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Co-eigenvector graphs

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ABSTRACT

Except for the empty graph, we show that the orthogonal matrix X of the adjacency matrix A determines that adjacency matrix completely, but not always uniquely. The proof relies on interesting properties of the Hadamard product $\Xi = X \circ X$. As a consequence of the theory, we show that irregular co-eigenvector graphs exist only if the number of nodes $N \geq 6$. Co-eigenvector graphs possess the same orthogonal eigenvector matrix X, but different eigenvalues of the adjacency matrix. Co-eigenvector graphs are the dual of co-spectral graphs, that share all eigenvalues of the adjacency matrix, but possess a different orthogonal eigenvector matrix. We deduce general properties of co-eigenvector graph and start to enumerate all co-eigenvector graphs on $N = 6$ and $N = 7$ nodes. Finally, we list many open problems.

1. Introduction

A graph $G(\mathcal{N}, \mathcal{L})$ is composed of a set $\mathcal{N}$ of $N = |\mathcal{N}|$ nodes and a set $\mathcal{L}$ of $L = |\mathcal{L}|$ links. An undirected and unweighted graph with N nodes can be represented by an $N \times N$

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symmetric adjacency matrix A. The element a_{ij} of the adjacency matrix A equals $a_{ij} = 1$ if there exists a link between node i and j, else $a_{ij} = 0$. We exclude self-loops, implying that A has zero diagonal elements, i.e. $a_{jj} = 0$ for $1 \leq j \leq N$. We call a graph simple if it is undirected without self-loops. Just as any symmetric matrix, the symmetric, zero-one adjacency matrix A possesses the eigenvalue decomposition

$$A = X\Lambda X^T \tag{1}$$

as reviewed in the introduction of [1]. The equality in (1) implies that all information at the left-hand side, that we call the *topology domain*, is also contained in the right-hand side, that we call the *spectral domain*. Most insight so far in graphs is gained in the topology domain that allows a straightforward drawing of a graph: nodes are interconnected by links and the picture of a graph is attractive and understandable to humans. The spectral domain, consisting of the set of orthogonal and normalized eigenvectors $x_1, x_2, \ldots, x_N$ stored as columns in the orthogonal eigenvector matrix X in (1) and the corresponding set of eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_N$ stored in the eigenvalue vector $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_N)$ in $\Lambda = \text{diag}(\lambda)$, is less intuitive for humans; the meaning of an eigenvector and eigenvalue of a graph is not obvious. However, as mentioned in the preface of [1], the relation $A = X\Lambda X^T$ represents a transformation of a similar nature as a Fourier transform, which suggests that some information is better or more adequately accessible in one domain and other information in the other domain. Besides the topology domain and the spectral domain, there exists a third equivalent representation, called the *geometric domain*, where each, possibly weighted, undirected graph is a simplex in the $N-1$ dimensional Euclidean space [2].

Most of the spectral results are obtained for eigenvalues, in particular, for the largest eigenvalue or spectral radius [3]. While the number of mathematical results on other eigenvalues is already considerably less than for the spectral radius, results on eigenvectors are scarce [4,5].

Earlier, Haemers and van Dam [6] have conjectured that, when the number of nodes $N \to \infty$, the eigenvalue vector $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_N)$ characterizes the graph almost surely, i.e. the probability that eigenvalue vector λ determines the graph tends to 1. The Haemers and van Dam conjecture practically means that the eigenvalue vector λ is a fingerprint of a real-world, large graph, that is comparable to a photoluminescence spectrum of a material (see e.g. [7]). Here, we present a kind of dual of the Haemers and van Dam conjecture and concentrate on the orthogonal eigenvector matrix X in (1) rather than on the eigenvalue vector λ. In particular, Theorem 2 in Section 4 demonstrates that, given the orthogonal eigenvector matrix X of the adjacency matrix A, the precise adjacency matrix is recovered, in contrast to a partial or approximated one as in network inference methods (see e.g. [8], [9]) that estimate the most likely underlying graph. Section 5 discusses consequences of Theorem 2: we will show that co-eigenvector graphs exist and that the orthogonal eigenvector matrix X does not always "uniquely" specifies a graph, because different graphs can possess the same orthogonal eigenvector matrix X.

We briefly review the orthogonal eigenvector matrix X of a symmetric matrix in Section 2, introduce the Hadamard product $\Xi = X \circ X$ and derive some properties of the matrix Ξ in Section 3, which we apply to the adjacency matrix of an undirected graph in Section 3.2. We provide the proof of Theorem 2 in Section 4 and analyze its consequences in Section 5. Section 6 deduces general properties of co-eigenvector graphs, for both regular and irregular graphs. Section 7 enumerates nearly all co-eigenvector graphs on $N = 6$ and $N = 7$ nodes. For $N < 6$, our enumeration algorithm did not find irregular co-eigenvector graphs. Proceeding with a higher number N of nodes rapidly becomes computationally challenging due to the huge increase in the number of unlabeled graph on N nodes. Section 8 concludes and poses open problems.

2. Eigenvectors and eigenvalues: brief review

Following the notation of [1], we denote by x_k the $N \times 1$ eigenvector of the symmetric matrix A belonging to the eigenvalue λ_k, normalized so that $x_k^T x_k = 1$. Here, in Section 2, A is any symmetric matrix and not necessarily equal to the adjacency matrix. The eigenvalues of an $N \times N$ symmetric matrix $A = A^T$ are real and can be ordered as $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_N$. Let X be the orthogonal matrix with eigenvectors of A in the columns,

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

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

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

where the element $X_{ij} = (x_j)_i$.

The relation $X^T X = I = X X^T$ (see e.g. [1, art. 247]) expresses, in fact, *double orthogonality*. The first equality $X^T X = I$ translates, with the Kronecker delta $\delta_{km} = 0$ if $k \neq m$, otherwise $\delta_{km} = \delta_{mm} = 1$, to the well-known orthogonality relation

$$x_k^T x_m = \sum_{j=1}^{N} (x_k)_j (x_m)_j = \delta_{km} \tag{3}$$

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

as $y_m = ((x_1)_m, (x_2)_m, \ldots, (x_N)_m)$. Then, the second orthogonality condition $XX^T = I$ implies orthogonality of the row vectors of X,

$$y_l^T y_j = \sum_{k=1}^{N} (x_k)_l (x_k)_j = \delta_{lj} \tag{4}$$

The $N \times N$ matrix $\Xi = X \circ X$, where $\circ$ denotes the Hadamard product,[1]

$$\Xi = \begin{bmatrix} (x_1)_1^2 & (x_2)_1^2 & (x_3)_1^2 & \cdots & (x_N)_1^2 \\ (x_1)_2^2 & (x_2)_2^2 & (x_3)_2^2 & \cdots & (x_N)_2^2 \\ (x_1)_3^2 & (x_2)_3^2 & (x_3)_3^2 & \cdots & (x_N)_3^2 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ (x_1)_N^2 & (x_2)_N^2 & (x_3)_N^2 & \cdots & (x_N)_N^2 \end{bmatrix} \tag{5}$$

will play an important role in this paper.

3. Function of a symmetric matrix and the stochastic matrix Ξ

From the general relation for diagonalizable matrices (see e.g. [11, p. 526]),

$$f(A) = \sum_{k=1}^{N} f(\lambda_k) x_k x_k^T \tag{6}$$

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

$$(f(A))_{jj} = \sum_{k=1}^{N} f(\lambda_k) (x_k)_j^2 \tag{7}$$

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

$$\begin{bmatrix} (f(A))_{11} \\ (f(A))_{22} \\ (f(A))_{33} \\ \vdots \\ (f(A))_{NN} \end{bmatrix} = \begin{bmatrix} (x_1)_1^2 & (x_2)_1^2 & (x_3)_1^2 & \cdots & (x_N)_1^2 \\ (x_1)_2^2 & (x_2)_2^2 & (x_3)_2^2 & \cdots & (x_N)_2^2 \\ (x_1)_3^2 & (x_2)_3^2 & (x_3)_3^2 & \cdots & (x_N)_3^2 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ (x_1)_N^2 & (x_2)_N^2 & (x_3)_N^2 & \cdots & (x_N)_N^2 \end{bmatrix} \begin{bmatrix} f(\lambda_1) \\ f(\lambda_2) \\ f(\lambda_3) \\ \vdots \\ f(\lambda_N) \end{bmatrix} \tag{8}$$

We write (8) in matrix form as $\psi = \Xi\chi$ with the vectors

[1] The Hadamard product [10] (entrywise product) of two matrices is $(A \circ B)_{ij} = A_{ij} B_{ij}$. If A and B are both diagonal matrices, then $AB = A \circ B$.

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

where the $N \times N$ matrix $\Xi = X \circ X$ is defined in (5). We denote by u the all-one vector.

Since $\Xi u = u$ and $\Xi^T u = u$, by "double orthogonality" of (3) and (4), and since each element $0 \leq (x_k)_j^2 \leq 1$, the matrix Ξ with squared eigenvector components of a diagonalizable matrix A is doubly[2]-stochastic [1] with largest eigenvalue equal to 1. The latter property follows from the Perron-Frobenius Theorem of non-negative matrices. The product[3] of two doubly-stochastic matrices is also a doubly-stochastic matrix. The doubly-stochastic matrix Ξ also provides a vehicle to generate sharp inequalities, for which we refer to the book of Marshall et al. [12].

The $N \times N$ doubly-stochastic matrix Ξ in (5) can have a rank that is lower than N, in contrast to the $N \times N$ orthogonal eigenvector matrix X, whose rank always equals N. The fact that Ξ is not necessary of full rank, i.e. $\det(\Xi) = 0$ is possible, is exploited in the proof of Theorem 2 in Section 4 for graph recovery.

3.1. Eigenstructure of the matrix Ξ

Let us denote the eigenvalue equation of the asymmetric[4] $N \times N$ matrix Ξ by

$$\Xi w_j = \xi_j w_j \tag{9}$$

Double-stochasticity combined with the Perron-Frobenius theorem tells us that $\xi_1 = 1 \geq |\xi_j|$ for any $j > 1$ and $w_1 = u$. Each eigenvalue ξ_j of the asymmetric matrix Ξ thus lies within the unit circle and is either real on $[-1, 1]$ or occurs in complex conjugate pairs, i.e. if $\mathrm{Im}\, \xi_j \neq 0$, then existence of ξ_j implies existence of its complex conjugate ξ_j^*. The corresponding eigenvector w_j^* of ξ_j^* follows by taking the complex conjugate of the eigenvalue equation (i.e. replacing i by $-i$), thus $\Xi w_j^* = \xi_j^* w_j^*$. All eigenvalues of Ξ^m, i.e. ξ_j^m for $1 \leq j \leq N$ and for any positive integer m, lie within the unit circle and the

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

[3] Indeed, let Ξ and Ψ be two $N \times N$ doubly-stochastic matrices. Then, left-multiplying both sides in $\Xi u = u$ by Ψ and using $\Psi u = u$ yields $\Psi \Xi u = u$. Similarly, left-multiplying both sides in $\Psi^T u = u$ by Ξ^T and using $\Xi^T u = u$ yields $(\Psi \Xi)^T u = u$. Finally, an element of $\Psi \Xi$ equals

$$0 \leq (\Psi \Xi)_{ij} = \sum_{k=1}^{N} \Psi_{ik} \Xi_{kj} \leq \min\left(\max_{1 \leq k \leq N} \Psi_{ik}, \max_{1 \leq k \leq N} \Xi_{kj} \right) \leq 1$$

which demonstrates the property.

[4] Since symmetric orthogonal eigenvector matrices exist [20], their corresponding symmetric Ξ matrices have real eigenvalues in the interval $[-1, 1]$.

largest eigenvalue $\xi_1 = 1$ possesses the all-one vector u as eigenvector. This fact follows from (a) the above eigenvalue equation and (b), separately, from the property that the product of two doubly-stochastic matrices is also a doubly-stochastic matrix. The trace of the matrix Ξ is $\text{trace}(\Xi) = \sum_{j=1}^{N} (x_j)_j^2 \geq 0$, implying that the sum of the eigenvalues of Ξ is non-negative. It follows from $\text{trace}\left(\Xi^2\right) = \sum_{j=1}^{N} \xi_j^2 = \sum_{i=1}^{N} \sum_{k=1}^{N} (x_k)_i^2 (x_i)_k^2$ that $\sum_{k=1}^{N} (\text{Re}\, \xi_k)^2 \geq \sum_{k=1}^{N} (\text{Im}\, \xi_k)^2$.

Since the matrix Ξ is asymmetric, the eigenvectors are not necessarily orthogonal, but only independent (provided that Ξ is not defective and that there exist N independent eigenvectors). We find from the eigenvalue equation (9) that (a) $w_k^T \Xi w_j = \xi_j w_k^T w_j$ and (b) $w_j^T \Xi w_k = \xi_k w_j^T w_k$ and subtraction

$$(\xi_j - \xi_k)\, w_k^T w_j = w_k^T \Xi w_j - w_j^T \Xi w_k = w_k^T \left(\Xi - \Xi^T\right) w_j$$

indicates that orthogonality between w_k and w_j, for $j \neq k$, only holds for symmetric matrices. Thus, $w_j^T w_k$ is not necessarily zero if $k \neq j$.

Lemma 1. *All eigenvectors w_j of a doubly-stochastic matrix Ξ with $j > 1$ are orthogonal to $w_1 = u$.*

Proof. Right-multiplying the transpose of the eigenvalue equation (9) by the all-one vector yields $w_j^T \Xi^T u = \xi_j w_j^T u$. After using $\Xi^T u = u$, we find that $0 = (\xi_j - 1)\, w_j^T u$, which implies that any eigenvector w_j, except for $w_1 = u$ belonging to $\xi_1 = 1$, is orthogonal to the all-one vector u. □

A consequence of Lemma 1 is that the sum of the components of an eigenvector w_j with $j > 1$ of a doubly-stochastic matrix is zero.

3.2. The matrix $\Xi = X \circ X$ of the adjacency matrix

We apply the general theory to the adjacency matrix A and refer to [1, art. 109] for the Laplacian matrix. Let us denote the vector $\lambda^k = \left(\lambda_1^k, \lambda_2^k, \ldots, \lambda_N^k\right)$ so that, for the function $f(z) = z^k$ in (8) where k is a non-negative integer, we can write (8) as

$$\text{diag}\left(\left(A^k\right)_{jj}\right) u = \Xi \lambda^k \tag{10}$$

where $u = (1, 1, \ldots, 1)$ is the all-one vector. From (10) and $u^T \Xi = u^T$, we find the well-known trace relation [1], namely that $u^T \text{diag}\left(\left(A^k\right)_{jj}\right) u = \text{trace}\left(A^k\right) = u^T \lambda^k = \sum_{j=1}^{N} \lambda_j^k$.

Formula (10) for integer powers $f(z) = z^k$ leads to nice formulae. Indeed, for $k = 0$, we find from (6) the *second* orthogonality relation (4); for $k = 1$ (since $a_{jj} = 0$, from which $\text{trace}(A) = \sum_{j=1}^{N} \lambda_j = 0$)

$$0 = \sum_{k=1}^{N} \lambda_k \left(x_k\right)_j^2 \text{ and } 0 = \Xi\lambda \tag{11}$$

that appeared earlier in [1, art. 96], while for $k = 2$ (since the degree of node j is $d_j = \left(A^2\right)_{jj}$)

$$d_j = \sum_{k=1}^{N} \lambda_k^2 \left(x_k\right)_j^2 \text{ and } d = \Xi\lambda^2 \tag{12}$$

For any adjacency matrix A without self-loops (i.e. $a_{jj} = 0$ for each $1 \le j \le N$), the instance (11)

$$\Xi\lambda = 0 \tag{13}$$

is the special case of the eigenvalue equation (9) in Section 3.1, where the eigenvalue vector $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_N)$ of the adjacency matrix A is the eigenvector of Ξ corresponding to eigenvalue zero. Lemma 1 states that $\lambda^T u = 0$ or $\sum_{j=1}^{N} \lambda_j = 0$. In addition, the eigenvalue equation (9) implies that $\det(\Xi) = 0$, which is equivalent to the fact that $\text{rank}(\Xi) \le N - 1$. Thus, the rank of the matrix Ξ for an adjacency matrix is at most $N - 1$.

We can write (10) for integers k ranging from $k = 0$ up to $k = N - 1$,

$$\begin{aligned} Y &= \begin{bmatrix} 1 & 0 & d_1 & \cdots & \left(A^k\right)_{11} & \cdots & \left(A^{N-1}\right)_{11} \\ 1 & 0 & d_2 & \cdots & \left(A^k\right)_{22} & \cdots & \left(A^{N-1}\right)_{22} \\ 1 & 0 & d_3 & \cdots & \left(A^k\right)_{33} & \cdots & \left(A^{N-1}\right)_{33} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ 1 & 0 & d_N & \cdots & \left(A^k\right)_{NN} & \cdots & \left(A^{N-1}\right)_{NN} \end{bmatrix} \\ &= \Xi. \begin{bmatrix} 1 & \lambda_1 & \lambda_1^2 & \cdots & \lambda_1^k & \cdots & \lambda_1^{N-1} \\ 1 & \lambda_2 & \lambda_2^2 & \cdots & \lambda_2^k & \cdots & \lambda_2^{N-1} \\ 1 & \lambda_3 & \lambda_3^2 & \cdots & \lambda_3^k & \cdots & \lambda_3^{N-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ 1 & \lambda_N & \lambda_N^2 & \cdots & \lambda_N^k & \cdots & \lambda_N^{N-1} \end{bmatrix} \end{aligned} \tag{14}$$

where $\left(A^k\right)_{jj}$ equals the number of closed walks of length k from node j and back to node j and the right-hand side matrix is an $N \times N$ Vandermonde matrix V.

3.3. Examples of particular graphs

(a) In a line topology or path on N nodes, only even closed walks are possible and $\left(A^k\right)_{jj} = 0$ for odd k. For finite N and even k, symmetry is broken and $\left(A^k\right)_{jj} \neq \left(A^k\right)_{ll}$ for any pair (l, j) of nodes, due to the end nodes. Since all eigenvalues of the adjacency

matrix of a path graph are distinct [1, Sec. 6.4], we deduce from (14) and the property $\text{rank}(C.D) \leq \min(\text{rank}(C), \text{rank}(D))$ that $\text{rank}(\Xi_{\text{path}}) = \left[\frac{N}{2}\right]$, where $[x]$ is the integer part of the real number x. The same result, $\text{rank}(\Xi_{\text{path}}) = \left[\frac{N}{2}\right]$, can also be obtained from the explicit analytic expression (e.g. [1, p. 203]) for the orthogonal eigenvector matrix X_{path}.

(b) For a regular graph with degree r, the degree vector is $d = r.u$ and the first and third column in the non-negative matrix Y in (14) are dependent. Hence, $\text{rank}(Y)$ is at most $N-2$ for regular graphs, but $\text{rank}(\Xi)$ can still be $N-1$ as shown in (c) below.

(c) The adjacency matrix of the complete graph $A_{K_N} = J - I$, where $J = u.u^T$ is the all-one matrix. For the complete graph K_N, the matrix Y in (14) can be computed analytically, because $\left(A^k_{K_N}\right)_{jj} = (J-I)^k_{jj} = \frac{1}{N}\left((N-1)^k - (-1)^k\right) + (-1)^k$, which is the same for any node j, as

$$Y_{K_N} = \left[u \quad 0 \quad (N-1)\,u \quad \cdots \quad \left(\tfrac{(N-1)^k-(-1)^k}{N} + (-1)^k\right) u \quad \cdots \quad \left((J-I)^{N-1}_{jj}\right) u \right]$$

Since all columns are multiples of the all-one vector u, we find that $\text{rank}(Y_{K_N}) = 1$. The adjacency matrix $A_{K_N} = J - I$ of the complete graph K_N has two eigenvalues: $N-1$ belonging to eigenvector $x_1 = u$ and -1 with multiplicity $N-1$. Hence, the rank of the Vandermonde matrix V in (14) is $\text{rank}(V) = 2$ and (14) is not effective to determine $\text{rank}(\Xi)$. Fortunately, the orthogonal eigenvector matrix of adjacency matrix $A_{K_N} = J - I$ can be computed analytically, in at least two ways.

The eigenvalue equation for $\lambda = -1$ is $(J-I)\,x = -x$, which is equivalent to $0 = Jx = u.u^T x$. Hence, any set of $N-1$ independent vectors $\{x_2, x_3, \ldots, x_N\}$ with a component sum equal to zero is possible. In other words, there are infinitely many orthogonal X-matrices for the complete graph K_N. Perhaps, the simplest *not normalized* eigenvector for the complete graph K_N is

$$\widetilde{x}_j = e_j - \frac{1}{j-1}\sum_{m=1}^{j-1} e_m \qquad \text{for } j > 1$$

where e_j is the basic vector with component $(e_j)_k = \delta_{jk}$. The eigenvector $\widetilde{x}_j$ satisfies the eigenvalue equation $(J-I)\,\widetilde{x}_j = -\widetilde{x}_j$ or $J\widetilde{x}_j = 0$, because $Je_j = u$. In addition, using $e_m^T e_k = \delta_{mk}$, the scalar product $\widetilde{x}_j^T \widetilde{x}_k = \delta_{jk}$ is

$$\begin{aligned}
\widetilde{x}_j^T \widetilde{x}_k &= \left(e_j^T - \frac{1}{j-1}\sum_{m=1}^{j-1} e_m^T\right)\left(e_k - \frac{1}{k-1}\sum_{l=1}^{k-1} e_l\right) \\
&= e_j^T e_k - \frac{1}{k-1}\sum_{l=1}^{k-1} e_j^T e_l - \frac{1}{j-1}\sum_{m=1}^{j-1} e_m^T e_k + \frac{1}{j-1}\frac{1}{k-1}\sum_{m=1}^{j-1}\sum_{l=1}^{k-1} e_m^T e_l \\
&= \delta_{jk} - \frac{1}{k-1}\sum_{l=1}^{k-1}\delta_{jl} - \frac{1}{j-1}\sum_{m=1}^{j-1}\delta_{mk} + \frac{1}{j-1}\frac{1}{k-1}\sum_{m=1}^{j-1}\sum_{l=1}^{k-1}\delta_{ml}
\end{aligned}$$

$$= \delta_{jk} - \frac{1}{k-1} 1_{\{j\in[1,k-1]\}} - \frac{1}{j-1} 1_{\{k\in[1,j-1]\}} + \frac{1}{j-1}\frac{1}{k-1} \sum_{m=1}^{j-1} 1_{\{m\in[1,k-1]\}}$$

If $j = k$, then

$$\widetilde{x}_k^T \widetilde{x}_k = 1 + \frac{1}{(k-1)^2} \sum_{m=1}^{k-1} 1_{\{m\in[1,k-1]\}} = 1 + \frac{1}{k-1} = \frac{k}{k-1}$$

Without loss of generality, we may assume that $j < k$ (else interchange j and k) and then, with $\sum_{m=1}^{j-1} 1_{\{m\in[1,k-1]\}} = j-1$, we find

$$\widetilde{x}_j^T \widetilde{x}_k = -\frac{1}{k-1} + \frac{1}{j-1}\frac{1}{k-1} \sum_{m=1}^{j-1} 1_{\{m\in[1,k-1]\}} = 0$$

Hence, the normalized eigenvector $x_j = \frac{\widetilde{x}_j}{\sqrt{\widetilde{x}_j^T \widetilde{x}_j}} = \sqrt{\frac{j-1}{j}} e_j - \frac{1}{\sqrt{j(j-1)}} \sum_{m=1}^{j-1} e_m$ and the corresponding orthogonal eigenvector matrix for the complete graph K_N is

$$X_{K_N} = \begin{bmatrix} \frac{1}{\sqrt{N}} & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{6}} & -\frac{1}{2\sqrt{3}} & -\frac{1}{2\sqrt{5}} & \cdots & -\frac{1}{\sqrt{N(N-1)}} \\ \frac{1}{\sqrt{N}} & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{6}} & -\frac{1}{2\sqrt{3}} & -\frac{1}{2\sqrt{5}} & \cdots & -\frac{1}{\sqrt{N(N-1)}} \\ \frac{1}{\sqrt{N}} & 0 & \sqrt{\frac{2}{3}} & -\frac{1}{2\sqrt{3}} & -\frac{1}{2\sqrt{5}} & \cdots & -\frac{1}{\sqrt{N(N-1)}} \\ \frac{1}{\sqrt{N}} & 0 & 0 & \frac{\sqrt{3}}{2} & -\frac{1}{2\sqrt{5}} & \cdots & -\frac{1}{\sqrt{N(N-1)}} \\ \frac{1}{\sqrt{N}} & 0 & 0 & 0 & \sqrt{\frac{5}{6}} & \cdots & -\frac{1}{\sqrt{N(N-1)}} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{1}{\sqrt{N}} & 0 & 0 & 0 & 0 & \cdots & \frac{N-1}{\sqrt{N}} \end{bmatrix} \tag{15}$$

and the rank of the corresponding matrix $\Xi_{K_N} = X_{K_N} \circ X_{K_N}$ is $\mathrm{rank}(\Xi_{K_N}) = N-1$. Barik et al. [13] have shown that only regular graphs, such as the complete graph K_N, for $N = 4k$ and $k \in \mathbb{N}_0$, and the regular bipartite graph $K_{2k,2k}$, are diagonalizable by a Hadamard matrix. An $n \times n$ Hadamard matrix H_n has as elements either -1 and 1 and obeys $H_n H_n^T = nI_n$, where the order n can only be $n = 1, 2$ or $n = 4k$, subject to the fact that Hadamard's conjecture, namely that there exists a Hadamard matrix H_{4k} for each integer k, holds. Hadamard's conjecture is still an open, unsolved problem. The normalized matrix $X_n = \frac{1}{\sqrt{n}} H_n$ is an orthogonal matrix, from which it follows that $|\det H_n| = n^{\frac{n}{2}}$, which is maximal among all $n \times n$ matrices with elements in absolute value less than or equal to 1 and the latter class includes all orthogonal matrices. Any relabeling (permutation of rows and columns) of a Hadamard matrix is again a Hadamard matrix; multiplying any row or column by -1 preserves the Hadamard properties. Following Barik et al. [13], let $H_n = \left[u|\widetilde{H}\right]$ so that $H_n e_1 = u$. Consider the diagonal matrix $D = I - e_1 e_1^T$, then

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

Hence, the Laplacian matrix of the complete graph K_n is $Q_{K_n} = nI - J = H_n D H_n^T$. Since K_n is a regular graph, the eigenvectors of the Laplacian Q and the adjacency matrix A are the same.[5] In conclusion, any Hadamard matrix with $H_n e_1 = u$ provides the orthogonal matrix for the complete graph K_n. Since $H_n \circ H_n = J = u.u^T$, we find that the corresponding $\text{rank}(\Xi_{K_n}) = 1$, which is the minimum possible rank for any Ξ matrix.

In summary, depending on the choice of the orthogonal eigenvector matrix for the complete graph K_N for $N = 4k$, we believe that the rank of the corresponding Ξ matrix may vary over all possible values: $1 \leq \text{rank}(\Xi_{K_N}) \leq N - 1$. However, we do not have a proof that $\text{rank}(\Xi_{K_N})$ can attain any integer in the interval $[1, N]$.

4. The orthogonal eigenvector matrix X determines the graphs

After the introduction in Section 2 and the discussion in 3, we now prove our main result:

Theorem 2. *Given the orthogonal eigenvector matrix X of the adjacency matrix A of an undirected, simple graph that is not the empty graph, then that adjacency matrix A can be retrieved.*

Since the empty graph trivially possesses any orthogonal X matrix with eigenvalue vector $\lambda = 0$, we exclude this extreme case. Theorem 2 implies that the orthogonal eigenvector matrix X of the adjacency matrix A of an undirected, simple graph specifies that graph, except for the empty graph.

Proof of Theorem 2. Given the orthogonal eigenvector matrix X of the adjacency matrix A of an undirected graph, the Hadamard product $\Xi = X \circ X$ in (5) can be computed.

If the matrix Ξ has $n \geq 1$ eigenvectors belonging to the zero eigenvalue, then $\text{rank}(\Xi) = N - n$ and the dimension n of the kernel or null space obeys $1 \leq n \leq N - 1$, because $1 \leq \text{rank}(\Xi) \leq N - 1$. The kernel space corresponding to Ξ is spanned by n linearly independent, real vectors $v_1, v_2, \ldots, v_n$ and each vector v_m of the kernel space is orthogonal to all the row vectors of the matrix Ξ. The eigenvalue vector λ, which obeys $\Xi\lambda = 0$ in (13), can thus be written as a linear combination of the n independent kernel vectors

$$\lambda = \sum_{m=1}^{n} \beta_m v_m \tag{16}$$

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

where β_m for $1 \le m \le n$ are real, unknown numbers. The adjacency matrix $A = X\Lambda X^T$ is constructed with (16) as

$$A = \sum_{m=1}^{n} \beta_m X \mathrm{diag}\,(v_m)\, X^T \tag{17}$$

and each element is $a_{ij} = \sum_{m=1}^{n} \beta_m \left(X \mathrm{diag}\,(v_m)\, X^T\right)_{ij}$.

We remark that $\left(X \mathrm{diag}\,(v_m)\, X^T\right)_{jj} = 0$ for any $1 \le j \le N$. Indeed, using $X \mathrm{diag}(q)\, X^T = \sum_{k=1}^{N} q_k x_k x_k^T$ and $\left(x_k x_k^T\right)_{ij} = (x_k)_i\,(x_k)_j$, yields

$$\left(X \mathrm{diag}\,(v_m)\, X^T\right)_{jj} = \left(\sum_{k=1}^{N} (v_m)_k\, x_k x_k^T\right)_{jj} = \sum_{k=1}^{N} (v_m)_k\, (x_k)_j^2$$

Row j of the eigenvalue equation (9) in Section 3.1 of the matrix Ξ (with $\Xi_{ij} = (x_j)_i^2$) equals $\sum_{k=1}^{N} (w_l)_k\, (x_k)_j^2 = \xi_l\, (w_l)_j$. Since each vector v_m of the kernel space belongs to eigenvalue $\xi_l = 0$ with multiplicity n in (9), we find that $\left(X \mathrm{diag}\,(v_m)\, X^T\right)_{jj} = 0$. Thus, the information that the diagonal elements, $a_{jj} = 0$ for $1 \le j \le N$, cannot be used to determine the unknowns $\beta_1, \beta_2, \ldots, \beta_n$. Hence, we must invoke the off-diagonal elements of the adjacency matrix.

Any selection of n off-diagonal elements $a_{ij} = \sum_{m=1}^{n} \beta_m \left(X \mathrm{diag}\,(v_m)\, X^T\right)_{ij}$, where $i \neq j$, can be chosen. Without loss of generality, we confine ourselves to n off-diagonal elements that lie on a particular row r, but also n elements a_{ij} on an upper-diagonal (with $j = i + k$ and $k > 0$) may be considered. Row r of the adjacency matrix A, up to column n, is written as the linear set, in which a_{rr} is omitted as equation and replaced by that of element $a_{r;n+1}$,

$$\begin{bmatrix} \left(X \mathrm{diag}\,(v_1)\, X^T\right)_{r1} & \left(X \mathrm{diag}\,(v_2)\, X^T\right)_{r1} & \cdots & \left(X \mathrm{diag}\,(v_n)\, X^T\right)_{r1} \\ \left(X \mathrm{diag}\,(v_1)\, X^T\right)_{r2} & \left(X \mathrm{diag}\,(v_2)\, X^T\right)_{r2} & \cdots & \left(X \mathrm{diag}\,(v_n)\, X^T\right)_{r2} \\ \vdots & \vdots & \ddots & \vdots \\ \left(X \mathrm{diag}\,(v_1)\, X^T\right)_{rn} & \left(X \mathrm{diag}\,(v_2)\, X^T\right)_{rn} & \cdots & \left(X \mathrm{diag}\,(v_n)\, X^T\right)_{rn} \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_n \end{bmatrix} = \begin{bmatrix} a_{r1} \\ a_{r2} \\ \vdots \\ a_{rn} \end{bmatrix} \tag{18}$$

The linear set (18) is sufficient to determine all remaining unknowns $\beta_1, \beta_2, \ldots, \beta_n$, provided that the rank of the left-hand side $n \times n$ matrix, say M, is n, else a row different from r of the adjacency matrix A must be taken (or generally a different selection of n off-diagonal elements). The $n \times n$ matrix M with $\mathrm{rank}(M) = n$ can be inverted and the unknowns $\beta_1, \beta_2, \ldots, \beta_n$ can be expressed in terms of the partial row vector $(a_{r1}, a_{r2}, \ldots, a_{rn})$. The only complicating factor is that the partial row vector $(a_{r1}, a_{r2}, \ldots, a_{rn})$ is not precisely known, only that each element is either zero or one. A recipe for any chosen row $1 \le r \le N$ is to (i) create all $2^n - 1$ possible partial, zero-one row vectors $(a_{r1}, a_{r2}, \ldots, a_{rn})$, excluding all zeros, (ii) determine all unknowns $\beta_1, \beta_2, \ldots, \beta_n$

by solving the set (18) and (iii) compute the eigenvalue vector λ from (16) and (iv) check whether the resulting matrix $X\,\mathrm{diag}(\lambda)\,X^T$ is a zero-one matrix, which is a possible adjacency matrix corresponding to the orthogonal eigenvector matrix X. Equation $\Xi\lambda = 0$ in (13) ensures that there must at least be one partial row vector $(a_{r1}, a_{r2}, \ldots, a_{rn})$ out of the $2^n - 1$ possible combinations that leads to a zero-one matrix.

We cannot exclude, however, that only one adjacency matrix is retrieved. In other words, it may happen that $l > 1$ different adjacency matrices of l different undirected graphs are found, that all possess the same orthogonal eigenvector matrix X, but a different eigenvalue vector λ. □

5. Consequences of Theorem 2

If $\mathrm{rank}(\Xi) < N - 1$, then the proof of Theorem 2 shows that the orthogonal eigenvector matrix X may specify more than one undirected graph. Such graphs are called "co-eigenvector graphs" and possess a same orthogonal eigenvector matrix X, but a different eigenvalue vector λ, as opposed to co-spectral graphs that have a same eigenvalue vector λ, but a different orthogonal eigenvector matrix X. Only if $\mathrm{rank}(\Xi) = N - 1$, the eigenvalue equation $\Xi\lambda = 0$ in (13) possesses one eigenvalue vector λ and we find immediately from Theorem 2

Corollary 1. *The orthogonal eigenvector matrix X of the adjacency matrix A of an undirected graph only specifies the graph uniquely if rank*$(\Xi) = N - 1$.

The proof of Theorem 2 fundamentally relies on the zero-one matrix structure when $\mathrm{rank}(\Xi) < N - 1$ to recover the adjacency matrix A from the orthogonal eigenvector matrix X and thus excludes an extension towards weighted graphs. However, if $\mathrm{rank}(\Xi) = N - 1$, then also a weighted adjacency matrix, apart from a scaling factor β, can be recovered.

Fig. 1 shows the metacode of a graph recovery algorithm, based on the proof of Theorem 2 in Section 4.

If $\mathrm{rank}(\Xi) = N - n$ with $n > 1$ and if $n = O(N^\gamma)$ for large N and $0 < \gamma \leq 1$, meaning that the dimension $n \simeq \alpha N^\gamma$ of the kernel space increases with the number N of nodes, then the proof of Theorem 2 and the corresponding metacode in Fig. 1 looses computational efficiency, because $2^n \sim 2^{\alpha N^\gamma}$ (in the loop in line 6 in Fig. 1) increases non-polynomially fast with size N of the graph, pointing towards (but not proving) the NP-hard nature of the graph recovery problem in the worst case. In the worst case of low $\mathrm{rank}(\Xi)$ or high n, one might argue that the proof of Theorem 2 is hardly better than the trivial method of finding the eigenvector λ by inversion of (1), i.e. finding the adjacency matrix A that diagonalizes $X^T A X = \Lambda$, by checking all $2^{\binom{N}{2}}$ possible $N \times N$ adjacency matrices. Since X is the orthogonal eigenvector matrix of "a particular" adjacency matrix, we certainly know that at least one of all possible $N \times N$ adjacency matrices converts $X^T A X$ to a diagonal matrix Λ. However, extensive simulations so far

GRAPH RECOVERY

input: orthogonal matrix X with N orthonormal eigenvectors of A
output: adjacency matrix A

1. $\Xi \leftarrow X \circ X$ Hadamard product
2. $n \leftarrow$ size of the kernel space of Ξ
3. v_i with $i \in \{1, 2, \cdots, n\} \leftarrow$ eigenvectors of Ξ obeying $\Xi v_i = 0$
4. $C_{(\{1,2,\ldots,N^2\},i)} \leftarrow \mathrm{vec}(X\mathrm{diag}(v_i)X^T)$ for $i \in \{1, 2, \cdots, n\}$
5. $M_{n\times n} \leftarrow n$ non-zero rows j of C,
   where $j \neq k(N+1)+1$, $k \in \{0, 1, \ldots, N-1\}$ —
   such that $\mathrm{rank}(M) = n$

6. **For** $(j \leftarrow 1$ to $2^n - 1)$ **do**
7. $\quad \hat{a}_{n\times 1} \leftarrow$ binary representation in n digits of j
8. $\quad \hat{\beta}_{n\times 1} \leftarrow M^{-1}\hat{a}$
9. $\quad \hat{\lambda}_{N\times 1} \leftarrow \sum_{i=1}^{n} \hat{\beta}_i v_i$
10. $\quad \hat{A}_{N\times N} \leftarrow X\mathrm{diag}(\hat{\lambda})X^T$
11. $\quad$ **If** ($\hat{A}$ contains only ones and zeros)
12. $\quad\quad$ return $\hat{\lambda}$, $\hat{A}$
13. $\quad$ **End If**
14. **End For**

Fig. 1. Metacode of the algorithm for graph recovery, given the orthogonal eigenvector matrix X.

indicate that $\mathrm{rank}(\Xi) < N-1$ occurs for relatively small graphs and is extremely rare for large N. In other words, for large graphs, nearly always $\mathrm{rank}(\Xi) = N-1$ holds, so that Corollary 1 applies.

Fig. 2 and 3 exemplify the existence of co-eigenvector graphs.

When $X = \frac{1}{\sqrt{n}} H_n$ is given for $n = 8$, then $\mathrm{rank}(\Xi) = 1$ as shown in Section 3.3 and the algorithm in Fig. 1 finds $2^{n-1} = 128$ labeled co-eigenvector graphs, that are all regular graphs with integer eigenvalues. Indeed, any regular graph has all eigenvectors, except for the principal eigenvector $x_1 = u$, orthogonal to the all-one vector u and thus shares a common basis of eigenvectors with the complete graph. Regular graphs are further examined in Section 6.1.

Fig. 4 presents some co-eigenvector graphs of the line or path topology.

6. Properties of co-eigenvector graphs

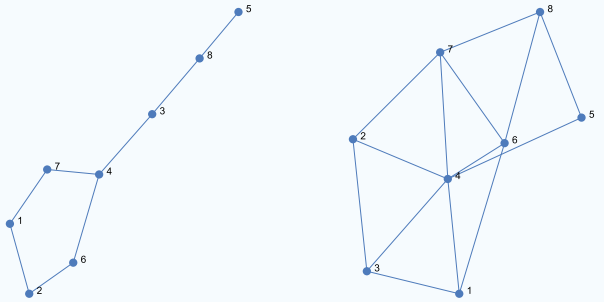
Section 4 has demonstrated that co-eigenvector graphs can exist, provided that $\mathrm{rank}(\Xi) < N-1$. In this Section 6, we deduce some properties of two co-eigenvector graphs $G_1(\mathcal{N}, \mathcal{L}_1)$ and $G_2(\mathcal{N}, \mathcal{L}_2)$ on N nodes, that possess the same eigenvectors, but a different set of eigenvalues:

$$\begin{cases} A_1 = X\Lambda_1 X^T = \sum_{i=1}^{N} \lambda_i(A_1)\, x_i x_i^T \\ A_2 = X\Lambda_2 X^T = \sum_{i=1}^{N} \lambda_i(A_2)\, x_i x_i^T \end{cases} \tag{19}$$

where the $N \times N$ diagonal matrices Λ_1 and Λ_2 contain on the main diagonal the eigenvalues of the adjacency matrices A_1 and A_2, respectively.

$$X = \begin{bmatrix} -0.1229 & -0.6015 & -0.1348 & -0.2361 & 0.3717 & 0.4237 & 0.3342 & 0.3461 \\ -0.1229 & 0.6015 & -0.1348 & -0.2361 & -0.3717 & 0.4237 & 0.3342 & 0.3461 \\ 0.4625 & 0 & -0.2935 & -0.5802 & 0 & -0.1881 & -0.4653 & 0.3338 \\ -0.6034 & 0 & -0.2508 & 0.1914 & 0 & -0.4989 & -0.1008 & 0.5266 \\ 0.1581 & 0 & -0.4919 & 0.5960 & 0 & 0.4606 & -0.3969 & 0.0906 \\ 0.3665 & -0.3717 & 0.3052 & 0.2745 & -0.6015 & -0.0978 & 0.1584 & 0.4031 \\ 0.3665 & 0.3717 & 0.3052 & 0.2745 & 0.6015 & -0.0978 & 0.1584 & 0.4031 \\ -0.3132 & 0 & 0.6216 & -0.0970 & 0 & 0.3542 & -0.5850 & 0.1960 \end{bmatrix}$$

G_1 G_2



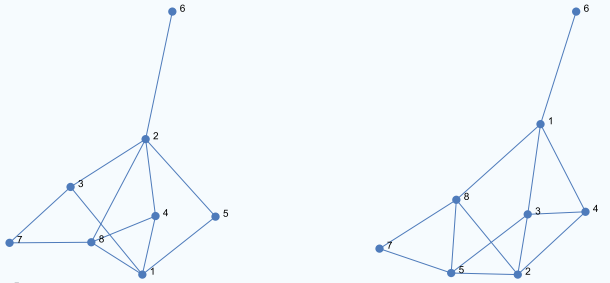
$\lambda(G_1) = [-1.9816\ -1.6180\ -1.2635\ -0.1627\ 0.6180\ 0.7691\ 1.4739\ 2.1648]$

$\lambda(G_2) = [-1.8360\ \ 0.6180\ \ 1.7733\ \ 0.4839\ \ -1.6180\ \ -1.8524\ \ -1.2199\ \ 3.6511]$

Fig. 2. Example of two co-eigenvector graphs.

$$X = \begin{bmatrix} -0.4466 & -0.0993 & 0.4895 & 0.2580 & -0.3541 & 0.4121 & 0.0986 & -0.4238 \\ -0.5064 & -0.1988 & -0.4582 & -0.0438 & 0.0923 & -0.3272 & -0.4012 & -0.4643 \\ 0.4177 & -0.1223 & -0.1963 & 0.4850 & -0.3963 & -0.4053 & 0.3262 & -0.3303 \\ 0.2086 & 0.5953 & -0.2222 & 0.3117 & 0.3773 & 0.3824 & -0.1069 & -0.3945 \\ 0.3275 & 0.2108 & -0.0450 & -0.5620 & -0.5754 & 0.1277 & -0.3378 & -0.2624 \\ 0.1740 & 0.1406 & 0.6590 & 0.1150 & 0.2030 & -0.4918 & -0.4478 & -0.1372 \\ -0.2624 & 0.4710 & 0.1052 & -0.3990 & 0.0815 & -0.3546 & 0.5950 & -0.2297 \\ 0.3460 & -0.5434 & 0.1232 & -0.3329 & 0.4333 & 0.1695 & 0.2069 & -0.4469 \end{bmatrix}$$

G_1 G_2



$\lambda(G_1) = [\ -2.9101\ \ -1.4136\ \ -0.6953\ \ -0.3811\ \ 0.4548\ \ 0.6653\ \ 0.8960\ \ 3.3841]$

$\lambda(G_2) = [-2.5665\ -0.7062\ 0.7428\ 2.2432\ -1.7438\ -0.8379\ -0.2201\ 3.0886]$

Fig. 3. Example of two other co-eigenvector graphs.

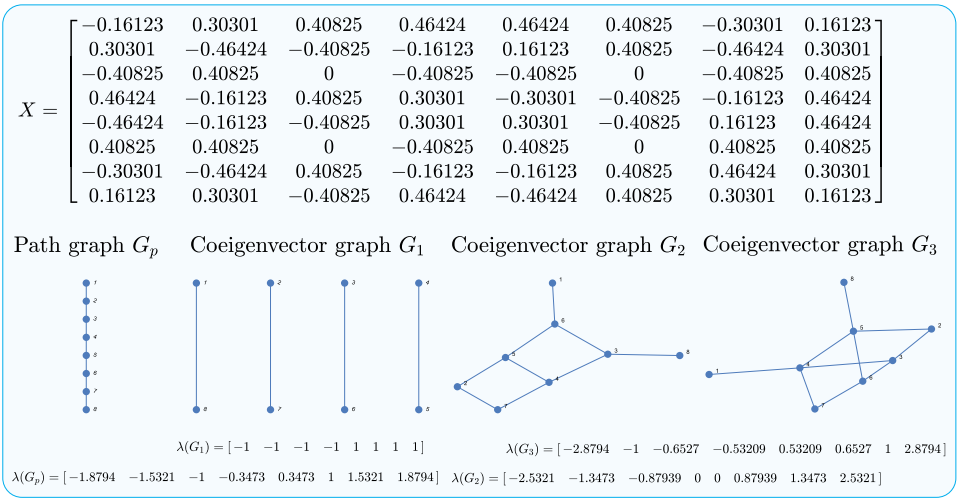


Fig. 4. Example of co-eigenvector graphs of a line topology on $N = 8$ nodes.

First, the sum of the adjacency matrices A_1 and A_2

$$A_1 + A_2 = \sum_{i=1}^{N} (\lambda_i(A_1) + \lambda_i(A_2))\, x_i x_i^T \tag{20}$$

again represents an adjacency matrix, provided that the existence of a link, i.e. $(A_1)_{ij} = 1$, between node i and j in the graph G_1 implies the non-existence of a link, i.e. $(A_2)_{ij} = 0$, in G_2. In other words, $A_1 + A_2$ is an adjacency matrix if the graphs G_1 and G_2 do not share common links (i.e. $|\mathcal{L}_1 \cap \mathcal{L}_2| = 0$). In Theorem 4 below, we derive the number of common links between two co-eigenvector graphs explicitly. Second, the product of the adjacency matrices A_1 and A_2

$$A_1 A_2 = \sum_{i=1}^{N} \lambda_i(A_1)\lambda_i(A_2) x_i x_i^T, \tag{21}$$

contains the same set of eigenvectors as A_1 and A_2 due to orthogonality of the eigenvectors. Lemma [1, p. 392] indeed tells us that if any two matrices B and C have a common complete set of eigenvectors, then B and C commute. Relation (21) may be regarded as another demonstration of that Lemma. The diagonal element $(A_1 A_2)_{ii} = \sum_{k=1}^{N} (A_1)_{ik}(A_2)_{ik}$ equals the number of common neighbors of node i in G_1 and G_2, i.e. each node k for which $(A_1)_{ik} = (A_2)_{ik} = 1$.

The $N \times N$ Hadamard product $A_c = A_1 \circ A_2$ represents the adjacency matrix of the graph $G_c(\mathcal{N}_c, \mathcal{L}_c)$, composed of common links $\mathcal{L}_c = \mathcal{L}_1 \cap \mathcal{L}_2$ between G_1 and G_2,

$$A_c = \left(\sum_{i=1}^{N} \lambda_i(A_1) x_i x_i^T \right) \circ \left(\sum_{j=1}^{N} \lambda_j(A_2) x_j x_j^T \right). \tag{22}$$

Using the distributive property of a Hadamard product [10, p. 32], we transform (22) as

$$A_c = \sum_{i=1}^{N}\sum_{j=1}^{N} \lambda_i(A_1)\lambda_j(A_2)\left(x_i x_i^T\right) \circ \left(x_j x_j^T\right).$$

The Hadamard product of outer products $x_i x_i^T$ and $x_j x_j^T$ is written [10] as

$$\left(x_i x_i^T\right) \circ \left(x_j x_j^T\right) = \mathrm{diag}(x_i) x_j x_j^T \mathrm{diag}(x_i) = \left(x_i \circ x_j\right)\left(x_i \circ x_j\right)^T$$

simplifying (22) further as

$$A_c = \sum_{i=1}^{N}\sum_{j=1}^{N} \lambda_i(A_1)\lambda_j(A_2)\left(x_i \circ x_j\right)\left(x_i \circ x_j\right)^T. \tag{23}$$

Definition 3. Two co-eigenvector graphs G_1 and G_2 are called non-overlapping if they do not share common links.

Another way to determine the number of common links between G_1 and G_2 is by summing the elements of the product $A_1 A_2$ on the main diagonal

$$2|\mathcal{L}_1 \cap \mathcal{L}_2| = \mathrm{trace}\left(A_1 A_2\right). \tag{24}$$

Theorem 4. *Consider two co-eigenvector graphs $G_1(\mathcal{N}, \mathcal{L}_1)$ and $G_2(\mathcal{N}, \mathcal{L}_2)$ on N nodes, defined by the $N \times N$ adjacency matrices A_1 and A_2, respectively. Graphs G_1 and G_2 are non-overlapping if their eigenvalue vectors are orthogonal.*

Proof. Since the graph G_c, with the $N \times N$ adjacency matrix A_c defined in (23), is composed of common links between G_1 and G_2, twice the number of common links between the co-eigenvector graphs G_1 and G_2 equals the sum of elements of A_c

$$2|\mathcal{L}_1 \cap \mathcal{L}_2| = u^T\left(A_1 \circ A_2\right)u = u^T A_c u \tag{25}$$

where u denotes the all-one vector. By substituting (23) into (25) we obtain

$$2|\mathcal{L}_1 \cap \mathcal{L}_2| = \sum_{i=1}^{N}\sum_{j=1}^{N} \lambda_i(A_1)\lambda_j(A_2) u^T \left(x_i \circ x_j\right)\left(x_i \circ x_j\right)^T u.$$

The inner product $\left(x_i \circ x_j\right)^T u = x_i^T x_j$ equals 1 if $i = j$, otherwise 0, because the eigenvectors of a symmetric adjacency matrix are orthogonal. Thus, relation (25) simplifies to

$$2|\mathcal{L}_1 \cap \mathcal{L}_2| = \left(\lambda(A_1)\right)^T \lambda(A_2). \tag{26}$$

Since "non-overlapping" in Definition 3 means that $|\mathcal{L}_1 \cap \mathcal{L}_2| = 0$, relation (26) completes the proof. □

Theorem 4 states that if two co-eigenvector graphs G_1 and G_2 do not share common links, their eigenvalue vectors $\lambda(A_1)$ and $\lambda(A_2)$ are orthogonal. The vectors $\lambda(A_1)$ and $\lambda(A_2)$ span the kernel space of the $N \times N$ matrix $\Xi = X \circ X$, as shown in the proof of Theorem 2, provided that $\text{rank}(\Xi) = N - 2$. The sum of two non-overlapping co-eigenvector graphs A_1 and A_2 is another co-eigenvector graph $A_s = A_1 + A_2$, with the eigenvalue vector $\lambda(A_s) = \lambda(A_1) + \lambda(A_2)$, as derived in (20). Thus, the eigenvalue vector $\lambda(A_s)$ also lies in the kernel space of the matrix Ξ, and, hence, $\text{rank}(\Xi) \leq N - 2$.

The Hadamard product in (23) allows us to determine the number of non-common links in G_1 and G_2.

Corollary 2. *Consider a pair of co-eigenvector graph $G_1(\mathcal{N}, \mathcal{L}_1)$ and $G_2(\mathcal{N}, \mathcal{L}_2)$ on N nodes with corresponding adjacency matrices A_1 and A_2, respectively. The number of non-common links in G_1 and G_2 is given by*

$$|\mathcal{L}_1 \setminus \mathcal{L}_2| + |\mathcal{L}_2 \setminus \mathcal{L}_1| = \sum_{i=1}^{N} \left(\lambda_i(A_1) - \lambda_i(A_2)\right)^2 \tag{27}$$

Proof. A graph $G_u\left(\mathcal{N}, (\mathcal{L}_1 \setminus \mathcal{L}_2) \cup (\mathcal{L}_2 \setminus \mathcal{L}_1)\right)$ contains only non-common links of G_1 and G_2 and has the corresponding $N \times N$ adjacency matrix $A_u = A_1 + A_2 - 2\,(A_1 \circ A_2)$. By using the identity $A \circ A = A$, that holds for any zero-one matrix, and importing (23), we obtain

$$\begin{aligned} A_u &= A_1 \circ A_1 + A_2 \circ A_2 - 2\,(A_1 \circ A_2) \qquad (28)\\ &= \sum_{i=1}^{N}\sum_{j=1}^{N} \left(\lambda_i(A_1)\lambda_j(A_1) + \lambda_i(A_2)\lambda_j(A_2) - 2\lambda_i(A_1)\lambda_j(A_2)\right)(x_i \circ x_j)\,(x_i \circ x_j)^T \end{aligned}$$

from which the number of not-common links in G_1 and G_2 is computed as the sum of elements of A_u

$$u^T A_u u = \sum_{i=1}^{N} \left(\lambda_i^2(A_1) + \lambda_i^2(A_2) - 2\lambda_i(A_1)\lambda_i(A_2)\right),$$

which completes the proof. □

An equivalent way to compute the number of not-common links in G_1 and G_2 is to subtract twice the number of common links in G_1 and G_2 from the sum of elements of $A_1 + A_2$

$$|\mathcal{L}_1 \setminus \mathcal{L}_2| + |\mathcal{L}_2 \setminus \mathcal{L}_1| = u^T\,(A_1 + A_2)\,u - 2 \cdot \text{trace}\,(A_1 A_2)\,, \tag{29}$$

which, after substituting (20) and (21) again leads to (27). The adjacency matrix A_u with only non-common links in G_1 and G_2 in (28), using the distributive property of the Hadamard product, can be transformed into

$$A_u = (A_1 - A_2) \circ (A_1 - A_2), \tag{30}$$

where relation (30) holds for adjacency matrices A_1 and A_2 of any two unweighted graphs G_1 and G_2.

6.1. Regular graphs

In a regular graph G_r on N nodes, defined by the $N \times N$ adjacency matrix A_r, each node has the same degree r. The complement graph G_r^c of G_r is also a regular graph with degree $q = N - 1 - r$ and the $N \times N$ adjacency matrix [1, p. 15] is

$$A_r^c = J - I - A_r, \tag{31}$$

where the $N \times N$ all-one matrix is denoted by $J = u.u^T$. Since each node in G_r has degree r, it holds that $A_r u = d_r = ru$. Thus, the principal eigenvalue $\lambda_1(A_r) = r$ corresponds to the principal eigenvector $x_1 = \frac{1}{\sqrt{N}}u$. The remaining $N - 1$ eigenvectors of A_r are orthogonal to u, implying that $u^T x_j = 0$ or

$$\sum_{i=1}^{N} (x_j)_i = 0, \tag{32}$$

where $1 < j \leq N$. The following theorem is also provided in [14, p. 15].

Theorem 5. *A regular graph G_r on N nodes with degree r and its complement graph G_r^c compose a pair of co-eigenvector graphs.*

Proof. By multiplying the $N \times N$ adjacency matrix A_r^c of the complement graph G_r^c, defined in (31), with the eigenvector x_j of A_r, where $j > 1$, we obtain

$$A_r^c x_j = (J - I - A_r)\, x_j.$$

From (32) we conclude that $Jx_j = uu^T x_j = 0$ and the above equation becomes

$$A_r^c x_j = (-1 - \lambda_j(A_r))\, x_j. \tag{33}$$

Additionally, multiplying the adjacency matrix A_c with the principal eigenvector $\frac{1}{\sqrt{N}}u$ yields

$$A_r^c \frac{1}{\sqrt{N}} u = (J - I - A_r) \frac{1}{\sqrt{N}} u = (N - 1 - r_1) \frac{1}{\sqrt{N}} u$$

showing that the adjacency matrix A_r^c shares the same eigenvectors with A_r, which completes the proof. □

Relation (33) shows that the adjacency matrix A_r^c of the complement graph G_r^c of a regular graph possesses the spectral decomposition

$$A_r^c = \frac{N-1-r}{N} uu^T + \sum_{j=2}^{N} (-1-\lambda_j(A_r))\, x_j x_j^T. \tag{34}$$

Theorem 4 states that the eigenvalue vectors $\lambda(A_r)$ and $\lambda(A_r^c)$ are orthogonal. Indeed, the inner product $(\lambda(A_r))^T\lambda(A_r^c)$ transforms, after using (34), into

$$\begin{aligned}(\lambda(A_r))^T\lambda(A_r^c) &= r(N-1-r) + \sum_{j=2}^{N} \lambda_j(A_r)\,(-1-\lambda_j(A_r)) \\ &= r\cdot N - \left(r + \sum_{j=2}^{N} \lambda_j(A_r)\right) - \left(r^2 + \sum_{j=2}^{N} (\lambda_j(A_r))^2\right).\end{aligned} \tag{35}$$

The adjacency matrix A_r represents a simple graph without self-loops and thus $\text{trace}(A_r) = \sum_{i=1}^{N} \lambda_i(A_r) = 0$. Further, the sum of squared eigenvalues is $\sum_{i=1}^{N} (\lambda_i(A_r))^2 = r\cdot N$, simplifying (35) to $(\lambda(A_r))^T \cdot \lambda(A_r^c) = 0$. The following Corollary is proved in [14, p. 15], while we provide another proof.

Corollary 3. *The eigenvectors of a regular graph G_r on N nodes and degree r are also eigenvectors of the complete graph K_N on N nodes, implying that a regular graph G_r and the complete graph K_N compose a pair of co-eigenvector graphs.*

Proof. The sum of adjacency matrices A_r of a regular graph G_r and A_r^c of its complement graph G_r^c establishes the adjacency matrix $J-I = A_r + A_r^c$ of the complete graph K_N, as directly follows from (31). By substituting (20) and (34), the previous relation transforms into

$$J - I = \left(\frac{r}{N} + \frac{N-1-r}{N}\right) \cdot uu^T + \sum_{j=2}^{N} (\lambda_j(A_r) + (-1-\lambda_j(A_r))) \cdot x_j x_j^T,$$

while after grouping terms, the adjacency matrix of the complete graph K_N becomes

$$J - I = \frac{N-1}{N} \cdot uu^T - \sum_{j=2}^{N} x_j \cdot x_j^T, \tag{36}$$

from which we observe that the complete graph K_N, together with a regular graph G_r (or with its complement graph G_r^c) compose a pair of co-eigenvector graphs, which completes the proof. □

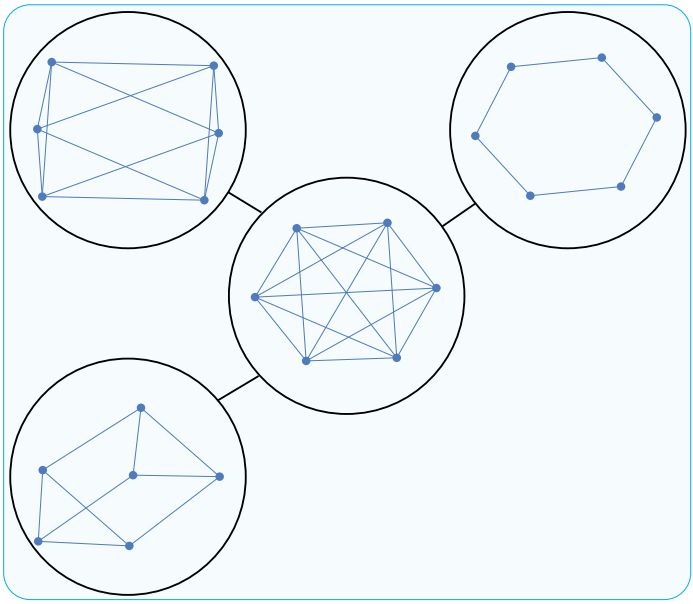


Fig. 5. Example of pairs of regular co-eigenvector graphs on $N = 6$ nodes. Each regular graph is enclosed in a circle, where circles are connected if the two corresponding regular graphs compose a pair of co-eigenvector graphs.

Corollary 4. *Not each set of eigenvectors of the complete graph K_N can represent the eigenvectors of a regular graph G_r.*

Proof. In Section 3.3, we have shown two orthogonal eigenvector matrices of the complete graph with maximally different $\text{rank}(\Xi) = 1$ and $\text{rank}(\Xi) = N - 1$. Corollary 1 tells us that the $N \times N$ eigenvector matrix X_{K_N} in (15) with $\text{rank}(\Xi) = N - 1$ determines the complete graph K_N uniquely. In other words, the eigenvectors in (15) cannot be the eigenvectors of a non-complete regular graph G_r, although the eigenvectors of any regular graph G_r can also be the eigenvectors of the complete graph K_N. As illustrated by X_{K_N} in (15), the reverse does not always hold, which completes the proof. □

Corollary 3 shows that a regular graph G_r together with the complete graph K_N compose a pair of co-eigenvector graphs. However, Corollary 4 informs us that two regular graphs G_{r_1} and G_{r_2} do not form a pair of co-eigenvector graphs, in general. Fig. 5 presents the pairs of co-eigenvector graphs of size $N = 6$ that are regular graphs.

6.2. Irregular co-eigenvector graphs

The definition of co-eigenvector graphs imposes a strong constraint on the $N \times N$ adjacency matrix A of an undirected graph G. The $N \times 1$ all-one vector u is [1, Sec. 3.3] the only eigenvector, corresponding to the principal eigenvalue $\lambda_1 = r$ of a regular graph G_r with degree r. Thus, a regular graph G_r and an irregular graph G_1 cannot form a

pair of co-eigenvector graphs. Therefore, it is relevant to study how often co-eigenvector graphs emerge among irregular graphs.

We consider the $N \times N$ adjacency matrix A_1 of a graph G_1 and the $N \times N$ adjacency matrix A_2 of a relabeled graph G_2, such that

$$A_2 = P^T A_1 P, \tag{37}$$

where the $N \times N$ permutation matrix P [1, p. 43] is an orthogonal matrix, satisfying $P^T P = I$. In other words, the adjacency matrices A_1 and A_2 define two isomorphic graphs. While G_1 and G_2 are co-spectral graphs and share the same set of eigenvalues, because a permutation does not influence eigenvalues [1], they are not a pair of different co-eigenvector graphs.

Graph relabeling does not affect the eigenvalues of an adjacency matrix. On the other side, two isomorphic graphs in general do not constitute a pair of co-eigenvector graphs.

Corollary 5. *Consider a pair of co-eigenvector graphs G_1 and G_2, with the corresponding $N \times N$ adjacency matrices A_1 and A_2. When using the same $N \times N$ permutation matrix P, the relabeled graphs G_1 and G_2 still compose a pair of co-eigenvector graphs.*

Proof. The i-th eigenvector x_i corresponds to the i-th eigenvalue $\lambda_i(A_1)$, but also to the i-th eigenvalue $\lambda_i(A_2)$. After permutation with P, the relabeled eigenvector $P^T x_i$ satisfies the eigenvector equation for both relabeled graphs

$$\begin{aligned} P^T A_1 P(P^T x_i) =& P^T A_1 x_i = \lambda_i(A_1)(P^T x_i) \\ P^T A_2 P(P^T x_i) =& P^T A_2 x_i = \lambda_i(A_2)(P^T x_i), \end{aligned}$$

where $i \in \mathcal{N}$. Thus, relabeled graphs G_1 and G_2 share eigenvectors, which completes the proof. □

Corollary 5 is understood geometrically. The N eigenvectors of an adjacency matrix A define a polytope on N points in the N-dimensional space. If two adjacency matrices A_1 and A_2 form a pair of co-eigenvector graphs, the $N \times N$ eigenvector matrix X of both adjacency matrices contains the same polytope in the N-dimensional space. The permutation matrix P changes the coordinate system, but not the nature of the polytope on N points.

7. Identifying co-eigenvector graphs

We identify pairs of co-eigenvector graphs of different size N. Firstly, for a fixed N, we create all possible unlabeled graphs. The first co-eigenvector graphs, that are *not* regular graphs, occur for $N = 6$. We present an algorithm, with metacode in Fig. 6, for identifying pairs of co-eigenvector graphs, among all possible connected, irregular graphs with N nodes based on permutation or relabeling (Section 6.2). The $N \times N$ adjacency matrix A of each possible unlabeled graph with N nodes is provided as input to the

```
CoEigenvectorGraphs(A_1, A_2, ... A_{N_u})

Input: A_1, A_2, ... A_{N_u}
Output: C
1. C ← O_{N_u × N_u}
2. for i ← 1 to N_u − 1
3.     for j ← i + 1 to N_u
4.         X_i ← N × N eigenvector matrix of A_i
5.         X_j ← N × N eigenvector matrix of A_j
6.         m ← 1
7.         while (C_ij = 0) and (m < N!)
8.             P_m ← N × N m-th permutation matrix
9.             T_i ← (P_m X_i)^T A_j (P_m X_i)
10.            T_j ← (P_m X_j)^T A_i (P_m X_j)
11.            if (I ∘ T_i = T_i) or (I ∘ T_j = T_j)
12.                C_ij ← 1, C_ji ← 1
13.            end if
14.            m ← m + 1
15.        end while
16.    end for
17. end for
18. return C
```

Fig. 6. Pseudocode for identifying co-eigenvector graphs among all possible unlabeled graphs with N nodes (in total N_u of them), provided as input.

algorithm. Using the double for loop (line 2-3), we examine each pair of graphs. Graph relabeling in (37) affects eigenvectors. Therefore, we need to account for each possible permutation whether a pair of non-isomorphic graphs share the same eigenvectors. In line 9, we define each possible $N \times N$ permutation matrix P and observe that the matrix $(PX_j)^T A_i (PX_j)$ is a diagonal matrix only if $(PX_j) = X_i$. The proposed algorithm returns the $N_u \times N_u$ matrix C, whose entry $C_{ij} = 1$ if graphs G_i and G_j share the same eigenvectors, otherwise $C_{ij} = 0$.

Computing all N_u unlabeled graphs on N nodes is intractable for large N, because their number increases as $O\left(\frac{2^{\binom{N}{2}}}{N!}\right)$. Furthermore, the proposed algorithm in Fig. 6 cannot guarantee that each pair of co-eigenvector graphs, for a given network size N, is identified. The limitation is due to the fact that some graphs may contain multiple sets of eigenvectors (i.e. multiple different orthogonal X-matrices), while the algorithm in Fig. 6 computes, for each adjacency matrix A_i, only one $N \times N$ eigenvector matrix X_i (line 4-5).

Some examples of irregular co-eigenvector graphs with $N = 6$ nodes are drawn in Fig. 7. The algorithm identified two triples of co-eigenvector graphs with $N = 6$ nodes. Fig. 8 overviews the identified irregular, connected and unlabeled, co-eigenvector graphs with $N = 7$ nodes.

8. Conclusion and open questions

The proof of Theorem 2 relies on the zero-one structure of the adjacency matrix and reveals that only unweighted graphs can be recovered when $\text{rank}(\Xi) < N-1$. The idea to

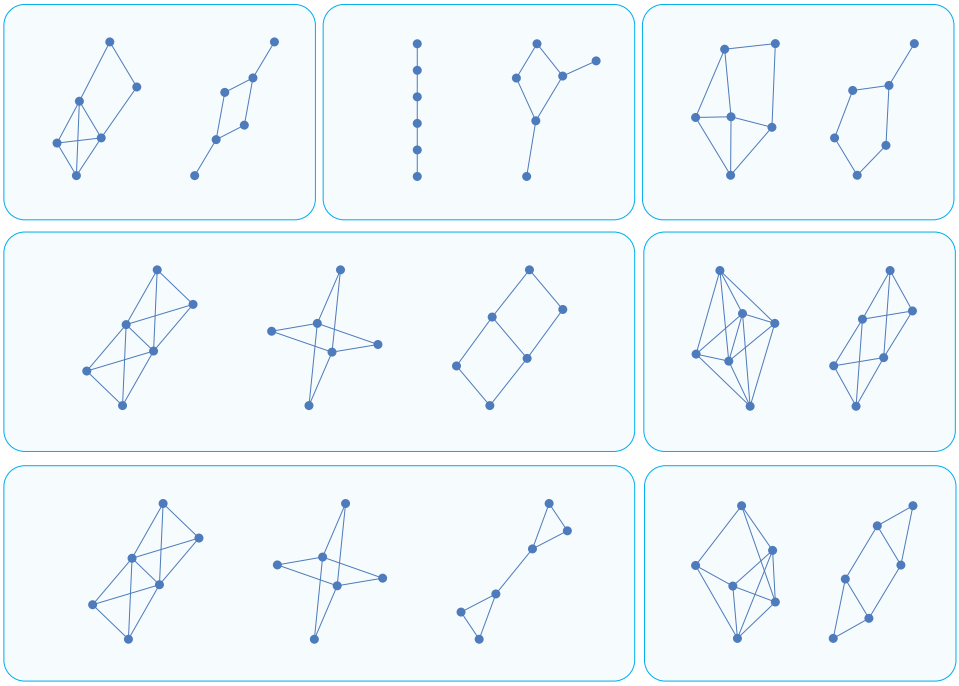


Fig. 7. Pairs of non-regular, unlabeled, co-eigenvector graphs with $N = 6$ nodes.

reconstruct the unweighted, undirected graph from the orthogonal eigenvector matrix X of the adjacency matrix A can be extended similarly to the orthogonal eigenvector matrix Z of the Laplacian $Q = \Delta - A$. The remainder of the paper has deduced properties of co-eigenvector graphs. In particular, irregular co-eigenvector graphs, that are less trivial to find than their regular companions, are found by a rather exhaustive algorithm, based on Theorem 2 and the rank of the matrix Ξ.

A deeper knowledge of the matrix Ξ is desirable. The meaning of the rank(Ξ) turns out to be difficult. For example, if the graph is connected, then rank(Ξ) can be smaller than $N - 1$. The reverse also is observed: if rank(Ξ) $= N - 1$, then the graph can be disconnected. The relation between rank(Ξ) and the number of distinct eigenvalues of the adjacency matrix A is also unclear. The relation to the diameter of the graph needs to be investigated. It is also unclear whether the matrix Ξ is diagonalizable. Since Ξ is doubly-stochastic, the underlying associated Markov graph is connected and the matrix Ξ is irreducible [15]. However, an irreducible matrix may still possess a Jordan block. Another question concerns the number of co-eigenvector graphs of size N and its relation to rank(Ξ). Simulations suggest that the less structure or symmetry a graph possesses, the higher the probability that rank(Ξ) $= N - 1$.

Earlier [16], the reconstructability coefficient θ was defined as the smallest value of m in $\widetilde{A} = \sum_{k=1}^{m} \lambda_k x_k x_k^T$ that allows us to exactly reconstruct the zero-one adjacency matrix A. Fig. 9 seems to suggest for small Erdős-Rényi graphs that there is hardly

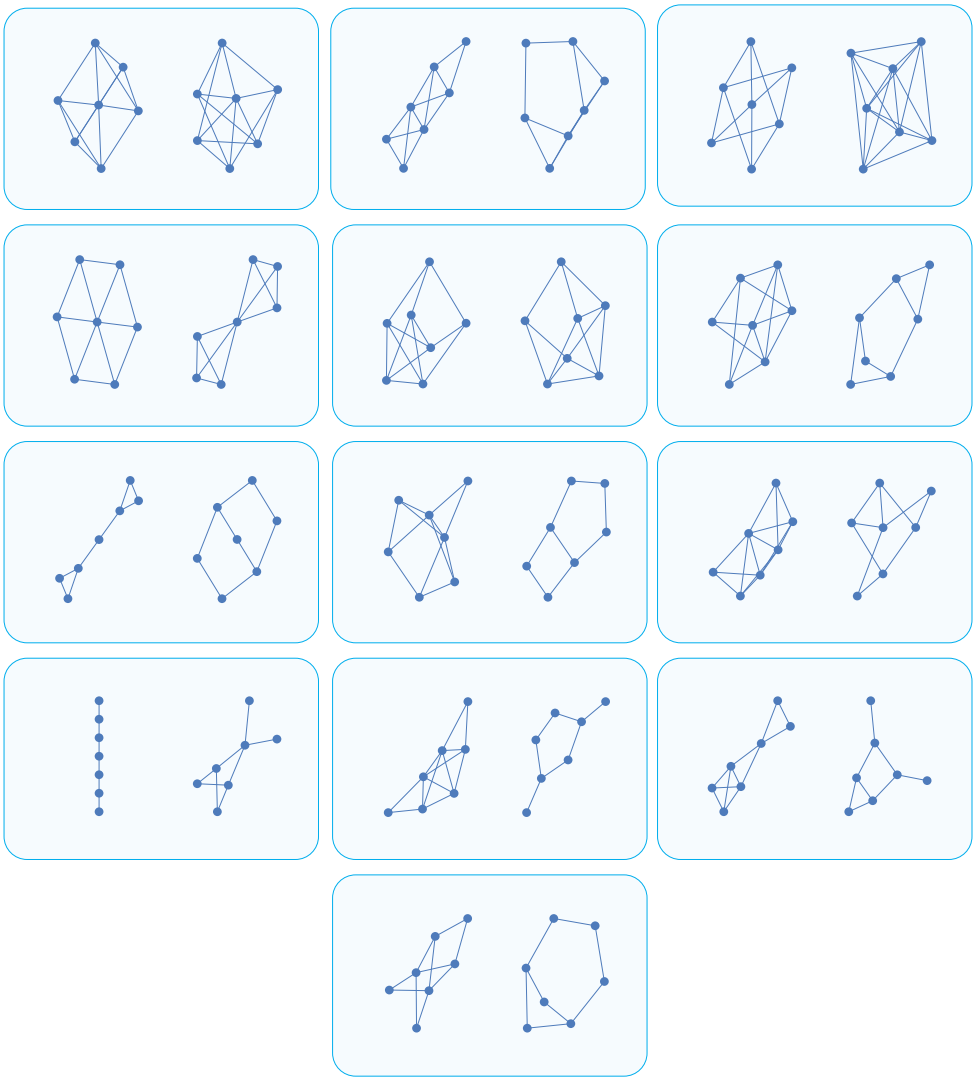


Fig. 8. Pairs of non-regular, unlabeled, co-eigenvector graphs with $N = 7$ nodes.

any correlation between the reconstructability coefficient θ and rank(Ξ). Perhaps, other graph classes or/and larger graphs may reveal a relation?

Furthermore, one may ask whether the confinement to undirected graphs, that possess a symmetric adjacency matrix, can be relaxed to directed graphs, whose general eigenvector matrix X may be complex. If that extension is favorable, one may consider Hermitian matrices, which may open possible applications to quantum mechanics and quantum computing. Data measured over time on complex networks is often related to a dynamic process that runs on the underlying graph. If that dynamic process is linear or proportional to the graph (as e.g. the flow of currents in a resistor or impedance network

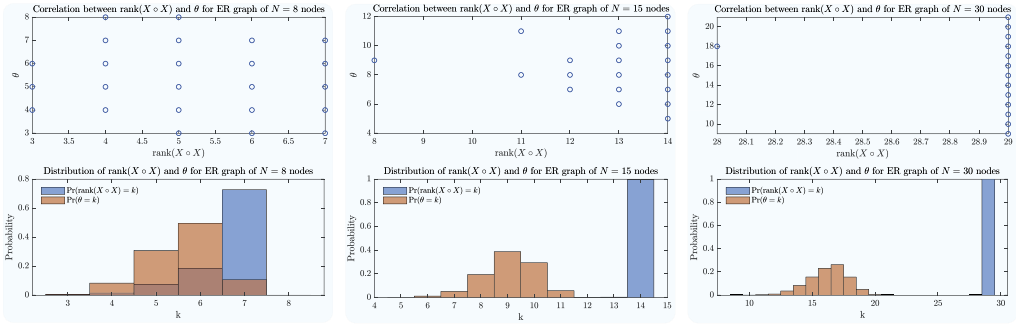


Fig. 9. Correlation between reconstructability coefficient θ and the rank(Ξ) for ER graphs with $N = 8$ (left-hand side figures), $N = 15$ (figures in the middle) and $N = 30$ nodes (right-hand side figures). The link density p is varied between $p = \frac{3 \log N}{4N}$ and $p = \frac{3 \log N}{2N}$, while 10^5 connected graphs are generated for each network size N.

[17]), then the eigendecomposition of the graph is reflected by that data and Theorem 2 may provide insight in the underlying topology on which data is collected.

At last, from an information theoretical point of view discussed in [18], Theorem 2 is not surprising, because the presentation of the orthogonal X matrix needs more digits (i.e. more information) than the zero-one adjacency matrix.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

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

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