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On the inverse of the adjacency matrix of a graph

Abstract

A real symmetric matrix $\mathbf{G}$ with zero diagonal encodes the adjacencies of the vertices of a graph G with weighted edges and no loops. A graph associated with a $n \times n$ non–singular matrix with zero entries on the diagonal such that all its $(n-1) \times (n-1)$ principal submatrices are singular is said to be a NSSD. We show that the class of NSSDs is closed under taking the inverse of $\mathbf{G}$. We present results on the nullities of one– and two–vertex deleted subgraphs of a NSSD. It is shown that a necessary and sufficient condition for two–vertex deleted subgraphs of G and of the graph $\Gamma(\mathbf{G}^{-1})$ associated with $\mathbf{G}^{-1}$ to remain NSSDs is that the submatrices belonging to them, derived from $\mathbf{G}$ and $\mathbf{G}^{-1}$, are inverses. Moreover, an algorithm yielding what we term plain NSSDs is presented. This algorithm can be used to determine if a graph G with a terminal vertex is *not* a NSSD.

Keywords

singular graph • adjacency matrix • nullity • SSP model • inverse of a graph • vertex–deleted subgraphs • NSSD

MSC:

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1. Introduction

The search for molecular graphs that conduct or bar conduction leads to the investigation of a class of graphs which we term NSSDs (Non–Singular graphs with a Singular Deck) with an invertible real symmetric adjacency matrix, having zero diagonal entries, that becomes singular on deleting any vertex. We study the remarkable properties of NSSDs and prove in Theorem 5 that the set of NSSDs is closed under taking the inverse of the adjacency matrix. Since conduction or insulation depends sensitively on the connecting pair of single atoms of the molecule in the circuit represented by the vertices x and y of the graph G, we choose to focus on the vertices x and y by using the block matrix for the adjacency matrix $\mathbf{G}$ of G:

$$\mathbf{G} = \begin{pmatrix} \mathbf{P}_{xy} & \mathbf{R}_{xy} \\ \mathbf{R}_{xy}^{\mathsf{T}} & \beta_{xy}\mathbf{U} \end{pmatrix}. \tag{1}$$

Note that the two last–labelled vertices of G are x and y, with $\mathbf{P}_{xy}$ a square matrix, $\mathbf{U} = \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$ and $\beta_{xy} = 0$ if and only if $\{x, y\}$ is a non–edge of the graph associated with $\mathbf{G}$.

The paper is organised as follows. In Section 2, we introduce the class of NSSDs and other relevant results from matrix theory. We show, in Section 3, that even paths P_{2k}, $k \in \mathbb{N}$, are NSSDs and for a NSSD G associated with adjacency matrix $\mathbf{G}$, there corresponds the graph $\Gamma(\mathbf{G}^{-1})$ which is also a NSSD. The vertices of the graph $\Gamma(\mathbf{G}^{-1})$ associated with the adjacency matrix $\mathbf{G}^{-1}$ (determined by the zero and non–zero pattern of the entries of $\mathbf{G}^{-1}$) are indexed according

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to the rows and columns of $\mathbf{G}$. We establish a set of equations which relate the submatrices of $\mathbf{G}$ and $\mathbf{G}^{-1}$. These equations are then used in Section 4 to construct the nullspace of one–vertex deleted subgraphs of $\mathbf{G}$ and of $\mathbf{G}^{-1}$, and to present results pertaining to these submatrices. In Section 5, we examine two–vertex deleted subgraphs of NSSDs. In particular, we determine the nullity of the matrix $\mathbf{G}^{-1} - \mathbf{v} - \mathbf{w}$, whose value depends on whether $\{v, w\}$ is an edge or a non-edge of G. Moreover, for a NSSD G, we show that the $(n-2) \times (n-2)$ submatrix $\mathbf{G} - \mathbf{v} - \mathbf{w}$ is the inverse of $\mathbf{G}^{-1} - \mathbf{v} - \mathbf{w}$ if and only if the edge $\{v, w\}$ is a pendant edge in G. In the last part of this section we present an algorithm yielding what we term a plain NSSD.

2. Preliminaries

Within the graph-theoretical SSP (Source-and-Sink Potential) model, transmission of electrons at a particular energy λ, through a molecular framework of carbon atoms (or molecular graph) G, connected to two semi–infinite wires in a circuit, depends sensitively on the electron energy, on the choice of single atom contacts (represented by vertices of the graph), and on the electronic structure of the molecule itself. A graph G has a vertex set $\mathcal{V}_G = \{1, 2, \dots, n\}$, representing the n arbitrarily labelled (carbon) atoms in the molecule, and a set $\mathcal{E}_G$ of $m(G)$ edges consisting of unordered pairs of distinct vertices. These edges represent the sigma bonds in the Π–electron system of the molecule. The complete graph on n vertices is denoted by K_n.

The linear transformations, which we choose to encode the structure of a graph G up to isomorphism, are the $n \times n$ real and symmetric edge-weighted adjacency matrices $\{\mathbf{G}\}$ of G. For an arbitrary labelling of the vertices of the graph G, the ij^{th} entry of an adjacency matrix $\mathbf{G}$ is non–zero if $\{i, j\}$ is an edge and zero otherwise. The diagonal entries are taken to be zero. The eigenvectors $\mathbf{x}$ satisfying $\mathbf{G}\mathbf{x} = \lambda\mathbf{x}$ yield the spectrum (or set of eigenvalues $\{\lambda\}$) of $\mathbf{G}$. If the edge weights of a molecular graph are taken to be one, then the eigenvalues are the electron energy levels in the Π–system represented by G as approximate solutions of Schrödinger's linear partial differential equation of the wave function of the quantum mechanical system describing the molecule. Different labellings of the vertices of G yield similar matrices and hence an invariant spectrum. Let $\mathbf{I}$ denote the identity matrix. The characteristic polynomial $\phi(\mathbf{M}, \lambda)$ of a square $n \times n$ matrix $\mathbf{M}$, over a field F, is $\det(\lambda\mathbf{I} - \mathbf{M})$, denoted also by $|\lambda\mathbf{I} - \mathbf{M}|$, which is a polynomial in λ of degree n whose roots (in the algebraic closure of F) are the eigenvalues of $\mathbf{M}$. The algebraic multiplicity of an eigenvalue λ is the number of times it appears in the spectrum of $\mathbf{M}$. If $\mathbf{M}$ is real and symmetric, then the eigenvalues are real.

Here we consider only $n \times n$ adjacency matrices $\{\mathbf{G}\}$ of parent graphs $\{G\}$ (and their vertex–deleted subgraphs) where $\mathbf{G}$ is a non–singular matrix with zero diagonal. We write $\Gamma(\mathbf{G})$ for the graph determined by matrix $\mathbf{G}$.

Definition 1.

A graph $G = \Gamma(\mathbf{G})$ is said to be a *NSSD* if $\mathbf{G}$ is a non–singular, real and symmetric matrix with each entry of the diagonal equal to zero, and such that all the $(n-1) \times (n-1)$ principal submatrices of $\mathbf{G}$ are singular.

The choice for the term NSSD will be clear from Theorem 5 by connotation with the polynomial reconstruction problem for Non-Singular graphs with both $\mathbf{G}$ and $\mathbf{G}^{-1}$ having a Singular Deck.

The bipartite graphs with non–singular 0–1 adjacency matrix form a subclass of the class of NSSDs. The complete graph K_2 associated with the 0–1 adjacency matrix is also a member, but K_n for $n \geq 3$ is not. We note that if $\mathbf{G}$ is the 0–1 adjacency matrix of K_2, then $\mathbf{G} = \mathbf{G}^{-1}$. Henceforth we consider NSSDs on at least 3 vertices.

The *nullity* of a $n \times n$ matrix $\mathbf{M}$, denoted by $\eta(\mathbf{M})$, is the dimension of the nullspace $\ker(\mathbf{M})$ of $\mathbf{M}$, that is the number of linearly independent non–zero vectors $\mathbf{x}$ satisfying $\mathbf{M}\mathbf{x} = \mathbf{0}$. Because $\mathbf{x} \in \ker(\mathbf{M})$, $\mathbf{x}$ is referred to as a *kernel eigenvector* of $\mathbf{M}$. Therefore, the nullity is the *geometric multiplicity* of the eigenvalue 0 of $\mathbf{M}$. For a real and symmetric matrix $\mathbf{G}$, the geometric multiplicity and the algebraic multiplicity of any of its eigenvalues coincide. Effectively this means that $\eta(\mathbf{M})$ is also the number of times that the eigenvalue 0 appears in the spectrum of $\mathbf{M}$. The $(n-1) \times (n-1)$ principal submatrix obtained from $\mathbf{G}$ by deleting the v^{th} row and column will be denoted by $\mathbf{G} - \mathbf{v}$, while $\mathbf{G} - \mathbf{v} - \mathbf{w}$ will denote the principal submatrix obtained from $\mathbf{G}$ by deleting the v^{th} and the w^{th} rows and columns. By *Cauchy's Inequalities for Hermitian matrices* (also referred to as the *Interlacing Theorem*) [3], deletion of a vertex changes the nullity of a graph by at most one.

3. Adjacency matrices $\mathbf{G}$ and $\mathbf{G}^{-1}$ of NSSDs

In this section we see how the algebraic properties of an adjacency matrix $\mathbf{G}$ of a labelled NSSD G determine particular combinatorial properties of G and of $\Gamma(\mathbf{G}^{-1})$.

A *terminal vertex* in a graph is a vertex which is adjacent to only one other vertex in the graph, a next–to–terminal (NTT) vertex. The edge joining a terminal vertex and a NTT vertex is called a *pendant edge*. A NSSD G cannot have two or more terminal vertices adjacent to the same NTT vertex v. Otherwise, $\mathbf{G} - \mathbf{v}$ would have nullity at least 2, and hence by the Interlacing Theorem, $\mathbf{G}$ would be singular.

A path P_n on n vertices admits a tridiagonal matrix representation. Fiedler [1] showed that P_n has distinct eigenvalues for any edge weights. We show that for a path P_n to be a NSSD, n must be even.

Lemma 2.

If P_n is the path on n vertices and $\mathbf{G}$ is the matrix representing P_n, then $\det(\mathbf{G}) = 0$ if and only if n is odd.

Proof. The matrix $\mathbf{G}$ would be in the form

$$\mathbf{G} = \begin{pmatrix} 0 & c_1 & 0 & 0 & 0 & \cdots & 0 \\ c_1 & 0 & c_2 & 0 & 0 & \cdots & 0 \\ 0 & c_2 & 0 & c_3 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots & \vdots \\ 0 & \cdots & 0 & 0 & c_{n-2} & 0 & c_{n-1} \\ 0 & \cdots & 0 & 0 & 0 & c_{n-1} & 0 \end{pmatrix}$$

where $c_i \neq 0$ for $i \in \{1, 2, \ldots, n-1\}$. If $\{v_1, v_2\}$ is a pendant edge, then $\det(\mathbf{G}) = -{c_1}^2 \det(\mathbf{G} - \mathbf{v_1} - \mathbf{v_2})$. This can be applied recursively until we are left with the determinant of either an isolated vertex if n is odd or of K_2 if n is even. Thus if n is odd, $\det(\mathbf{G}) = 0$, while if n is even, $\det(\mathbf{G}) = (-1)^{\frac{n}{2}}(c_1 c_3 \cdots c_{n-1})^2 \neq 0$. □

Proposition 3.

The path P_n is a NSSD if and only if n is even.

Proof. Let P_n be a path on n vertices where n is odd. Then by Lemma 2, P_n is singular and hence P_n is not a NSSD. Now suppose n is even. Then, by Lemma 2, P_n is non–singular. Moreover, removing a terminal vertex from P_n results in the odd path P_{n-1}, which is singular by Lemma 2. Removing any non–terminal vertex from P_n results in the graph H, which is the disjoint union of two paths P_a and P_b, where, without loss of generality, a is even and b is odd. The characteristic polynomial $\phi(\mathbf{H}, \lambda)$ is the product of the characteristic polynomials of the matrices associated with P_a and P_b, and 0 is a root of the latter. Thus, if n is even, all vertex–deleted subgraphs of P_n have a singular matrix representing them, and hence P_n is a NSSD. □

NSSDs are special in their relation to their matrix inverse. In Theorem 5, we show that this class of graphs is closed under taking inverses. We make use of the following lemma.

Lemma 4.

For a NSSD G, the nullity of $\mathbf{G} - \mathbf{v}$ is equal to one for all $v \in \mathcal{V}_G$.

Proof. By Definition 1, for a NSSD G, the $(n-1) \times (n-1)$ principal submatrices $\{\mathbf{G} - \mathbf{v}\}$ of $\mathbf{G}$ are singular, for all $v \in \mathcal{V}_G$. Thus 0 is in the spectrum of $\mathbf{G} - \mathbf{v}$. As a consequence of the Interlacing Theorem, the nullity of $\mathbf{G} - \mathbf{v}$ is one. □

Theorem 5.

For a NSSD G with associated adjacency matrix $\mathbf{G}$, the graph $\Gamma(\mathbf{G}^{-1})$ is also a NSSD.

Proof. The zero and non–zero pattern of the entries in $\mathbf{G}^{-1}$ is reflected in the adjugate $\mathrm{adj}(\mathbf{G})$ of $\mathbf{G}$. For all $v \in \mathcal{V}_G$, the v^{th} diagonal entry of $\mathrm{adj}(\mathbf{G})$ is $\det(\mathbf{G} - \mathbf{v})$ which is zero since the nullity of $\mathbf{G} - \mathbf{v}$ is one by Lemma 4. Thus, each diagonal entry of $\mathbf{G}^{-1}$ is zero. Since each diagonal entry of $\mathbf{G} = (\mathbf{G}^{-1})^{-1}$ is zero, then all $(n-1) \times (n-1)$ principal submatrices of $\mathbf{G}^{-1}$ are singular. Since $\mathbf{G}^{-1}$ is non-singular, it satisfies the axioms of Definition 1. □

This establishes a duality between $\mathbf{G}$ and $\mathbf{G}^{-1}$, so that either of the two can assume a principal role.

Corollary 6.

The matrices $\mathbf{G}$ and $\mathbf{G}^{-1}$ are real and symmetric with each entry on the respective diagonals equal to zero if and only if $\Gamma(\mathbf{G})$ and $\Gamma(\mathbf{G}^{-1})$ are both NSSDs.

Proof. Assume first that $\mathbf{G}$ and $\mathbf{G}^{-1}$ are $n \times n$ real symmetric matrices with each entry on the respective diagonals equal to zero. Since the i^{th} diagonal entry of $\mathbf{G}^{-1}$ is zero for all $i = 1, \dots, n$, then $\det(\mathbf{G} - \mathbf{i}) = 0$. Now $\mathbf{G}$ is non–singular, and hence $\eta(\mathbf{G}) = 0$. As a consequence of the Interlacing Theorem, $\eta(G - i) = 1$ for all $i = 1, \dots, n$. Thus, all $(n-1) \times (n-1)$ principal submatrices of $\mathbf{G}$ are singular, implying that G is a NSSD. By Theorem 5, $\Gamma(\mathbf{G}^{-1})$ is also a NSSD.
The converse follows from Definition 1. □

We note that if a NSSD G is disconnected, then each component of G is also a NSSD. Moreover, $\Gamma(\mathbf{G}^{-1})$ is also a disconnected NSSD with corresponding NSSD components. Therefore we can limit our considerations to connected NSSDs.
The matrix

$$\mathbf{G}^{-1} = \begin{pmatrix} \mathbf{L}_{xy} & \mathbf{S}_{xy} \\ \mathbf{S}_{xy}^{\mathsf{T}} & \alpha_{xy}\mathbf{U} \end{pmatrix} \tag{2}$$

is conformal with the matrix $\mathbf{G}$ in (1). Here, $\mathbf{L}_{xy}$ is a square matrix, and $\alpha_{xy} = 0$ if and only if $\{x, y\}$ is a non–edge of $\Gamma(\mathbf{G}^{-1})$.
We denote by $\mathbf{0}$ a matrix each of whose entries is zero. Since $\mathbf{G}\mathbf{G}^{-1} = \mathbf{I}$, then the following relations hold.

Lemma 7.

$$\mathbf{P}_{xy}\mathbf{L}_{xy} + \mathbf{R}_{xy}\mathbf{S}_{xy}^{\mathsf{T}} = \mathbf{I} \tag{3}$$

$$\mathbf{R}_{xy}^{\mathsf{T}}\mathbf{S}_{xy} + \alpha_{xy}\beta_{xy}\mathbf{I} = \mathbf{I} \tag{4}$$

$$\mathbf{P}_{xy}\mathbf{S}_{xy} + \alpha_{xy}\mathbf{R}_{xy}\mathbf{U} = \mathbf{0} \tag{5}$$

$$\mathbf{L}_{xy}\mathbf{R}_{xy} + \beta_{xy}\mathbf{S}_{xy}\mathbf{U} = \mathbf{0} \tag{6}$$

Henceforth we shall write

$$\mathbf{G} = \begin{pmatrix} \mathbf{P}_{xy} & \mathbf{R}_x & \mathbf{R}_y \\ \mathbf{R}_x^{\mathsf{T}} & 0 & \beta_{xy} \\ \mathbf{R}_y^{\mathsf{T}} & \beta_{xy} & 0 \end{pmatrix}, \qquad \text{with } \mathbf{P}_{xy} \text{ square} \tag{7}$$

and

$$\mathbf{G}^{-1} = \begin{pmatrix} \mathbf{L}_{xy} & \mathbf{S}_x & \mathbf{S}_y \\ \mathbf{S}_x^{\mathsf{T}} & 0 & \alpha_{xy} \\ \mathbf{S}_y^{\mathsf{T}} & \alpha_{xy} & 0 \end{pmatrix}, \qquad \text{with } \mathbf{L}_{xy} \text{ square.} \tag{8}$$

4. One–vertex–deleted subgraphs of NSSDs

The results in this section follow, whether $\{x, y\}$ is an edge ($\beta_{xy} \neq 0$) or a non–edge ($\beta_{xy} = 0$) in G, with the adjacency matrix $\mathbf{G}$ written in the form (1).
From (5), we see how $\mathbf{S}_y$ relates to $\mathbf{R}_x$ and $\mathbf{S}_x$ relates to $\mathbf{R}_y$.

Lemma 8.
Let x and y be two vertices of a NSSD G with adjacency matrix $\mathbf{G}$. Then $\mathbf{P}_{xy}\mathbf{S}_y = -\alpha_{xy}\mathbf{R}_x$ and $\mathbf{P}_{xy}\mathbf{S}_x = -\alpha_{xy}\mathbf{R}_y$.

Furthermore, (4) relates $\mathbf{S}_{xy}$ to $\mathbf{R}_{xy}$.

Lemma 9.
Let x and y be two vertices of a NSSD G with adjacency matrix $\mathbf{G}$. Then $\langle \mathbf{R}_x, \mathbf{S}_y\rangle = \langle \mathbf{R}_y, \mathbf{S}_x\rangle = 0$ and $\langle \mathbf{R}_x, \mathbf{S}_x\rangle = \langle \mathbf{R}_y, \mathbf{S}_y\rangle = 1 - \alpha_{xy}\beta_{xy}$.

We note that for particular vertices $x, y \in \mathcal{V}_G$ with vertex labelling determined by (7) and (8), $\mathbf{R}_x$ and $\mathbf{S}_y$ are orthogonal, and similarly for $\mathbf{R}_y$ and $\mathbf{S}_x$. Moreover, if $\alpha_{xy}\beta_{xy} = 1$, $\mathbf{R}_x$ and $\mathbf{S}_x$ are also orthogonal, and the same holds for $\mathbf{R}_y$ and $\mathbf{S}_y$. A kernel eigenvector of $\mathbf{G} - \mathbf{y}$ can be obtained from (5). Note that post–multiplying a two–column matrix by $\mathbf{U}$ has the effect of interchanging the two columns.

Proposition 10.
Let x and y be two vertices of a NSSD G with adjacency matrix $\mathbf{G}$. Then $\begin{pmatrix} \mathbf{S}_y \\ \alpha_{xy} \end{pmatrix}$ generates the nullspace of $\mathbf{G} - \mathbf{y}$.

Proof. Irrespective of the value of β_{xy},

$$(\mathbf{G} - \mathbf{y}) \begin{pmatrix} \mathbf{S}_y \\ \alpha_{xy} \end{pmatrix} = \begin{pmatrix} \mathbf{P}_{xy} & \mathbf{R}_x \\ \mathbf{R}_x^{\mathsf{T}} & 0 \end{pmatrix} \begin{pmatrix} \mathbf{S}_y \\ \alpha_{xy} \end{pmatrix}. \tag{9}$$

By Lemmas 8 and 9, $(\mathbf{G} - \mathbf{y}) \begin{pmatrix} \mathbf{S}_y \\ \alpha_{xy} \end{pmatrix} = \begin{pmatrix} \mathbf{0} \\ 0 \end{pmatrix}$. □

By duality, there is a similar result for $\mathbf{G}^{-1}$.

Proposition 11.
Let x and y be two vertices of a NSSD G with adjacency matrix $\mathbf{G}$. Then $\begin{pmatrix} \mathbf{R}_y \\ \beta_{xy} \end{pmatrix}$ generates the nullspace of $\mathbf{G}^{-1} - \mathbf{y}$.

5. Two–vertex–deleted subgraphs of NSSDs

The adjacency matrices of $G - x - y$ and $\Gamma(\mathbf{G}^{-1} - \mathbf{x} - \mathbf{y})$ are $\mathbf{P}_{xy}$ and $\mathbf{L}_{xy}$ respectively. As a consequence of the Interlacing Theorem, since $\eta(\mathbf{G}^{-1} - \mathbf{y}) = 1$, we expect the nullity of $\mathbf{L}_{xy}$ to be either zero, one or two.
Following [4], let the characteristic polynomials of $\mathbf{G}$, $\mathbf{G} - \mathbf{x}$, $\mathbf{G} - \mathbf{y}$ and $\mathbf{G} - \mathbf{x} - \mathbf{y}$ be denoted by $s(\lambda)$, $t(\lambda)$, $u(\lambda)$ and $v(\lambda)$, which will be written simply as s, t, u, v respectively, when there is no risk of ambiguity. Let g_s, g_t, g_u and g_v denote $\eta(\mathbf{G})$, $\eta(\mathbf{G} - \mathbf{x})$, $\eta(\mathbf{G} - \mathbf{y})$ and $\eta(\mathbf{G} - \mathbf{x} - \mathbf{y})$ respectively, which correspond to the number of zero roots of the real functions $s(\lambda)$, $t(\lambda)$, $u(\lambda)$, $v(\lambda)$, respectively.
To determine the possible changes in nullity when any two vertices x and y are deleted from a graph G, we make use of an identity due to Jacobi [2].

Lemma 12 [2].

Let x and y be two distinct vertices of a graph G. The entry $j(\lambda)$ (often written as j) of the adjugate of $\lambda\mathbf{I}-\mathbf{G}$ in the x, y position, for the real symmetric matrix $\mathbf{G}$, satisfies

$$j^2 = ut - sv \tag{10}$$

Jacobi's identity requires that $ut - sv$, which is j^2, has an even number of roots. This condition on the root $\lambda = 0$ imposes restrictions on the possible value of the nullity of $\mathbf{G}$ and its principal submatrices.

Theorem 13.

Let x and y be any two distinct vertices of a NSSD G. It is impossible to have the nullity of $\mathbf{G}-\mathbf{x}-\mathbf{y}$ equal to one.

Proof. For a NSSD G, by Definition 1 $g_s = 0$, and the Interlacing Theorem implies that $g_t = g_u = 1$. The multiplicity of the root $\lambda = 0$ of the real function $u(\lambda)t(\lambda)$ is 2. Suppose $g_v = 1$. Then the number of zero roots of $s(\lambda)v(\lambda)$ is 1. But then j^2 has only one root equal to zero, that is, j^2 has an odd number of zero roots, a contradiction. □

5.1. Relations among the submatrices of $\mathbf{G}$ and $\mathbf{G}^{-1}$

As a result of Theorem 13 and by duality of $\mathbf{G}$ and $\mathbf{G}^{-1}$, we have:

Corollary 14.

Let x and y be any two distinct vertices of a NSSD G with adjacency matrix $\mathbf{G}$ written as in (7).

(i) The nullity of $\mathbf{P}_{xy}$ associated with the graph $G-x-y$ is equal to zero or two.

(ii) The nullity of $\mathbf{L}_{xy}$ associated with the graph $\Gamma(\mathbf{G}^{-1}-\mathbf{x}-\mathbf{y})$ is equal to zero or two.

In Theorems 26 and 27, the conditions on the structure of the graph for the two different values of the nullity will be characterised. To proceed, we require some further results.
We first determine the rank of $\mathbf{R}_{xy}$, $\mathbf{S}_{xy}$ and $\mathbf{P}_{xy}\mathbf{L}_{xy}$.

Lemma 15.

Let x and y be any two distinct vertices of a NSSD G. Let $\mathbf{G}$ and $\mathbf{G}^{-1}$ be expressed as in (7) and (8) respectively. If $\alpha_{xy}\beta_{xy} \neq 1$, then

(i) $\mathbf{R}_x$ and $\mathbf{R}_y$ are linearly independent;

(ii) $\mathbf{S}_x$ and $\mathbf{S}_y$ are linearly independent.

Proof. For $\alpha_{xy}\beta_{xy} \neq 1$, then by (4), since the rank of $\mathbf{I}$ is two, it follows that the rank of each of $\mathbf{R}_{xy}$ and $\mathbf{S}_{xy}$ is at least two. The rank is exactly two since each of the matrices $\mathbf{R}_{xy}$ and $\mathbf{S}_{xy}$ has two columns. □

The square matrices $\mathbf{L}_{xy}$, $\mathbf{P}_{xy}$, $\mathbf{R}_{xy}\mathbf{S}_{xy}^{\mathsf{T}}$ and $\mathbf{P}_{xy}\mathbf{L}_{xy}$ are all of order $n-2$. Since, for all conformal matrices $\mathbf{M}$ and $\mathbf{N}$, the matrices $\mathbf{MN}$, $\mathbf{NM}$ and $\mathbf{N}^{\mathsf{T}}\mathbf{M}^{\mathsf{T}}$ have the same non–zero eigenvalues, the eigenvalues of $\mathbf{R}_{xy}\mathbf{S}_{xy}^{\mathsf{T}}$ and $\mathbf{P}_{xy}\mathbf{L}_{xy}$ can be determined immediately from (4) and (3), respectively.

Theorem 16.

The spectrum of $\mathbf{R}_{xy}\mathbf{S}_{xy}^{\mathsf{T}}$ is $\{(1-\alpha_{xy}\beta_{xy})^2, 0^{n-4}\}$, while the spectrum of $\mathbf{P}_{xy}\mathbf{L}_{xy}$ is $\{(\alpha_{xy}\beta_{xy})^2, 1^{n-4}\}$, where the superscripts indicate the multiplicity of the particular eigenvalue in the spectrum.

Corollary 17.

If $\mathbf{P}_{xy}\mathbf{L}_{xy} = \mathbf{I}$, then $\alpha_{xy}\beta_{xy} = 1$.

Proof. When $\mathbf{P}_{xy}\mathbf{L}_{xy} = \mathbf{I}$, its spectrum is $\{1^{n-2}\}$, and hence $\alpha_{xy}\beta_{xy} = 1$. □

The eigenvectors of matrices $\mathbf{P}_{xy}\mathbf{L}_{xy}$ and $\mathbf{L}_{xy}\mathbf{P}_{xy}$ associated with the eigenvalue $\alpha_{xy}\beta_{xy}$ can also be determined. We make use of the fact that $\mathsf{U}^2 = \mathbf{I}$.

Theorem 18.

If $\alpha_{xy}\beta_{xy} \neq 1$, the columns of $\mathbf{R}_{xy}$ are linearly independent eigenvectors associated with the eigenvalue $\alpha_{xy}\beta_{xy}$ of the matrix $\mathbf{P}_{xy}\mathbf{L}_{xy}$ and the columns of $\mathbf{S}_{xy}$ are linearly independent eigenvectors associated with the eigenvalue $\alpha_{xy}\beta_{xy}$ of the matrix $\mathbf{L}_{xy}\mathbf{P}_{xy}$.

Proof. Recall (5) and (6):

$$\begin{aligned} \mathbf{P}_{xy}\mathbf{S}_{xy} + \alpha_{xy}\mathbf{R}_{xy}\mathsf{U} &= \mathbf{0} \\ \mathbf{L}_{xy}\mathbf{R}_{xy} + \beta_{xy}\mathbf{S}_{xy}\mathsf{U} &= \mathbf{0} \end{aligned}$$

Thus

$$\mathbf{P}_{xy}\mathbf{S}_{xy}\mathsf{U} = -\alpha_{xy}\mathbf{R}_{xy} \tag{11}$$

and

$$\mathbf{L}_{xy}\mathbf{R}_{xy}\mathsf{U} = -\beta_{xy}\mathbf{S}_{xy}. \tag{12}$$

Pre-multiplying (11) by $\mathbf{L}_{xy}$ and post-multiplying it by U, we obtain

$$(\mathbf{L}_{xy}\mathbf{P}_{xy})\mathbf{S}_{xy} = -\alpha_{xy}\mathbf{L}_{xy}\mathbf{R}_{xy}\mathsf{U} = \alpha_{xy}\beta_{xy}\mathbf{S}_{xy}$$

Similarly, pre-multiplying (12) by $\mathbf{P}_{xy}$ and post-multiplying it by U, we obtain

$$(\mathbf{P}_{xy}\mathbf{L}_{xy})\mathbf{R}_{xy} = -\beta_{xy}\mathbf{P}_{xy}\mathbf{S}_{xy}\mathsf{U} = \alpha_{xy}\beta_{xy}\mathbf{R}_{xy}$$

Since the columns of $\mathbf{R}_{xy}$ and $\mathbf{S}_{xy}$ are linearly independent by Lemma 15, the result follows. □

Remark 19.

Note that if $\alpha_{xy}\beta_{xy} = 1$, both matrices $\mathbf{P}_{xy}\mathbf{L}_{xy}$ and $\mathbf{L}_{xy}\mathbf{P}_{xy}$ would have only the eigenvalue 1 repeated $n-2$ times. Furthermore, if $\mathbf{P}_{xy}\mathbf{L}_{xy}$ and $\mathbf{L}_{xy}\mathbf{P}_{xy}$ would be diagonalisable, the eigenvectors associated with them would be, for instance, the columns of $\mathbf{I}$, and $\mathbf{P}_{xy}\mathbf{L}_{xy} = \mathbf{L}_{xy}\mathbf{P}_{xy} = \mathbf{I}$.

We now obtain the minimum polynomial of $\mathbf{P}_{xy}\mathbf{L}_{xy}$ and $\mathbf{R}_{xy}\mathbf{S}_{xy}^{\mathsf{T}}$ respectively.

Proposition 20.

Let x and y be any two distinct vertices of a NSSD G. Then $\left(\mathbf{P}_{xy}\mathbf{L}_{xy}\right)^2 = (1+\alpha_{xy}\beta_{xy})\mathbf{P}_{xy}\mathbf{L}_{xy} - (\alpha_{xy}\beta_{xy})\mathbf{I}$. Moreover, the minimum polynomial of $\mathbf{P}_{xy}\mathbf{L}_{xy}$ is

$$m_{\mathbf{PL}}(x) = \begin{cases} x^2 - (1+\alpha_{xy}\beta_{xy})x + \alpha_{xy}\beta_{xy}, & \text{if } \mathbf{P}_{xy}\mathbf{L}_{xy} \neq \mathbf{I} \\ x - 1, & \text{if } \mathbf{P}_{xy}\mathbf{L}_{xy} = \mathbf{I} \end{cases}$$

Proof.

$$\begin{aligned}(\mathbf{P}_{xy}\mathbf{L}_{xy})(\mathbf{P}_{xy}\mathbf{L}_{xy}) &= \mathbf{P}_{xy}(\mathbf{I}-\mathbf{S}_{xy}\mathbf{R}_{xy}^{\mathsf{T}})\mathbf{L}_{xy} && \text{by (3)}\\ &= \mathbf{P}_{xy}\mathbf{L}_{xy}-(\mathbf{P}_{xy}\mathbf{S}_{xy})(\mathbf{R}_{xy}^{\mathsf{T}}\mathbf{L}_{xy})\\ &= \mathbf{P}_{xy}\mathbf{L}_{xy}-(-\alpha_{xy}\mathbf{R}_{xy}\mathbf{U})(\mathbf{R}_{xy}^{\mathsf{T}}\mathbf{L}_{xy}) && \text{by (5)}\\ &= \mathbf{P}_{xy}\mathbf{L}_{xy}+\alpha_{xy}\mathbf{R}_{xy}\mathbf{U}(-\beta_{xy}\mathbf{U}\mathbf{S}_{xy}^{\mathsf{T}}) && \text{by (6)}\\ &= \mathbf{P}_{xy}\mathbf{L}_{xy}-\alpha_{xy}\beta_{xy}\mathbf{R}_{xy}\mathbf{S}_{xy}^{\mathsf{T}}\end{aligned}$$

But from (3), $\alpha_{xy}\beta_{xy}\mathbf{R}_{xy}\mathbf{S}_{xy}^{\mathsf{T}} = \alpha_{xy}\beta_{xy}(\mathbf{I}-\mathbf{P}_{xy}\mathbf{L}_{xy})$. Thus $(\mathbf{P}_{xy}\mathbf{L}_{xy})^2+\alpha_{xy}\beta_{xy}\mathbf{I} = (1+\alpha_{xy}\beta_{xy})\mathbf{P}_{xy}\mathbf{L}_{xy}$, so that if $\mathbf{P}_{xy}\mathbf{L}_{xy}\neq\mathbf{I}$, $m_{\mathbf{PL}}(x) = x^2-(1+\alpha_{xy}\beta_{xy})x+\alpha_{xy}\beta_{xy}$.
If $\mathbf{P}_{xy}\mathbf{L}_{xy}=\mathbf{I}$, then $m_{\mathbf{PL}}(x) = x-1$. □

Similarly, by (4) we have

Proposition 21.
Let x and y be any two distinct vertices of a NSSD G. Then $\left(\mathbf{R}_{xy}\mathbf{S}_{xy}^{\mathsf{T}}\right)^2 = (1-\alpha_{xy}\beta_{xy})\mathbf{R}_{xy}\mathbf{S}_{xy}^{\mathsf{T}}$. Moreover, the minimum polynomial of $\mathbf{R}_{xy}\mathbf{S}_{xy}^{\mathsf{T}}$ is

$$m_{\mathbf{RS}^{\mathsf{T}}}(x) = \begin{cases} x^2-(1-\alpha_{xy}\beta_{xy})x, & \text{if } \mathbf{R}_{xy}\mathbf{S}_{xy}^{\mathsf{T}}\neq\mathbf{0}\\ x, & \text{if } \mathbf{R}_{xy}\mathbf{S}_{xy}^{\mathsf{T}}=\mathbf{0}\end{cases}$$

Corollary 22.
The matrix $\mathbf{P}_{xy}\mathbf{L}_{xy}$ is not diagonalizable if and only if $\alpha_{xy}\beta_{xy}=1$ and $\mathbf{P}_{xy}\mathbf{L}_{xy}\neq\mathbf{I}$.

Proof. From Proposition 20, if $\mathbf{P}_{xy}\mathbf{L}_{xy}=\mathbf{I}$ then $\alpha_{xy}\beta_{xy}=1$ and $m_{\mathbf{PL}}(x)=x-1$ has a simple root. If $\mathbf{P}_{xy}\mathbf{L}_{xy}\neq\mathbf{I}$, then $m_{\mathbf{PL}}(x) = x^2-(1+\alpha_{xy}\beta_{xy})x+\alpha_{xy}\beta_{xy}$. This quadratic equation has two equal roots if and only if $\alpha_{xy}\beta_{xy}=1$. Hence, the result follows. □

We note that, in general, it does not necessarily follow that the product $\mathbf{P}_{xy}\mathbf{L}_{xy}$ is diagonalizable when $\mathbf{P}_{xy}$ and $\mathbf{L}_{xy}$ are separately diagonalizable. Moreover, using a similar argument to that applied in Corollary 22, the matrix $\mathbf{R}_{xy}\mathbf{S}_{xy}^{\mathsf{T}}$ is not diagonalisable if and only if $\alpha_{xy}\beta_{xy}=1$ and $\mathbf{R}_{xy}\mathbf{S}_{xy}^{\mathsf{T}}\neq\mathbf{0}$.
The following results follow immediately.

Corollary 23.

(i) $\alpha_{xy}\beta_{xy}=0$ if and only if $\mathbf{P}_{xy}\mathbf{L}_{xy}$ and $\mathbf{R}_{xy}\mathbf{S}_{xy}^{\mathsf{T}}$ are projections;
(ii) $\alpha_{xy}\beta_{xy}=-1$ if and only if $(\mathbf{P}_{xy}\mathbf{L}_{xy})^2=\mathbf{I}$ and $\mathbf{P}_{xy}\mathbf{L}_{xy}\neq\mathbf{I}$;
(iii) $\alpha_{xy}\beta_{xy}=1$ if and only if $(\mathbf{P}_{xy}\mathbf{L}_{xy}-\mathbf{I})^2=\mathbf{0}$ (that is, $\mathbf{P}_{xy}\mathbf{L}_{xy}-\mathbf{I}$ is a nilpotent matrix of degree 1 or 2).

For any two vertices x and y of a graph G, we obtain the following result depending on whether $\{x,y\}$ is an edge or a non–edge.

Proposition 24.
Let x and y be two vertices of a connected NSSD G on at least three vertices with adjacency matrix $\mathbf{G}$. Let $\mathbf{G}$ and $\mathbf{G}^{-1}$ be expressed as in (7) and (8) respectively. Then
(i) $\mathbf{L}_{xy}\mathbf{R}_x=\mathbf{L}_{xy}\mathbf{R}_y=\mathbf{0}, \mathbf{R}_x\neq\mathbf{0}$ and $\mathbf{R}_y\neq\mathbf{0}$, if $\{x,y\}$ is a non–edge of G;
(ii) $\mathbf{L}_{xy}\mathbf{R}_x=-\beta_{xy}\mathbf{S}_y$ and $\mathbf{L}_{xy}\mathbf{R}_y=-\beta_{xy}\mathbf{S}_x$, if $\{x,y\}$ is an edge of G;
(iii) $\mathbf{P}_{xy}\mathbf{S}_x=\mathbf{P}_{xy}\mathbf{S}_y=\mathbf{0}, \mathbf{S}_x\neq\mathbf{0}$ and $\mathbf{S}_y\neq\mathbf{0}$, if $\{x,y\}$ is a non–edge of $\Gamma(\mathbf{G}^{-1})$;
(iv) $\mathbf{P}_{xy}\mathbf{S}_x=-\alpha_{xy}\mathbf{R}_y$ and $\mathbf{P}_{xy}\mathbf{S}_y=-\alpha_{xy}\mathbf{R}_x$, if $\{x,y\}$ is an edge of $\Gamma(\mathbf{G}^{-1})$.

Proof.

(i) If $\beta_{xy}=0$, then both $\mathbf{R}_x$ and $\mathbf{R}_y$ are not $\mathbf{0}$, otherwise $\mathbf{G}^{-1}$ is singular. Also, by (6), $\mathbf{L}_{xy}\mathbf{R}_{xy}=\mathbf{0}$.

(ii) If $\beta_{xy} \neq 0$, then $\mathbf{R}_x$ or $\mathbf{R}_y$ may be $\mathbf{0}$ but not both, otherwise K_2 will be a component and G would be a disconnected graph. Also, $\mathbf{L}_{xy}\mathbf{R}_{xy} = -\beta_{xy}\mathbf{S}_{xy}\mathbf{U}$, and post–multiplying $\mathbf{S}_{xy}$ by $\mathbf{U}$ interchanges the two columns of $\mathbf{S}_{xy}$.

Similarly, by (5) and by duality of $\mathbf{G}$ and $\mathbf{G}^{-1}$, (iii) and (iv) follow. □

In the case when $\beta_{xy} \neq 0$, the inverse $\mathbf{L}_{xy}^{-1}$ of $\mathbf{L}_{xy}$ can be expressed in terms of the submatrices of $\mathbf{G}$ and $\mathbf{G}^{-1}$. The same holds for the inverse $\mathbf{P}_{xy}^{-1}$ of $\mathbf{P}_{xy}$ when $\alpha_{xy} \neq 0$. We show this in the following proposition.

Proposition 25.

Let x and y be two vertices of a NSSD G with adjacency matrix $\mathbf{G}$. Let $\mathbf{G}$ and $\mathbf{G}^{-1}$ be expressed as in (7) and (8) respectively. Then
(i) if $\beta_{xy} \neq 0$, $\mathbf{L}_{xy}^{-1} = \mathbf{P}_{xy} - \frac{1}{\beta_{xy}}\mathbf{R}_{xy}\mathbf{U}\mathbf{R}_{xy}^{\mathsf{T}}$;
(ii) if $\alpha_{xy} \neq 0$, $\mathbf{P}_{xy}^{-1} = \mathbf{L}_{xy} - \frac{1}{\alpha_{xy}}\mathbf{S}_{xy}\mathbf{U}\mathbf{S}_{xy}^{\mathsf{T}}$.

Proof. From (6) and (3),

$$\mathbf{L}_{xy}\mathbf{R}_{xy} = -\beta_{xy}\mathbf{S}_{xy}\mathbf{U}$$
$$\mathbf{L}_{xy}\mathbf{R}_{xy}\mathbf{U}\mathbf{R}_{xy}^{\mathsf{T}} = -\beta_{xy}\mathbf{S}_{xy}\mathbf{R}_{xy}^{\mathsf{T}} = -\beta_{xy}(\mathbf{I} - \mathbf{L}_{xy}\mathbf{P}_{xy}),$$

and hence

$$\mathbf{L}_{xy}(\mathbf{P}_{xy} - \tfrac{1}{\beta_{xy}}\mathbf{R}_{xy}\mathbf{U}\mathbf{R}_{xy}^{\mathsf{T}}) = \mathbf{I}. \qquad (13)$$

Similarly, from (5) and (3), $\mathbf{P}_{xy}(\mathbf{L}_{xy} - \frac{1}{\alpha_{xy}}\mathbf{S}_{xy}\mathbf{U}\mathbf{S}_{xy}^{\mathsf{T}}) = \mathbf{I}$. □

Recall that the nullity is the number of eigenvalues equal to zero. The next result characterises the two possible values of $\eta(\mathbf{L}_{xy})$ obtained in Corollary 14 (ii).

Theorem 26.

Let x and y be two vertices of a NSSD G with adjacency matrix $\mathbf{G}$. Then the nullity of $\mathbf{G}^{-1} - \mathbf{x} - \mathbf{y}$ is
$$\begin{cases} 0 \text{ if and only if } \{x, y\} \text{ is an edge of } G \\ 2 \text{ if and only if } \{x, y\} \text{ is a non–edge of } G. \end{cases}$$

Proof. For $\beta_{xy} \neq 0$, $\{x, y\}$ is an edge of G and by Proposition 25, $\mathbf{L}_{xy}$ (that is, $\mathbf{G}^{-1} - \mathbf{x} - \mathbf{y}$) is non–singular and hence has nullity equal to zero.
For $\beta_{xy} = 0$, $\{x, y\}$ is a non–edge of G. By (6), $\mathbf{L}_{xy}\mathbf{R}_{xy} = \mathbf{0}$. Hence $\ker(\mathbf{L}_{xy})$ is generated by $\mathbf{R}_x$ and $\mathbf{R}_y$, which are linearly independent by Lemma 15 where $\alpha_{xy}\beta_{xy} \neq 1$ is assumed. □

By the duality of $\mathbf{G}$ and $\mathbf{G}^{-1}$, an identical argument using (5) characterises the two possible values of $\eta(\mathbf{P}_{xy})$ obtained in Corollary 14 (i).

Theorem 27.

Let x and y be two vertices of a NSSD G with adjacency matrix $\mathbf{G}$. Then the nullity of $\mathbf{G} - \mathbf{x} - \mathbf{y}$ is
$$\begin{cases} 0 \text{ if and only if } \{x, y\} \text{ is an edge of } \Gamma(\mathbf{G}^{-1}) \\ 2 \text{ if and only if } \{x, y\} \text{ is a non–edge of } \Gamma(\mathbf{G}^{-1}). \end{cases}$$

As a consequence of Propositions 24 and 25, we have

Corollary 28.

Provided that $\alpha_{xy}\beta_{xy} \neq 0$,
(i) $\frac{1}{\alpha_{xy}}\mathbf{P}_{xy}$ and $\beta_{xy}\mathbf{L}_{xy}^{-1}$ give the same image when operating on $\mathbf{S}_x$ and $\mathbf{S}_y$;
(ii) $\frac{1}{\beta_{xy}}\mathbf{L}_{xy}$ and $\alpha_{xy}\mathbf{P}_{xy}^{-1}$ give the same image when operating on $\mathbf{R}_x$ and $\mathbf{R}_y$.

Proof. When $\beta_{xy} \neq 0$ (and hence $\mathbf{L}_{xy}^{-1}$ exists), from (6), (7) and (8) we obtain

$$\mathbf{R}_x = -\beta_{xy}\mathbf{L}_{xy}^{-1}\mathbf{S}_y \text{ and } \mathbf{R}_y = -\beta_{xy}\mathbf{L}_{xy}^{-1}\mathbf{S}_x.$$

When $\alpha_{xy} \neq 0$, from (5) we have

$$-\frac{1}{\alpha_{xy}}\mathbf{P}_{xy}\mathbf{S}_y = \mathbf{R}_x \text{ and } -\frac{1}{\alpha_{xy}}\mathbf{P}_{xy}\mathbf{S}_x = \mathbf{R}_y.$$

Thus

$$\frac{1}{\alpha_{xy}}\mathbf{P}_{xy}\mathbf{S}_y = \beta_{xy}\mathbf{L}_{xy}^{-1}\mathbf{S}_y \text{ and } \frac{1}{\alpha_{xy}}\mathbf{P}_{xy}\mathbf{S}_x = \beta_{xy}\mathbf{L}_{xy}^{-1}\mathbf{S}_x,$$

implying that $\frac{1}{\alpha_{xy}}\mathbf{P}_{xy}$ and $\beta_{xy}\mathbf{L}_{xy}^{-1}$ have the same effect when operating on $\mathbf{S}_x$ and $\mathbf{S}_y$, provided that $\alpha_{xy}\beta_{xy} \neq 0$. □

5.2. The case $\mathbf{P}_{xy}\mathbf{L}_{xy} = \mathbf{I}$

We note that although both $\mathbf{P}_{xy}$ and $\mathbf{L}_{xy}$ are real and symmetric, the product $\mathbf{P}_{xy}\mathbf{L}_{xy}$ remains real and symmetric if and only if $\mathbf{P}_{xy}$ and $\mathbf{L}_{xy}$ commute. This is the case when $\mathbf{P}_{xy}\mathbf{L}_{xy} = \mathbf{I}$, which warrants special attention.

Proposition 29.
One of the column vectors $\mathbf{R}_x$ and $\mathbf{R}_y$ is $\mathbf{0}$ and one of the column vectors $\mathbf{S}_x$ and $\mathbf{S}_y$ is $\mathbf{0}$ if and only if $\mathbf{P}_{xy}\mathbf{L}_{xy} = \mathbf{I}$.

Proof. We note that $\mathbf{P}_{xy}\mathbf{L}_{xy} = \mathbf{I}$ if and only if $\mathbf{P}_{xy}^{-1} = \mathbf{L}_{xy}$ and $\mathbf{L}_{xy}^{-1} = \mathbf{P}_{xy}$. Since both $\mathbf{P}_{xy}$ and $\mathbf{L}_{xy}$ would thus have nullity zero, $\alpha_{xy} \neq 0$ and $\beta_{xy} \neq 0$ by Theorem 26 and Theorem 27. From Proposition 25, $\mathbf{L}_{xy}^{-1} = \mathbf{P}_{xy} - \frac{1}{\beta_{xy}}\mathbf{R}_{xy}\mathbf{U}\mathbf{R}_{xy}^{\mathsf{T}}$ and $\mathbf{P}_{xy}^{-1} = \mathbf{L}_{xy} - \frac{1}{\alpha_{xy}}\mathbf{S}_{xy}\mathbf{U}\mathbf{S}_{xy}^{\mathsf{T}}$. Thus $\mathbf{P}_{xy}\mathbf{L}_{xy} = \mathbf{I}$ if and only if $\mathbf{R}_{xy}\mathbf{U}\mathbf{R}_{xy}^{\mathsf{T}} = \mathbf{0}$ and $\mathbf{S}_{xy}\mathbf{U}\mathbf{S}_{xy}^{\mathsf{T}} = \mathbf{0}$. Consider the expression $\mathbf{R}_{xy}\mathbf{U}\mathbf{R}_{xy}^{\mathsf{T}}$:

$$\mathbf{R}_{xy}\mathbf{U}\mathbf{R}_{xy}^{\mathsf{T}} = \begin{pmatrix}\mathbf{R}_x & \mathbf{R}_y\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}\mathbf{R}_x^{\mathsf{T}}\\ \mathbf{R}_y^{\mathsf{T}}\end{pmatrix} = \mathbf{R}_y\mathbf{R}_x^{\mathsf{T}} + \mathbf{R}_x\mathbf{R}_y^{\mathsf{T}}$$

and hence $\mathbf{R}_{xy}\mathbf{U}\mathbf{R}_{xy}^{\mathsf{T}} = \mathbf{0}$ if and only if

$$\mathbf{R}_y\mathbf{R}_x^{\mathsf{T}} + \mathbf{R}_x\mathbf{R}_y^{\mathsf{T}} = \mathbf{0}. \tag{14}$$

If we let $\mathbf{R}_x = \begin{pmatrix}c_1 & c_2 & \cdots & c_{n-2}\end{pmatrix}^{\mathsf{T}}$ and $\mathbf{R}_y = \begin{pmatrix}d_1 & d_2 & \cdots & d_{n-2}\end{pmatrix}^{\mathsf{T}}$, then $\mathbf{R}_y\mathbf{R}_x^{\mathsf{T}}$ is a matrix of rank at most one with diagonal entries $\{d_ic_i\}$, for $i = 1, \ldots, n-2$. Similarly, $\mathbf{R}_x\mathbf{R}_y^{\mathsf{T}}$ has diagonal entries $\{c_id_i\}$. Also $\left(\mathbf{R}_x\mathbf{R}_y^{\mathsf{T}}\right)^{\mathsf{T}} = \mathbf{R}_y\mathbf{R}_x^{\mathsf{T}} = -\mathbf{R}_x\mathbf{R}_y^{\mathsf{T}}$, and hence $\mathbf{R}_x\mathbf{R}_y^{\mathsf{T}}$ is skew–symmetric. It follows that each diagonal entry c_id_i of $\mathbf{R}_x\mathbf{R}_y^{\mathsf{T}}$ (for $i = 1, \ldots, n-2$) is zero.
If $c_i = 0$ for all $i = 1, \ldots, n-2$, then $\mathbf{R}_x = \mathbf{0}$. So suppose there is some $k \in \{1, \ldots, n-2\}$ such that $c_k \neq 0$, so that $\mathbf{R}_x \neq \mathbf{0}$. This implies that $d_k = 0$ (since the diagonal entries are all zero), and consequently the k^{th} row of $\mathbf{R}_y\mathbf{R}_x^{\mathsf{T}}$ is the zero vector. But $\mathbf{R}_y\mathbf{R}_x^{\mathsf{T}}$ is skew–symmetric, and thus all the entries c_kd_i $(i = 1, \ldots, n-2)$ in the k^{th} column of $\mathbf{R}_y\mathbf{R}_x^{\mathsf{T}}$ are zero. Since $c_k \neq 0$, then $d_i = 0$ for all $i = 1, \ldots, n-2$ and hence $\mathbf{R}_y = \mathbf{0}$.
Thus $\mathbf{R}_{xy}\mathbf{U}\mathbf{R}_{xy}^{\mathsf{T}} = \mathbf{0}$ if and only if either $\mathbf{R}_x = \mathbf{0}$ or $\mathbf{R}_y = \mathbf{0}$. Using a similar argument, $\mathbf{S}_{xy}\mathbf{U}\mathbf{S}_{xy}^{\mathsf{T}} = \mathbf{0}$ if and only if either $\mathbf{S}_x = \mathbf{0}$ or $\mathbf{S}_y = \mathbf{0}$. □

Proposition 30.
Let x and y be any two distinct vertices of a NSSD G. If $\mathbf{P}_{xy}\mathbf{L}_{xy} = \mathbf{I}$ then, without loss of generality, y is a terminal vertex adjacent to the NTT vertex x in G and x is a terminal vertex adjacent to the NTT vertex y in $\Gamma(\mathbf{G}^{-1})$.

Proof. By Proposition 29, $\mathbf{P}_{xy}\mathbf{L}_{xy} = \mathbf{I}$ if and only if one of $\mathbf{R}_x$ and $\mathbf{R}_y$ is $\mathbf{0}$ and one of $\mathbf{S}_x$ and $\mathbf{S}_y$ is $\mathbf{0}$. Without loss of generality, we consider $\mathbf{R}_y = \mathbf{0}$ and note that the argument that follows can be repeated in the case when $\mathbf{R}_x = \mathbf{0}$ by interchanging the roles of x and y.

By Proposition 11, $\begin{pmatrix} \mathbf{R}_y \\ \beta_{xy} \end{pmatrix}$, which has only one non–zero entry (namely β_{xy}), generates the nullspace of $\mathbf{G}^{-1}-\mathbf{y}$. Thus $(\mathbf{G}^{-1}-\mathbf{y})\begin{pmatrix} \mathbf{R}_y \\ \beta_{xy} \end{pmatrix} = \mathbf{0}$ implies that the last column of $\mathbf{G}^{-1}-\mathbf{y}$ must be composed of zero entries. Since $\mathbf{G}^{-1}-\mathbf{y}$ is a symmetric matrix, even the entries in the last row must be all zero. Thus, the entries in the x^{th} column and row of $\mathbf{G}^{-1}-\mathbf{y}$ are all zero, and the x^{th} column and row of $\mathbf{G}^{-1}$ have a non–zero entry only in the y^{th} entry (since $\alpha_{xy} \neq 0$). Hence vertex x in $\Gamma(\mathbf{G}^{-1})$ is a terminal vertex adjacent only to vertex y. From Proposition 10 or Proposition 24 ((ii) or (iv)), $\mathbf{S}_x$ is also a zero vector and by the duality of $\mathbf{G}$ and $\mathbf{G}^{-1}$, it follows that y is a terminal vertex in G. □

The converse of Proposition 30 is also true.

Proposition 31.

If a NSSD G has a terminal vertex y, then $\Gamma(\mathbf{G}^{-1})$ has a terminal vertex x and $\mathbf{P}_{xy}\mathbf{L}_{xy} = \mathbf{I}$.

Proof. Using the same notation as in (7), $\mathbf{R}_y = \mathbf{0}$. Since G is non–singular, $\beta_{xy} \neq 0$.
The matrix product $\mathbf{G}^{-1}\mathbf{G} = \mathbf{I}$ can be written as

$$\begin{pmatrix} \mathbf{L}_{xy} & \mathbf{S}_x & \mathbf{S}_y \\ \mathbf{S}_x^{\mathsf{T}} & 0 & \alpha_{xy} \\ \mathbf{S}_y^{\mathsf{T}} & \alpha_{xy} & 0 \end{pmatrix} \begin{pmatrix} \mathbf{P}_{xy} & \mathbf{R}_x & \mathbf{0} \\ \mathbf{R}_x^{\mathsf{T}} & 0 & \beta_{xy} \\ \mathbf{0}^{\mathsf{T}} & \beta_{xy} & 0 \end{pmatrix} = \begin{pmatrix} \mathbf{I} & \mathbf{0} & \mathbf{0} \\ \mathbf{0}^{\mathsf{T}} & 1 & 0 \\ \mathbf{0}^{\mathsf{T}} & 0 & 1 \end{pmatrix}$$

In particular, $\mathbf{L}_{xy}\mathbf{P}_{xy} + \mathbf{S}_x\mathbf{R}_x^{\mathsf{T}} = \mathbf{I}$ and $\beta_{xy}\mathbf{S}_x = \mathbf{0}$, so $\mathbf{S}_x = \mathbf{0}$ and $\mathbf{L}_{xy}\mathbf{P}_{xy} = \mathbf{I}$. Since $\mathbf{L}_{xy}$ and $\mathbf{P}_{xy}$ are inverses of each other, they commute. □

From Corollary 23, together with Propositions 30 and 31, we have proved the following theorem.

Theorem 32.

Let x and y be any two distinct vertices of a NSSD G. Then $\mathbf{P}_{xy}\mathbf{L}_{xy} = \mathbf{I}$ if and only if, without loss of generality, y is a terminal vertex adjacent to a NTT vertex x of G and x is a terminal vertex adjacent to a NTT vertex y of $\Gamma(\mathbf{G}^{-1})$.

Combining the results of Corollary 22, Corollary 23 (iii) and Theorem 32, we classify pairs of vertices x and y in a NSSD into three different types according to the values of $\mathbf{P}_{xy}\mathbf{L}_{xy}$ and $\alpha_{xy}\beta_{xy}$.

Classification 33.

Let x and y be two vertices of a NSSD G with adjacency matrix $\mathbf{G}$. Let $\mathbf{G}$ and $\mathbf{G}^{-1}$ be expressed as in (7) and (8) respectively. Depending on the values of $\mathbf{P}_{xy}\mathbf{L}_{xy}$ and $\alpha_{xy}\beta_{xy}$, the vertex pair x and y can be one of three types:

Type I: $\mathbf{P}_{xy}\mathbf{L}_{xy} = \mathbf{I}$

Type II: $\alpha_{xy}\beta_{xy} \neq 1$

Type III: $\mathbf{P}_{xy}\mathbf{L}_{xy} \neq \mathbf{I}$ *and* $\alpha_{xy}\beta_{xy} = 1$

The interplay between the values of $\mathbf{P}_{xy}\mathbf{L}_{xy}$ and $\alpha_{xy}\beta_{xy}$ for vertex pairs of Type I or II is given through Corollary 17, whereby $\mathbf{P}_{xy}\mathbf{L}_{xy} = \mathbf{I}$ implies that $\alpha_{xy}\beta_{xy} = 1$, and hence $\alpha_{xy}\beta_{xy} \neq 1$ implies that $\mathbf{P}_{xy}\mathbf{L}_{xy} \neq \mathbf{I}$. A vertex pair of Type I or II corresponds to the case when $\mathbf{P}_{xy}\mathbf{L}_{xy}$ is diagonalisable. Note that a vertex pair is of Type I if and only if it forms a pendant edge (Theorem 32). A vertex pair of Type III corresponds to the case when $\mathbf{P}_{xy}\mathbf{L}_{xy}$ is not diagonalisable (Corollary 22) and therefore the Jordan Normal Form of $\mathbf{P}_{xy}\mathbf{L}_{xy}$ is $\begin{pmatrix} \mathbf{I} & \mathbf{0} & \mathbf{0} \\ \mathbf{0}^{\mathsf{T}} & 1 & 1 \\ \mathbf{0}^{\mathsf{T}} & 0 & 1 \end{pmatrix}$.

The spectrum of $\mathbf{P}_{xy}\mathbf{L}_{xy}$, given in Theorem 16, indicates that when $\alpha_{xy}\beta_{xy} \neq 0, \mathbf{P}_{xy}\mathbf{L}_{xy}$ has full rank. Therefore each of the square matrices $\mathbf{P}_{xy}$ and $\mathbf{L}_{xy}$ have full rank. This is a particular case of Theorem 26 for $\alpha_{xy}\beta_{xy} \neq 0$, which yields that $\mathbf{L}_{xy}$ is non–singular. Indeed, in the special case when $\mathbf{P}_{xy}\mathbf{L}_{xy} = \mathbf{I}$, $\mathbf{P}_{xy}$ and $\mathbf{L}_{xy}$ are not only non–singular, but one is the inverse of the other. Since we also know that both $\mathbf{P}_{xy}$ and $\mathbf{L}_{xy}$ have all their diagonal entries equal to zero, we can say more.

Theorem 34.

If $\mathbf{P}_{xy}\mathbf{L}_{xy} = \mathbf{I}$, then both $\Gamma(\mathbf{P}_{xy})$ and $\Gamma(\mathbf{L}_{xy})$ are NSSDs.

Proof. Let G be a NSSD. Since $\mathbf{P}_{xy}\mathbf{L}_{xy} = \mathbf{I}$, $\mathbf{P}_{xy} = \mathbf{L}_{xy}^{-1}$ and $\mathbf{L}_{xy} = \mathbf{P}_{xy}^{-1}$. Also, both $\mathbf{P}_{xy}$ and $\mathbf{L}_{xy}$ have the entries of their respective diagonals equal to zero, which, by Corollary 6, is a necessary and sufficient condition for $\Gamma(\mathbf{P}_{xy})$ and $\Gamma(\mathbf{L}_{xy})$ to be both NSSDs. □

From Theorems 32 and 34, we have:

Corollary 35.

Let G be a NSSD and let x and y be adjacent vertices in G. If one of x and y is a terminal vertex in G, then both $G - x - y$ and $\Gamma(\mathbf{G}^{-1} - \mathbf{x} - \mathbf{y})$ are NSSDs.

For a NSSD G associated with the adjacency matrix $\mathbf{G}$ written as in (7), the inverse adjacency matrix $\mathbf{G}^{-1}$ can be written as in (8). For $x, y \in \mathcal{V}_G$, if there exists an edge $\{x, y\}$ in G and $\Gamma(\mathbf{G}^{-1})$ such that $\alpha_{xy}\beta_{xy} = 1$, then by Theorem 34, the graphs $\Gamma(\mathbf{P}_{xy})$ and $\Gamma(\mathbf{L}_{xy})$ are still NSSDs. Equivalently, for a terminal vertex y in G adjacent to x, by Corollary 35, the graphs $G - x - y$ and $\Gamma(\mathbf{G}^{-1} - \mathbf{x} - \mathbf{y})$ are still NSSDs. A pendant edge can be removed from $G - x - y$, leaving another NSSD H. The procedure is repeated on H and other intermediate subgraphs obtained in the process, until either there are no more terminal vertices or the adjacency matrix of the intermediate subgraph of G corresponds to the adjacency matrix of K_2. The resulting graph thus obtained is termed a '*plain NSSD*'. We present the above iterative process in the following algorithm.

Algorithm 36.

To determine a plain NSSD.
Input NSSD G (either in graphical form or through its adjacency matrix $\mathbf{G}$)

Step 1. If G is either K_2 or has no terminal vertices, then go to Step 3.

Step 2. Otherwise suppose v is a terminal vertex adjacent to vertex w. Replace G by $G - v - w$ and go to Step 1.

Step 3. Output is plain NSSD G.

We note that since we have no more than one terminal vertex adjacent to the same NTT vertex in a NSSD G, then the algorithm will not produce any isolated vertices.
Although the input of the algorithm is meant to be a NSSD, any graph can be processed. *A fortiori*, if we apply the algorithm to a graph G and the output is *not* a NSSD, then we can conclude that the original graph is *not* a NSSD, by the contrapositive of Corollary 35.

6. An Example

Consider the matrix $\mathbf{G}$ and its inverse $\mathbf{G}^{-1}$:

$$\mathbf{G} = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 \end{pmatrix}, \qquad \mathbf{G}^{-1} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & -1 & 1 & 0 & -1 & 1 \\ 0 & 0 & 0 & -1 & 0 & 1 \\ -1 & 0 & 0 & 1 & 1 & 0 \end{pmatrix}$$

Since both matrices have each of their diagonal entries equal to zero, they are both NSSDs by Corollary 6. The graphs G and $\Gamma(\mathbf{G}^{-1})$ associated with $\mathbf{G}$ and $\mathbf{G}^{-1}$ respectively are depicted in Figure 1.

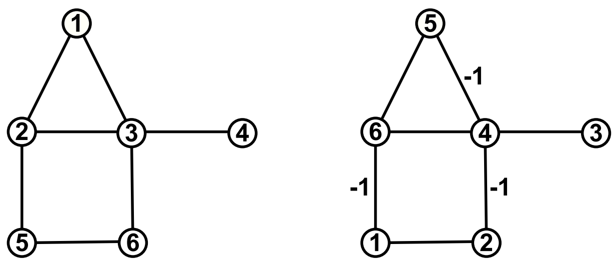

Fig 1. The NSSDs G and $\Gamma(\mathbf{G}^{-1})$.

We note that the edge $\{5, 6\}$ has weight 1 in both G and $\Gamma(\mathbf{G}^{-1})$, and hence $\alpha_{56}\beta_{56} = 1$. Expressing the above matrices as in (1), we have

$$\mathbf{P}_{56} = \begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \mathbf{L}_{56} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 1 \\ 0 & -1 & 1 & 0 \end{pmatrix}, \mathbf{R}_{56} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{pmatrix}, \mathbf{S}_{56} = \begin{pmatrix} 0 & -1 \\ 0 & 0 \\ 0 & 0 \\ -1 & 1 \end{pmatrix}$$

It can be shown that $\mathbf{P}_{56}\mathbf{L}_{56} \neq \mathbf{I}$ and $(\mathbf{P}_{56}\mathbf{L}_{56} - \mathbf{I})^2 = \mathbf{0}$. Thus, we conclude that $\{5, 6\}$ is not a pendant edge in neither G nor $\Gamma(\mathbf{G}^{-1})$. Indeed, none of the columns of $\mathbf{R}_{56}$ or $\mathbf{S}_{56}$ is $\mathbf{0}$. The vertex pair 5 and 6 is of Type III as described in Classification 33.

The edge $\{3, 4\}$ also has weight 1 in both G and $\Gamma(\mathbf{G}^{-1})$, and hence $\alpha_{34}\beta_{34} = 1$ as well. Focusing on this edge, we obtain:

$$\mathbf{P}_{34} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \mathbf{L}_{34} = \begin{pmatrix} 0 & 1 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 1 & 0 \end{pmatrix}, \mathbf{R}_{34} = \begin{pmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 0 \\ 1 & 0 \end{pmatrix} \mathbf{S}_{34} = \begin{pmatrix} 0 & 0 \\ 0 & -1 \\ 0 & -1 \\ 0 & 1 \end{pmatrix}$$

It can be shown that $\mathbf{P}_{34}\mathbf{L}_{34} = \mathbf{I}$. Thus, we conclude that $\{3, 4\}$ is a pendant edge in both G and $\Gamma(\mathbf{G}^{-1})$. In fact, the second column of $\mathbf{R}_{34}$ and the first column of $\mathbf{S}_{34}$ are both $\mathbf{0}$. The vertex pair 3 and 4 is of Type I.

An example of a Type II vertex pair is 2 and 5, since $\{2, 5\}$ is an edge in G but not in $\Gamma(\mathbf{G}^{-1})$, and hence $\alpha_{25}\beta_{25} \neq 1$.

Moreover, we note that neither G nor $\Gamma(\mathbf{G}^{-1})$ is a plain NSSD. If we apply the algorithm to both graphs G and $\Gamma(\mathbf{G}^{-1})$, we obtain the plain NSSD K_2 in both cases.

7. Conclusion

In the search for omni–conductors in nano–molecules, the need for the analysis of an adjacency matrix **G** (for a molecular graph G) which is real and symmetric with zero diagonal became evident. We introduce the class of NSSDs, which turn out to have the additional property that even $\Gamma(\mathbf{G}^{-1})$ is a NSSD. An interplay among the corresponding principal submatrices of **G** and $\mathbf{G}^{-1}$ of order $n-1$ and $n-2$ reveal special properties for NSSDs with terminal vertices. This subclass of NSSDs is reducible to plain NSSDs by consecutive deletions of pendant edges arising in the interim subgraphs obtained in the process. Moreover, the algorithm can be applied to any graph G. If any intermediate subgraph H, obtained by repeated removal of pendant edges, is *not* a NSSD, then the parent graph G cannot be a NSSD. Thus, this algorithm provides a method to test if a graph G having pendant edges is *not* a NSSD by considering a usually much smaller subgraph of G.

References

[1] M. Fiedler, A characterization of tridiagonal matrices. Linear Algebra Appl., 2 (1969), 191–197.
[2] I. Gutman and O.E. Polansky, Mathematical Concepts in Organic Chemistry. Springer-Verlag, Berlin, 1986.
[3] W.H. Haemers, Interlacing eigenvalues and graphs. Linear Algebra Appl. 227–228 (1995), 593–616.
[4] I. Sciriha, M. Debono, M. Borg, P. Fowler, and B.T. Pickup, Interlacing–extremal graphs. Ars Math. Contemp. 6(2) (2013), 261–278.