_k I\right)}\right)$$

$$\times\left(\xi\frac{\det\left(\left(A_{\backslash\{N\}}-\lambda_k I\right)_{\backslash\text{ row }N-1\backslash\text{ col }q}\right)}{\det\left(A_{\backslash\{N-1,N\}}-\lambda_k I\right)}+\theta\frac{\det\left(\left(A_{\backslash\{N-1\}}-\lambda_k I\right)_{\backslash\text{ row }N\backslash\text{ col }q}\right)}{\det\left(A_{\backslash\{N-1,N\}}-\lambda_k I\right)}\right)$$

$$=\eta\xi+\zeta\theta+\eta\xi\sum_{q=1}^{N-2}\frac{\det^2\left(\left(A_{\backslash\{N\}}-\lambda_k I\right)_{\backslash\text{ row }N-1\backslash\text{ col }q}\right)}{\det^2\left(A_{\backslash\{N-1,N\}}-\lambda_k I\right)}$$

$$+\left(\eta\theta+\zeta\xi\right)\sum_{q=1}^{N-2}\frac{\det\left(\left(A_{\backslash\{N\}}-\lambda_k I\right)_{\backslash\text{ row }N-1\backslash\text{ col }q}\right)\det\left(\left(A_{\backslash\{N-1\}}-\lambda_k I\right)_{\backslash\text{ row }N\backslash\text{ col }q}\right)}{\det^2\left(A_{\backslash\{N-1,N\}}-\lambda_k I\right)}$$
$$+\zeta\theta\sum_{q=1}^{N-2}\frac{\det^2\left(\left(A_{\backslash\{N-1\}}-\lambda_k I\right)_{\backslash\text{ row }N\backslash\text{ col }q}\right)}{\det^2\left(A_{\backslash\{N-1,N\}}-\lambda_k I\right)}$$

Hence,

$$0=\eta\xi S+\zeta\theta R+\left(\eta\theta+\zeta\xi\right)V$$

We need to solve η,ζ,ξ and θ from the quadratic set

$$\begin{cases}\eta^2 S+\zeta^2 R+2\eta\zeta V=1\\ \xi^2 S+\theta^2 R+2\xi\theta V=1\\ \eta\xi S+\zeta\theta R+\left(\eta\theta+\zeta\xi\right)V=0\end{cases}$$

From the first two equations, we first solve

$$\eta=\frac{-\zeta V\pm\sqrt{\left(\zeta V\right)^2-S\left(\zeta^2 R-1\right)}}{S}$$
$$\xi=\frac{-\theta V\pm\sqrt{\left(\theta V\right)^2-S\left(\theta^2 R-1\right)}}{S}$$

Substituted into the last equation,

$$0=\frac{\left(-\zeta V\pm\sqrt{\left(\zeta V\right)^2-S\left(\zeta^2 R-1\right)}\right)\left(-\theta V\pm\sqrt{\left(\theta V\right)^2-S\left(\theta^2 R-1\right)}\right)}{S}+\zeta\theta R$$
$$+\left(-2\zeta\theta V\pm\theta\sqrt{\left(\zeta V\right)^2-S\left(\zeta^2 R-1\right)}\pm\zeta\sqrt{\left(\theta V\right)^2-S\left(\theta^2 R-1\right)}\right)\frac{V}{S}$$

which is

$$0=\sqrt{\left(\left(\zeta V\right)^2-S\left(\zeta^2 R-1\right)\right)\left(\left(\theta V\right)^2-S\left(\theta^2 R-1\right)\right)}+\zeta\theta\left(RS-V^2\right)$$

and

$$\sqrt{V^2-SR+\frac{S}{\theta^2}}=\frac{V^2-RS}{\sqrt{V^2-SR+\frac{S}{\zeta^2}}}$$

Squaring

$$V^2 - SR + \frac{S}{\theta^2} = \frac{\left(V^2 - RS\right)^2}{V^2 - SR + \frac{S}{\zeta^2}}$$

and simplifying yields

$$\theta^2 + \zeta^2 = \frac{S}{RS - V^2}$$

The Cauchy-Schwarz inequality [3, (A.72) on p. 333] confirms that $RS > V^2$. Hence, the point (θ, ζ) lies on a circle with center at the origin of the θ-ζ plane and with radius equal to $\sqrt{\frac{S}{RS-V^2}}$. By choosing the positive root, we express θ as a function of ζ,

$$\theta = \sqrt{\frac{S}{RS - V^2} - \zeta^2}$$

After substitution into $\xi = \frac{-\theta V \pm \sqrt{S - \theta^2 (RS - V^2)}}{S}$, we express θ, ξ and η as functions of ζ as

$$\theta = \frac{\sqrt{S - \zeta^2 \left(RS - V^2\right)}}{\sqrt{RS - V^2}}$$

$$\eta = \frac{-\zeta V \pm \sqrt{S - \zeta^2 \left(RS - V^2\right)}}{S}$$

$$\xi = \frac{-V\sqrt{S - \zeta^2 \left(RS - V^2\right)}}{S\sqrt{(RS - V^2)}} \pm \frac{\zeta\sqrt{(RS - V^2)}}{S}$$

Choosing $(x_k)_N = \zeta = 0$ and positive signs before squareroot, leads to the simplest expressions,

$$\theta = \frac{\sqrt{S}}{\sqrt{RS-V^2}} \quad \eta = \frac{1}{\sqrt{S}} \quad \xi = \frac{-V}{\sqrt{S}\sqrt{(RS-V^2)}}$$

Finally, for the eigenvector x_k, we find $(x_k)_N = 0$ and for $1 \leq q \leq N-1$

$$(x_k)_q = \frac{(-1)^{q-N} \det\left(\left(A_{\setminus\{N\}} - \lambda_k I\right)_{\setminus \text{row } N-1 \setminus \text{col } q}\right)}{\sqrt{\sum_{j=1}^{N} \det^2\left(\left(A_{\setminus\{N\}} - \lambda_k I\right)_{\setminus \text{row } N-1 \setminus \text{col } j}\right)}}$$

which is the same as (7) if $m_k = 1$ and for the eigenvector x_{k+1}, it holds that $(x_{k+1})_{N-1} = \frac{-V}{\sqrt{S}\sqrt{(RS-V^2)}}$, $(x_{k+1})_N = \frac{\sqrt{S}}{\sqrt{RS-V^2}}$ and for $1 \leq q \leq N-2$

$$(-1)^{q-N} (x_{k+1})_q = \frac{-V}{\sqrt{S}\sqrt{RS - V^2}} \frac{\det\left(\left(A_{\setminus\{N\}} - \lambda_k I\right)_{\setminus \text{row } N-1 \setminus \text{col } q}\right)}{\det\left(A_{\setminus\{N-1,N\}} - \lambda_k I\right)}$$

$$+\frac{\sqrt{S}}{\sqrt{RS-V^2}}\frac{\det\left(\left(A_{\backslash\{N-1\}}-\lambda_k I\right)_{\backslash\,\text{row}\,N\backslash\,\text{col}\,q}\right)}{\det\left(A_{\backslash\{N-1,N\}}-\lambda_k I\right)}$$

The close-form, after substitution of R, S and V, does not seem to simplify so nicely as for the eigenvector x_k, mainly due to $RS - V^2$. However, Theorem 3 on the *square* of the eigenvector components presents rather elegant formulae, that suggest that further simplification may exist. Nevertheless, we omit here further efforts.

Appendix D. Additions to Theorem 1

Another way to rewrite the determinant in (35) is

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

where the $(N-1)\times 1$ vector $w_{\backslash m}=(w_1,\dots,w_{m-1},w_{m+1},\dots,w_N)$ is obtained from the $N\times 1$ vector w after removing the m-th component. Invoking Schur's block determinant relation [3, art. 217] yields[12]

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

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

$$\det\left(A-\lambda_k I\right)_{\text{row}\,m=b}=\det\left(A_{\backslash\{m\}}-\lambda_k I\right)\left(b_m-b_{\backslash m}^T\left(A_{\backslash\{m\}}-\lambda_k I\right)^{-1}(a_m)_{\backslash m}\right)\tag{47}$$

where $(a_m)_{\backslash m}=(a_{1m},\dots,a_{m-1;m},a_{m+1,m},\dots,a_{Nm})$ and $(A-\lambda I)^{-1}$ is the resolvent [3, art. 215]. Using (47) in (35) transforms (34) to

$$(x_k)_j=\frac{\beta_k}{b_j-b_{\backslash j}^T\left(A_{\backslash\{j\}}-\lambda_k I\right)^{-1}(a_j)_{\backslash j}}\tag{48}$$

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

[12] 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 $\lambda=-1$.

If $b = e_m$, the basic vector with all zero components, except that the m-th component is 1, then (48) reduces with $\beta_k = b^T x_k = (x_k)_m$, for $j \neq m$, to

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

else, for $j = m$, we find from (48) an identity, because $b_{\backslash m} = 0$. Interchanging m and j, the ratio $\frac{(x_k)_j}{(x_k)_m}$, expressed in two ways, leads to

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

When the vector b equals a row vector in A, it can be shown (see e.g. [28], [3, art. 259]) that

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

Indeed, let $b = (A - \lambda_k I)_{\text{row}=N}$, then

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

Since $\det(A - \lambda_k I) = \det \begin{bmatrix} \left(A_{\backslash\{N\}} - \lambda_k I\right) & a_N \\ (a_N)_{\backslash N}^T & a_{NN} - \lambda_k \end{bmatrix} = 0$, we deduce that

$$\lambda_k = a_{NN} - a_{\backslash N}^T \left(A_{\backslash\{N\}} - \lambda_k I\right)^{-1} (a_N)_{\backslash N}$$

which is equation in [3, top on p. 370], derived differently.

Appendix E. About the determinant det Ξ

Adding all rows in Ξ' in (32) to the last row and using (40) yields

$$\det \Xi' = \begin{vmatrix} \det\left(A_{G\backslash\{1\}} - \lambda_1 I\right) & \det\left(A_{G\backslash\{1\}} - \lambda_2 I\right) & \cdots & \det\left(A_{G\backslash\{1\}} - \lambda_N I\right) \\ \det\left(A_{G\backslash\{2\}} - \lambda_1 I\right) & \det\left(A_{G\backslash\{2\}} - \lambda_2 I\right) & \cdots & \det\left(A_{G\backslash\{2\}} - \lambda_N I\right) \\ \vdots & \vdots & \ddots & \vdots \\ -c_A'(\lambda_1) & -c_A'(\lambda_2) & \cdots & -c_A'(\lambda_N) \end{vmatrix}$$

In contrast to adding all rows to the last row and invoking $\sum_{n=1}^{N} \det\left(A_{\setminus\{n\}} - \lambda I\right) = -c'_A(\lambda)$ in (40), adding all the columns to the last column results, with (2) and (15),

$$\sum_{k=1}^{N} \det\left(A_{G\setminus\{q\}} - \lambda_k I\right) = \left(\sum_{k=1}^{N} \prod_{l=1;l\neq k}^{N} (\lambda_l I - A)\right)_{qq} = -\left(c'_A(A)\right)_{qq}$$
$$= -\sum_{k=1}^{N} k c_k \left(A^{k-1}\right)_{qq}$$

in

$$\det \Xi' = \begin{vmatrix} \det\left(A_{G\setminus\{1\}} - \lambda_1 I\right) & \det\left(A_{G\setminus\{1\}} - \lambda_2 I\right) & \cdots & -\left(c'_A(A)\right)_{11} \\ \det\left(A_{G\setminus\{2\}} - \lambda_1 I\right) & \det\left(A_{G\setminus\{2\}} - \lambda_2 I\right) & \cdots & -\left(c'_A(A)\right)_{22} \\ \vdots & \vdots & \ddots & \vdots \\ -c'_A(\lambda_1) & -c'_A(\lambda_2) & \cdots & -\sum_{k=1}^{N} c'_A(\lambda_k) \end{vmatrix}$$

Given that λ_k is a simple eigenvalue, it remains to find conditions on the graph G for $\det \Xi'$ to be zero.

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