The Adjacency Matrices of Complete
and Nutful Graphs

Irene Sciriha[⋆] , **Alexander Farrugia,** **John Baptist Gauci**

University of Malta, Department of Mathematics, Msida MSD2080, Malta

`irene.sciriha-aquilina@um.edu.mt, alex.farrugia@um.edu.mt, john-baptist.gauci@um.edu.mt`

Abstract

A real symmetric matrix $\mathbf{G}$ with zero entries on its diagonal is an adjacency matrix associated with a graph G (with weighted edges and no loops) if and only if the non–zero entries correspond to edges of G. An adjacency matrix $\mathbf{G}$ belongs to a generalized–nut graph G if every entry in a vector in the nullspace of $\mathbf{G}$ is non–zero. A graph G is termed NSSD if it corresponds to a non–singular adjacency matrix $\mathbf{G}$ with a singular deck $\{\mathbf{G} - \mathbf{v}\}$, where $\mathbf{G} - \mathbf{v}$ is the submatrix obtained from $\mathbf{G}$ by deleting the vth row and column. An NSSD G whose deck consists of generalized–nut graphs with respect to $\mathbf{G}$ is referred to as a $\mathbf{G}$–nutful graph. We prove that a $\mathbf{G}$–nutful NSSD is equivalent to having a NSSD with $\mathbf{G}^{-1}$ as the adjacency matrix of the complete graph. If the entries of $\mathbf{G}$ for a $\mathbf{G}$–nutful graph are restricted to 0 or 1, then the graph is known as nuciferous, a concept that has arisen in the context of the quantum mechanical theory of the conductivity of non–singular Carbon molecules according to the SSP model. We characterize nuciferous graphs by their inverse and the nullities of their one– and two–vertex deleted subgraphs. We show that a $\mathbf{G}$–nutful graph is a NSSD which is either K_2 or has no pendant edges. Moreover, we reconstruct a labelled NSSD either from the nullspace generators of the ordered one–vertex deleted subgraphs or from the determinants of the ordered two–vertex deleted subgraphs.

1 Introduction

The discovery of fullerenes triggered fast developments in carbon physics and chemistry. Different directions of research have focused on individual molecules. In this paper we discuss the structural and algebraic constraints on molecular graphs that act as conductors or else as insulators independent of the connectivity of the circuit wires to the atoms. Because of the difficulty in connecting a wire to a particular atom in a molecule, it would be practical and experimentally convenient if the structure of the molecule is such that any two single atom contacts enable conduction through the molecule or else if every pair bars conduction. The former molecules are termed *distinct omni–conductors* and the latter *distinct omni–insulators*. If the ends of the two semi–infinite wires connecting the molecule in a circuit are in contact with one atom only, instead of with two distinct atoms, the connection is said to be *ipso*.

In a molecular graph $G(\mathcal{V}_G, \mathcal{E}_G)$ of order n, the vertices in the vertex set $\mathcal{V}_G = \{1, 2, \ldots, n\}$ represent the arbitrarily labelled Carbon atoms in the Π–electron system of the molecule and the edges in the edge set $\mathcal{E}_G$ consist of the sigma bonds in the system.

The structure of a graph G, up to isomorphism, will be encoded in this paper by the $n \times n$ real and symmetric edge–weighted adjacency matrices $\{\mathbf{G}\}$ of G with zero entries on the diagonal. Any real symmetric matrix $\mathbf{G}$ with zero diagonal is associated with the loopless graph G, denoted also by $\Gamma(\mathbf{G})$, in which $\{i, j\}$ is a non–edge if and only if the ij^{th} entry of $\mathbf{G}$ is 0. In the case where the edge weights are all one, $\mathbf{G}$ will be denoted by $\mathbf{A}$. A graph G with an adjacency matrix $\mathbf{G}$ is a *generalized–nut graph* if every entry in a vector in the null–space of $\mathbf{G}$ is non–zero. If a graph G corresponds to a non–singular adjacency matrix $\mathbf{G}$ having singular one–vertex deleted submatrices $\{\mathbf{G} - \mathbf{v}\}$ (where $\mathbf{G} - \mathbf{v}$ is the submatrix obtained from $\mathbf{G}$ by deleting the vth row and column), then we say that the graph G belongs to the class of *NSSD*s (introduced in [1] and defined here in Definition 2.2). These graphs turn out to be such that both $\mathbf{G}$ and $\mathbf{G}^{-1}$ have zero diagonal. This sets up a duality between $\mathbf{G}$ and $\mathbf{G}^{-1}$, and any of the two can take the principal role. We use the term *plain NSSD* to refer to a graph which is either K_2 or an NSSD with no pendant edges. If a NSSD G happens to have all one–vertex deleted subgraphs consisting entirely of generalized–nut graphs with respect to $\mathbf{G}$, then we say that the graph is $\mathbf{G}$–*nutful*.

The graphs considered in the study of conductivity are chemical graphs, that is, connected molecular graphs with maximum vertex degree at most three. This is motivated

by Hückel theory, whereby graphs associated with Π molecular systems must have degree less than four. However, in this paper, we consider molecular graphs with no restriction on the maximum vertex degree.

In the SSP (Source–and–Sink Potential) model for ballistic conduction in nano–materials, any wave of electron flow through a molecule is set up by the incoming, reflected and transmitted waves. At a particular molecular energy λ of a specific molecule, the transmission of electrons through a specific Carbon molecular framework depends sensitively on the single atom contacts. The SSP theory predicts that conductivity at the Fermi energy level ($\lambda = 0$) through non–singular chemical graphs occurs for distinct contacts i and j if and only if the ij^{th} entry of the inverse $\mathbf{A}^{-1}$ of the 0–1 adjacency matrix $\mathbf{A}$ with zero diagonal is non–zero [11]. Therefore, the zero and non–zero pattern of the entries in $\mathbf{A}^{-1}$ determines the vertex contacts for insulation and conduction respectively. Thus, for a distinct omni–conductor which happens to be also an ipso omni–insulator, the inverse was proved (in [11]) to belong to the complete graph K_n with no loops at any vertex. In [11], the SSP model is shown to relate $K_n = \Gamma(\mathbf{G}^{-1})$ with a *nuciferous* graph G (Definition 3.1).

In this paper, we extend the results of [11] to any real symmetric adjacency matrix $\mathbf{G}$ of G with zero diagonal. One of our main results is Theorem 3.8, stating that a NSSD G is $\mathbf{G}$–nutful if and only if $\Gamma(\mathbf{G}^{-1}) = K_n$. In the proofs leading to Theorem 3.8, invariants of the adjacency matrix of G were used that will enable the reconstruction of a NSSD.

The paper is organised as follows. In Section 2, terminology related to graphs and their submatrices is presented formally. In Section 3, we prove Theorem 3.8 and show that a $\mathbf{G}$–nutful graph is a plain NSSD. The methods we develop in these proofs shed light on the interplay between the combinatorial properties of the one– and two–vertex deleted subgraphs relative to the matrix $\mathbf{G}$ associated with the parent NSSD $G = \Gamma(\mathbf{G})$ and the related submatrices of $\mathbf{G}$. In Section 4 we show how a NSSD can be constructed from these graph invariants.

2   Preliminaries

The set of eigenvalues $\{\lambda\}$ of $\mathbf{G}$ (also called the *spectrum* of $\mathbf{G}$) and the associated eigenvectors $\mathbf{x}$ are determined by $\mathbf{G}\mathbf{x} = \lambda\mathbf{x}$, where $\mathbf{x} \neq \mathbf{0}$. It is noted that different labellings of the vertices of G yield similar matrices and thus an invariant spectrum.

We recall that for any square $n \times n$ matrix $\mathbf{M}$, the characteristic polynomial $\phi(\mathbf{M}, \lambda)$

(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 *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 $\mathbf{x}$, called *kernel eigenvectors* of $\mathbf{M}$, such that $\mathbf{M}\mathbf{x} = \mathbf{0}$.

For a graph $G = \Gamma(\mathbf{G})$, the vertices can be partitioned into $\mathbf{G}$–*core* and $\mathbf{G}$–*core-forbidden* vertices for $\mathbf{G}$. A vertex of G corresponding to a non–zero entry in *some* kernel eigenvector $\mathbf{x}$ is said to be a $\mathbf{G}$–*core vertex* ($\mathbf{G}$–CV) for the adjacency matrix $\mathbf{G}$ associated with G. A $\mathbf{G}$–core-forbidden vertex ($\mathbf{G}$–CFV), for the matrix $\mathbf{G}$ associated with G, corresponds to a zero entry in *every* kernel eigenvector of $\mathbf{G}$. The nature of the vertex is the key to determine the effect on the nullity of $\mathbf{G}$ when the vertex is deleted.

We denote by $\mathbf{G} - \mathbf{v}$ the $(n-1) \times (n-1)$ principal submatrix obtained from $\mathbf{G}$ by deleting the vth row and column. By *Cauchy's Inequalities for Hermitian matrices* (also referred to as the *Interlacing Theorem*) [4], deletion of a vertex changes the nullity of a graph by at most one. On deleting a $\mathbf{G}$–core vertex in a singular graph $\Gamma(\mathbf{G})$, one of the vectors in a basis for the nullspace of $\mathbf{G}$ is destroyed. Together with the Interlacing Theorem, this leads to the next result, which we shall make use of, sometimes implicitly.

Lemma 2.1. [7] *Let G be a graph with adjacency matrix $\mathbf{G}$ of nullity η. Then*

(i) v is a $\mathbf{G}$–core vertex for $\mathbf{G}$ if and only if the nullity of $\mathbf{G} - \mathbf{v}$ is $\eta - 1$;

(ii) v is a $\mathbf{G}$–core-forbidden vertex if and only if the nullity of $\mathbf{G} - \mathbf{v}$ is either η or $\eta + 1$.

Our focus will be a subclass of the class of graphs termed NSSDs, introduced in [1]. For a graph to be a NSSD, it must have the following characteristics:

Definition 2.2. [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.*

Definition 2.3. *A NSSD is said to be* plain *if it is either K_2 or has no pendant edge.*

The next result is a direct consequence of the Interlacing Theorem.

Lemma 2.4. *For a NSSD G, the nullity of $\mathbf{G} - \mathbf{v}$ is equal to one for all $v \in \mathcal{V}_G$.*

In [1], it was shown that NSSDs are closed under the inverse operation.

Theorem 2.5. [1] *For a NSSD G with associated adjacency matrix* $\mathbf{G}$, *the graph* $\Gamma(\mathbf{G}^{-1})$ *is also a NSSD.*

Following [1], we shall let the last two vertices of a labelled NSSD G be x and y and write

$$\mathbf{G} = \begin{pmatrix} \mathbf{P}_{xy} & \mathbf{R}_x & \mathbf{R}_y \\ \mathbf{R}_x^t & 0 & \beta_{xy} \\ \mathbf{R}_y^t & \beta_{xy} & 0 \end{pmatrix}, \qquad \text{with } \mathbf{P}_{xy} \text{ square} \qquad (1)$$

and

$$\mathbf{G}^{-1} = \begin{pmatrix} \mathbf{L}_{xy} & \mathbf{S}_x & \mathbf{S}_y \\ \mathbf{S}_x^t & 0 & \alpha_{xy} \\ \mathbf{S}_y^t & \alpha_{xy} & 0 \end{pmatrix}, \qquad \text{with } \mathbf{L}_{xy} \text{ square.} \qquad (2)$$

In the following definition, we introduce another class $\{N\}$ of graphs with $\mathbf{N}$ singular which we shall refer to in the sequel.

Definition 2.6. *A graph N having adjacency matrix* $\mathbf{N}$ *with each entry of the diagonal equal to zero is said to be a* generalized–nut graph *if no entry in any kernel eigenvector of* $\mathbf{N}$ *is zero.*

As an aside, we note that no generalized–nut graphs exist on 2, 3 or 4 vertices. For 5 or more vertices, the problem of their existence is still open.

It follows immediately that the nullity of the matrix $\mathbf{N}$ associated with a generalized–nut graph N is one. In the literature (see for example [5, 8, 12]), a *nut graph* refers to the particular case when the entries of the adjacency matrix $\mathbf{A}$ are restricted to 0 and 1. Nut graphs turn out to be connected, of order at least seven, to be non–bipartite and to have neither vertices of degree one nor $\mathbf{A}$–core–forbidden vertices [12, 6]. Other studies on nut graphs can be found in [5]. For weighted adjacency matrices, see [10].

By association with the word *nut*, we define the class of $\mathbf{G}$–*nutful* graphs, which is a subclass of NSSDs. We shall show its relation to generalized–nut graphs in Corollary 3.6.

Definition 2.7. *A* $\mathbf{G}$–*nutful graph G is either* K_2 *or a NSSD on at least three vertices having all two vertex–deleted subgraphs of the same nullity.*

In the sequel we shall denote the $(n-2) \times (n-2)$ principal submatrix obtained from $\mathbf{G}$ by deleting the vth and the wth rows and columns by $\mathbf{G} - \mathbf{v} - \mathbf{w}$.

In [1], it is shown that it is impossible that for a NSSD G, the nullity of $\mathbf{G} - \mathbf{v} - \mathbf{w}$ takes the value of one for any two distinct vertices v and w of G. We shall determine, in Lemma 3.5, the common value of the nullity of $G - v - w$ for any two distinct vertices v and w of a $\mathbf{G}$–nutful graph G.

3   The Inverse of a Complete NSSD

Relative to the 0–1 adjacency matrix $\mathbf{A}$, the class of nuciferous graphs was introduced in [11] as that of the molecular graphs that are distinct omni–conductors and also ipso omni–insulators.

Definition 3.1. [11] *Let $\mathbf{A}$ be the 0–1 adjacency matrix of a graph G. If $\mathbf{A}$ is non-singular, the diagonal entries of $\mathbf{A}^{-1}$ are zero and the off-diagonal entries of $\mathbf{A}^{-1}$ are non–zero and real, then the graph G is said to be a* nuciferous graph.

The graph $\Gamma(\mathbf{A}^{-1})$ associated with a nuciferous graph with adjacency matrix $\mathbf{A}$ is thus the complete graph K_n with weighted edges and no loops. One such candidate is K_2, in which case $\mathbf{A}^{-1} = \mathbf{A}$, so that K_2 is both a complete graph and a nuciferous graph. To date we know of no other nuciferous graphs [2, 11].

¿From Theorem 2.5, a key result in [1], it follows that the complete graph $K_n = \Gamma(\mathbf{A}^{-1})$, determined by the inverse of the 0–1 adjacency matrix $\mathbf{A}$ of a nuciferous graph G, is a NSSD.

Motivated by the algebraic properties of a nuciferous graph G, we generalize the relation of $\mathbf{G}$ with $\mathbf{G}^{-1}$ for a NSSD associated with a real and symmetric matrix. We explore the properties of the inverse of an adjacency matrix associated with the complete graph K_n when this belongs to the class of NSSDs.

3.1   Nutful Graphs

In this section we justify the use of the terms nut graphs, generalized–nut graphs, nuciferous and nutful graphs. We consider an adjacency matrix $\mathbf{H}$ belonging to a complete graph K_n so that $\Gamma(\mathbf{H})$ is a NSSD, henceforth referred to as the complete NSSD K_n. Note that $\mathbf{H}^{-1}$ need not be associated with a nuciferous graph since the adjacency matrix $\mathbf{H}$ is not necessarily the inverse of a 0–1 symmetric matrix.

Lemma 3.2. *Let the complete NSSD K_n have adjacency matrix $\mathbf{H}$. Then the graph $\Gamma(\mathbf{H}^{-1}-\mathbf{y})$ is a generalized–nut graph for all $y \in \mathcal{V}_{K_n}$.*

Proof. Let a complete NSSD (with weighted edges) K_n have adjacency matrix $\mathbf{H}$. Since $\Gamma(\mathbf{H}) = K_n$ is a NSSD, by Theorem 2.5, $\Gamma(\mathbf{H}^{-1})$ is also a NSSD, and thus $\mathbf{H}^{-1}-\mathbf{y}$ has all diagonal entries equal to zero. In [1, Proposition 4.4], it was proved that the one–dimensional nullspace of $\mathbf{H}^{-1}-\mathbf{y}$ is generated by the eigenvector $\begin{pmatrix} \mathbf{R}_y \\ \beta_{xy} \end{pmatrix}$ for all $x, y \in \mathcal{V}_{K_n}$. Since $\Gamma(\mathbf{H}) = K_n$, the entries of $\mathbf{R}_y$ and β_{xy} are all non–zero, and hence all the entries of the eigenvector $\begin{pmatrix} \mathbf{R}_y \\ \beta_{xy} \end{pmatrix}$ are non–zero. By Definition 2.6, $\Gamma(\mathbf{H}^{-1}-\mathbf{y})$ is a generalized–nut graph. $\qquad\square$

The result [11, Theorem 7.9], stating that $G - v$ is a nut graph if G is nuciferous of order at least 3, is a special case of Lemma 3.2.

Proposition 3.3. *Let the complete NSSD K_n have adjacency matrix $\mathbf{H}$. Then the graph $\Gamma(\mathbf{H}^{-1})$ is $(\mathbf{H}^{-1})$–nutful.*

Proof. Since K_n is a NSSD, then $\mathbf{H}^{-1}$ exists and by Theorem 2.5, $\Gamma(\mathbf{H}^{-1})$ is also a NSSD. By Lemma 3.2, $\Gamma(\mathbf{H}^{-1}-\mathbf{y})$ is a generalized–nut graph for all $y \in \mathcal{V}_{K_n}$, and thus it has no zero entry in any vector in the nullspace of its adjacency matrix $\mathbf{H}^{-1}-\mathbf{y}$. It follows that all the vertices $x \in \mathcal{V}_{K_n-y}$ are $(\mathbf{H}^{-1}-\mathbf{y})$–core–vertices, and by Lemma 2.1, $\eta(\mathbf{H}^{-1}-\mathbf{x}-\mathbf{y}) = 0$ for all vertices x and y. $\qquad\square$

Now we consider the reverse process. Given a $\mathbf{G}$–nutful graph G, what are the possible graphs associated with $\mathbf{G}^{-1}$? To answer this question we need to establish some more results on nutful graphs.

Using the techniques applied in [7], we prove the following general result.

Proposition 3.4. *Given a non–singular matrix $\mathbf{G}$ associated with a NSSD G, $\mathbf{G}^{-1}$ can be obtained from the ordered kernel eigenvectors of $\{\mathbf{G} - \mathbf{i}\}$ for $i \in \mathcal{V}_G$.*

Proof. Let the order of a NSSD G be n. For $n \leq 2$, the only non–singular graph is K_2, having each vertex–deleted subgraph isomorphic to the singular graph K_1, with kernel eigenvector (ζ_1), $\zeta_1 \neq 0$.

If $n > 2$, then, for each vertex $i \in \mathcal{V}_G$, $i = 1, \ldots, n$, let the adjacency matrix $\mathbf{G} - \mathbf{i}$ of $G - i$ have kernel eigenvector $\boldsymbol{\zeta}^{(i)}$ such that $(\mathbf{G} - \mathbf{i})\boldsymbol{\zeta}^{(i)} = \mathbf{0}$, where $\boldsymbol{\zeta}^{(i)} = \begin{pmatrix} \zeta_1^{(i)} & \cdots & \zeta_{i-1}^{(i)} & \zeta_{i+1}^{(i)} & \cdots & \zeta_n^{(i)} \end{pmatrix}^{\mathsf{T}} \neq \mathbf{0}$.

Let $\mathbf{z}^{(i)}$ be obtained from $\boldsymbol{\zeta}^{(i)}$ by inserting a zero entry at position i in $\boldsymbol{\zeta}^{(i)}$. Let $\mathbf{c}_i^{\mathsf{T}}$ be the ith row in the adjacency matrix $\mathbf{G}$ of G (with zero in the ith position), and let

$\mathbf{Z} = \begin{pmatrix} \mathbf{z^{(1)}} & \mathbf{z^{(2)}} & \dots & \mathbf{z^{(n)}} \end{pmatrix}$. Then

$$
\mathbf{GZ} = \begin{pmatrix} \mathbf{c}_1^{\mathsf{T}} \\ \mathbf{c}_2^{\mathsf{T}} \\ \vdots \\ \mathbf{c}_n^{\mathsf{T}} \end{pmatrix} \begin{pmatrix} \mathbf{z^{(1)}} & \mathbf{z^{(2)}} & \dots & \mathbf{z^{(n)}} \end{pmatrix} = \begin{pmatrix} \mathbf{c}_1^{\mathsf{T}} \\ \mathbf{c}_2^{\mathsf{T}} \\ \vdots \\ \mathbf{c}_n^{\mathsf{T}} \end{pmatrix} \begin{pmatrix} 0 & \zeta_1^{(2)} & \dots & \zeta_1^{(n)} \\ \zeta_2^{(1)} & 0 & \dots & \zeta_2^{(n)} \\ \vdots & \vdots & \ddots & \vdots \\ \zeta_n^{(1)} & \zeta_n^{(2)} & \dots & 0 \end{pmatrix}. \tag{3}
$$

For $i \neq j$, the ij^{th} entry $\mathbf{c}_i^{\mathsf{T}} \mathbf{z^{(j)}} = 0$, since $\boldsymbol{\zeta}^{(j)}$ is an eigenvector of $\mathbf{G} - \mathbf{j}$. If for some i, $\mathbf{c}_i^{\mathsf{T}} \mathbf{z^{(i)}} = 0$, then $\mathbf{G} \mathbf{z^{(i)}} = \mathbf{0}$, contradicting that $\mathbf{G}$ is non–singular. Hence the only non–zero elements of the product $\mathbf{GZ}$ in (3) are the diagonal elements $\mathbf{c}_i^{\mathsf{T}} \mathbf{z^{(i)}}$. Thus

$$
\mathbf{G}^{-1} = \begin{pmatrix} \dfrac{\mathbf{z^{(1)}}}{\mathbf{c}_1^{\mathsf{T}} \mathbf{z^{(1)}}} & \dfrac{\mathbf{z^{(2)}}}{\mathbf{c}_2^{\mathsf{T}} \mathbf{z^{(2)}}} & \dots & \dfrac{\mathbf{z^{(n)}}}{\mathbf{c}_n^{\mathsf{T}} \mathbf{z^{(n)}}} \end{pmatrix} = \mathbf{Z} \operatorname{Diag} \left(\dfrac{1}{\mathbf{c}_1^{\mathsf{T}} \mathbf{z^{(1)}}}, \dfrac{1}{\mathbf{c}_2^{\mathsf{T}} \mathbf{z^{(2)}}}, \dots, \dfrac{1}{\mathbf{c}_n^{\mathsf{T}} \mathbf{z^{(n)}}} \right)
$$

and

$$
\mathbf{G} = \operatorname{Diag} \left(\mathbf{c}_1^{\mathsf{T}} \mathbf{z^{(1)}}, \mathbf{c}_2^{\mathsf{T}} \mathbf{z^{(2)}}, \dots, \mathbf{c}_n^{\mathsf{T}} \mathbf{z^{(n)}} \right) \mathbf{Z}^{-1},
$$

where $\operatorname{Diag} \left(\alpha_1, \alpha_2, \dots, \alpha_n \right)$ is a diagonal matrix with diagonal entries α_i, $i = 1, \dots, n$.

The values of $\mathbf{c}_i^{\mathsf{T}} \mathbf{z^{(i)}}$ need not be known to construct the edges of G because the $k\ell^{\text{th}}$ entry of $\mathbf{Z}^{-1}$ is non–zero if and only if $\{k, \ell\}$ is an edge.

The reconstruction is thus complete. $\qquad\square$

The proof of Proposition 3.3 shows that if $\mathbf{H}$ belongs to K_n, then for the $\mathbf{H}^{-1}$–nutful graph, the common value of the nullity of $\mathbf{H}^{-1} - \mathbf{x} - \mathbf{y}$ for all vertices x and y is zero. Indeed, this value of the nullity will be shown to be a characterization of $\mathbf{G}$–nutful graphs.

Lemma 3.5. *For a $\mathbf{G}$–nutful graph G, the nullity of $\mathbf{G} - \mathbf{x} - \mathbf{y}$ is equal to zero for all $x, y \in \mathcal{V}_G$.*

Proof. We consider a $\mathbf{G}$–nutful graph G. From Lemma 2.4 and as a consequence of the Interlacing Theorem, for a pair of vertices x and y in G, $\eta(\mathbf{G} - \mathbf{x} - \mathbf{y})$ is equal to either zero, one or two.

For all $y \in \mathcal{V}_G$, $\eta(\mathbf{G} - \mathbf{y}) = 1$ and, by definition of a $\mathbf{G}$–nutful graph, $\mathbf{G} - \mathbf{y}$ has a kernel eigenvector whose entries are all non–zero. Each vertex x of $G - y$ corresponds to a $(\mathbf{G} - \mathbf{y})$–core vertex. By Lemma 2.1, deleting a core vertex decreases the nullity by one, and hence $\eta(\mathbf{G} - \mathbf{x} - \mathbf{y})$ is equal to zero. Thus, at least one vertex pair x, y is such that $\eta(\mathbf{G} - \mathbf{x} - \mathbf{y}) = 0$. However, by Definition 2.7, $\eta(\mathbf{G} - \mathbf{x} - \mathbf{y})$ is a constant, and hence must be the same for all pairs of vertices x, y in G. $\qquad\square$

We have thus justified the relation between $\mathbf{G}$–nutful graphs and generalized–nut graphs.

Corollary 3.6. *Each vertex–deleted subgraph of a* **G**–*nutful graph G is a generalized–nut graph.*

There are certain orders, k, of graphs for which generalized–nut graphs do not exist, and thus by Corollary 3.6, there would not be any nutful graphs on $k + 1$ vertices.

We can now prove the converse of Proposition 3.3.

Proposition 3.7. *Let* **G** *be the adjacency matrix of a* **G**–*nutful graph G. Then the graph associated with the matrix* **G**$^{-1}$ *is* K_n.

Proof. We consider a **G**–nutful graph G. Since G is a NSSD, then by Theorem 2.5, $\Gamma(\mathbf{G}^{-1})$ is also a NSSD. Also, by Lemma 2.4, $\eta(\mathbf{G} - \mathbf{y}) = 1$ for all $y \in \mathcal{V}_G$, and by Lemma 3.5, $\eta(\mathbf{G} - \mathbf{x} - \mathbf{y}) = 0$ for all $x, y \in \mathcal{V}_G$. Thus, each vertex x in $G - y$ is a $(\mathbf{G} - \mathbf{y})$–core vertex, and, as a consequence of Lemma 2.1, each entry of any kernel eigenvector $\boldsymbol{\zeta}^{(y)}$ of $\mathbf{G} - \mathbf{y}$ is non–zero. This holds for all the vertices of G, and following the same line of proof as in Proposition 3.4, the columns $\mathbf{z}^{(\mathbf{y})}$ of $\mathbf{G}^{-1}$ can be obtained from $\boldsymbol{\zeta}^{(y)}$ by inserting a zero entry in the yth position. Thus, all the diagonal entries of $\mathbf{G}^{-1}$ are zero and all the off–diagonal entries of $\mathbf{G}^{-1}$ are non–zero. Hence $\Gamma(\mathbf{G}^{-1}) = K_n$. □

¿From Propositions 3.3 and 3.7, we deduce:

Theorem 3.8. *Let G be a graph with adjacency matrix* **G**. *Then G is a* **G**–*nutful graph if and only if* $\Gamma(\mathbf{G}^{-1}) = K_n$.

In [1, Proposition 5.19], it is proven that if y is a terminal vertex adjacent to vertex x in a NSSD G, then x is a terminal vertex adjacent to y in $\Gamma(\mathbf{G}^{-1})$. Recall that a plain NSSD is either K_2 or a NSSD with no pendant edge.

Corollary 3.9. *A* **G**–*nutful graph G is a plain NSSD.*

Proof. Suppose y is a terminal vertex adjacent to x in G. Then $\Gamma(\mathbf{G}^{-1})$ has a pendant edge by [1, Proposition 5.19], a contradiction to Theorem 3.8 unless $\Gamma(\mathbf{G}^{-1}) = K_2$, in which case $G = K_2$. □

3.2 Nuciferous Graphs

The properties of nuciferous graphs discussed in [11] suggest that these graphs are a subclass of the class of **G**–nutful graphs.

Theorem 3.10. *Let G be a nuciferous graph with associated 0–1 adjacency matrix $\mathbf{A}$. Then G is an $\mathbf{A}$–nutful graph.*

Proof. We consider a nuciferous graph G. Note that $\mathbf{A}$ is a non–singular, real and symmetric matrix with each entry of the diagonal equal to zero. By Definition 3.1, the diagonal entries of $\mathbf{A}^{-1}$ are zero, and hence the entries on the diagonal of adj($\mathbf{A}$) are all zero. Thus, for all vertices $v \in \mathcal{V}_G$, $\det(\mathbf{A} - \mathbf{v}) = 0$, implying that $\eta(\mathbf{A} - \mathbf{v}) \geq 1$. As a consequence of the Interlacing Theorem, $\eta(\mathbf{A} - \mathbf{v}) = 1$. Hence, $G = \Gamma(\mathbf{A})$ is a NSSD.

Since the graph associated with $\Gamma(\mathbf{A}^{-1})$ is K_n, the result follows by applying Proposition 3.3. $\qquad\square$

As for the case of $\mathbf{G}$–nutful graphs, the result that follows justifies the name '*nuciferous*' chosen for this class of graphs.

Corollary 3.11. *Each vertex–deleted subgraph of a nuciferous graph is a nut graph or K_1.*

Proof. By Theorem 3.10, a nuciferous graph G is a $\mathbf{A}$–nutful graph. If G has at most two vertices, then the only graph corresponding to a non–singular matrix $\mathbf{A}$ is K_2, whose vertex–deleted subgraphs are K_1. Each vertex–deleted subgraph of a $\mathbf{A}$–nutful graph G on at least three vertices is a generalized–nut graph by Corollary 3.6. Thus, each vertex deleted subgraph of a nuciferous graph is a nut graph. $\qquad\square$

We have thus shown that, for a nuciferous graph, the nullities of $\mathbf{A}$, $\mathbf{A} - \mathbf{x}$, $\mathbf{A} - \mathbf{y}$ and $\mathbf{A} - \mathbf{x} - \mathbf{y}$ are equal to 0, 1, 1 and 0, respectively. This is one of the characterizations of nuciferous graphs given in the following theorem, which is a direct consequence of Theorems 3.8 and 3.10 and of Corollary 3.11.

Theorem 3.12. *The following statements are equivalent for a graph G with associated 0–1 adjacency matrix $\mathbf{A}$:*

  (i) The graph G is nuciferous.

 (ii) The adjacency matrix $\mathbf{A}$ is non–singular and each vertex–deleted subgraph of G is a nut graph.

(iii) The graph $\Gamma(\mathbf{A}^{-1})$ is the complete graph with weighted edges and no loops.

(iv) The nullities of $\mathbf{A}$, $\mathbf{A} - \mathbf{x}$, $\mathbf{A} - \mathbf{y}$ and $\mathbf{A} - \mathbf{x} - \mathbf{y}$ are equal to 0, 1, 1 and 0, respectively, for all pairs of vertices x and y in $\mathcal{V}_G$.

4 Reconstructions

In the proofs of Propositions 3.4 and 3.7, a NSSD is reconstructed from graph invariants. Here we propose minimal sets of data that are required to reconstruct a particular NSSD. Following the terminology for *Ulam's Reconstruction Conjecture*, we call the set of one–vertex deleted subgraphs of G the *deck* of G. The *Polynomial Reconstruction Problem* attempts to recover $\phi(\mathbf{G}, \lambda)$ from the polynomial deck $\{\phi(\mathbf{G} - \mathbf{v}, \lambda) : v \in \mathcal{V}_G\}$. Since $\phi'(\mathbf{G}, \lambda) = \sum_{v \in \mathcal{V}_G} \phi(\mathbf{G} - \mathbf{v}, \lambda)$, then the problem is reduced to obtaining the constant a_0 of the characteristic polynomial $\phi(\mathbf{G}, \lambda)$. A *singular deck* is one consisting entirely of subgraphs having a singular adjacency matrix $\{\mathbf{G} - \mathbf{v}\}$. If for some $v \in \mathcal{V}_G$, $\eta(\mathbf{G} - \mathbf{v}) \geq 2$, then as a consequence of the Interlacing Theorem, zero is an eigenvalue of $\mathbf{G}$ and $a_0 = 0$. Therefore what remains to be considered for a singular deck is one consisting of subgraphs $G - v$ each of which has an adjacency matrix of nullity one [7].

A variant of the Reconstruction Conjecture is to reconstruct a non–singular NSSD G from the *ordered* kernel eigenvectors of $\{\mathbf{G} - \mathbf{v} : v \in \mathcal{V}_G\}$. This is presented in Theorem 4.1, and its proof follows immediately from Proposition 3.4.

Theorem 4.1. *A NSSD G is reconstructible from the ordered kernel eigenvectors of the adjacency matrices $\{\mathbf{G} - \mathbf{v}\}$.*

Each column of the adjugate $\text{adj}(\mathbf{M})$ of a $n \times n$ matrix $\mathbf{M}$ of nullity one lies in the nullspace of $\mathbf{M}$. Since the rank of $\mathbf{M}$ is $n-1$, the determinant of at least one $(n-1) \times (n-1)$ submatrix of $\mathbf{M}$ is non–zero. It follows that $\text{adj}(\mathbf{M}) \neq \mathbf{0}$. Therefore the rank of $\text{adj}(\mathbf{M})$ is one.

For a NSSD G, the entries of an eigenvector of $\mathbf{G} - \mathbf{y}$ for $y \in \mathcal{V}_G$, associated with the zero eigenvalue, are (up to sign) determinants of $(n - 2) \times (n - 2)$ submatrices of $\mathbf{G}$. Let the kth diagonal entry of $\text{adj}(\mathbf{G} - \mathbf{y})$ for the NSSD G be $|\mathbf{P}_{ky}|$. The matrix $\text{adj}(\mathbf{G} - \mathbf{y})$ is real and symmetric since $\mathbf{G}$ is real and symmetric. It follows that the $k\ell^{\text{th}}$ entry of $\text{adj}(\mathbf{G} - \mathbf{y})$ can be expressed in terms of the kth and ℓ^{th} diagonal entries of $\text{adj}(\mathbf{G} - \mathbf{y})$ [9].

Lemma 4.2. *The $k\ell^{\text{th}}$ entry of $\text{adj}(\mathbf{G} - \mathbf{y})$ is $\pm\sqrt{(|\mathbf{P}_{yk}| \, |\mathbf{P}_{y\ell}|)}$ where $|\mathbf{P}_{yk}|$ is the determinant of the principal submatrix of $\mathbf{G}$ obtained from $\mathbf{G}$ by deleting the kth and y^{th} rows and columns, and similarly for $|\mathbf{P}_{y\ell}|$.*

Proof. If G is a NSSD, then the rank of adj$(\mathbf{G} - \mathbf{y})$ is equal to one. Hence all nonzero rows of adj$(\mathbf{G} - \mathbf{y})$ are real multiples of each other and so are the nonzero columns. Since $\mathbf{G} - \mathbf{y}$ is real and symmetric, if

$$\text{adj}(\mathbf{G} - \mathbf{y}) = \begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} & \cdots & \mathbf{A}_{1\,n-1} \\ \mathbf{A}_{21} & \mathbf{A}_{22} & \cdots & \mathbf{A}_{2\,n-1} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{A}_{n-1\,1} & \mathbf{A}_{n-1\,2} & \cdots & \mathbf{A}_{n-1\,n-1} \end{pmatrix} = (\mathbf{A}_{ij})_{n-1 \times n-1}$$

where $\mathbf{A}_{ij}$ is the ij^{th} cofactor matrix of $\mathbf{G} - \mathbf{y}$, then

$$\mathbf{A}_{k\ell}^2 = \mathbf{A}_{kk}\mathbf{A}_{\ell\ell} = |\mathbf{P}_{yk}|\,|\mathbf{P}_{y\ell}|$$

as required. □

Note that the yth column of adj$(\mathbf{G})$ is $|\mathbf{G}| \begin{pmatrix} \mathbf{S}_y \\ \alpha_{xy} \\ 0 \end{pmatrix}$ and is proportional to $\mathbf{z}^{(\mathbf{y})}$ (defined in Proposition 3.4). Also, we can use Jacobi's Identity [3] to obtain the entries of the matrix $\mathbf{G}$ (up to sign) in terms of the submatrices of $\mathbf{G}^{-1}$ (and similarly for the matrix $\mathbf{G}^{-1}$) as shown in the following result. Simply stated, Jacobi's identity is $j^2 = ut - sv$, where j is the xy^{th} entry of the adjugate of $\lambda\mathbf{I} - \mathbf{G}$ and s, t, u, v are the characteristic polynomials in λ of $\mathbf{G}, \mathbf{G} - \mathbf{x}, \mathbf{G} - \mathbf{y}$ and $\mathbf{G} - \mathbf{x} - \mathbf{y}$, respectively. We remark that for a matrix $\mathbf{M}$, $\|\mathbf{M}\|$ denotes the absolute value of the determinant $|\mathbf{M}|$ of $\mathbf{M}$.

Theorem 4.3. *Let G be a NSSD with adjacency matrix $\mathbf{G}$. Using the same notation for $\mathbf{G}$ and $\mathbf{G}^{-1}$ as in (1) and (2), then*

$$\mathbf{G} = \sqrt{\|\mathbf{G}\|} \begin{pmatrix} 0 & \pm\sqrt{\|\mathbf{L}_{12}\|} & \cdots & \pm\sqrt{\|\mathbf{L}_{1n}\|} \\ \pm\sqrt{\|\mathbf{L}_{21}\|} & 0 & \cdots & \pm\sqrt{\|\mathbf{L}_{2n}\|} \\ \vdots & \vdots & \ddots & \vdots \\ \pm\sqrt{\|\mathbf{L}_{n-1\,1}\|} & \pm\sqrt{\|\mathbf{L}_{n-1\,2}\|} & \cdots & \pm\sqrt{\|\mathbf{L}_{n-1\,n}\|} \\ \pm\sqrt{\|\mathbf{L}_{n\,1}\|} & \pm\sqrt{\|\mathbf{L}_{n\,2}\|} & \cdots & 0 \end{pmatrix}$$

and

$$\mathbf{G}^{-1} = \frac{1}{\sqrt{\|\mathbf{G}\|}} \begin{pmatrix} 0 & \pm\sqrt{\|\mathbf{P}_{12}\|} & \cdots & \pm\sqrt{\|\mathbf{P}_{1n}\|} \\ \pm\sqrt{\|\mathbf{P}_{21}\|} & 0 & \cdots & \pm\sqrt{\|\mathbf{P}_{2n}\|} \\ \vdots & \vdots & \ddots & \vdots \\ \pm\sqrt{\|\mathbf{P}_{n-1\,1}\|} & \pm\sqrt{\|\mathbf{P}_{n-1\,2}\|} & \cdots & \pm\sqrt{\|\mathbf{P}_{n-1\,n}\|} \\ \pm\sqrt{\|\mathbf{P}_{n\,1}\|} & \pm\sqrt{\|\mathbf{P}_{n\,2}\|} & \cdots & 0 \end{pmatrix}$$

Proof. Let x and y be two (distinct) vertices of a NSSD G. Using Jacobi's identity $j^2 = ut - sv$, and by definition of a NSSD G, $u = t = 0$ for $\lambda = 0$. Now $v = |\mathbf{P}_{xy}|$ and $s = |\mathbf{G}|$. Also j is the xy^{th} entry of the adjugate of $\mathbf{G}$, which can be obtained from

$\mathbf{G}^{-1}$. Specifically the xy^{th} entry of G^{-1} is $\dfrac{j}{|\mathbf{G}|} = \pm\dfrac{\sqrt{-sv}}{|\mathbf{G}|} = \pm\dfrac{\sqrt{|\mathbf{G}|\,|\mathbf{P}_{xy}|}}{|\mathbf{G}|} = \pm\dfrac{\sqrt{\|\mathbf{P}_{xy}\|}}{\sqrt{\|\mathbf{G}\|}}$.
Similarly, since G^{-1} corresponds to a NSSD, the xy^{th} entry of $\mathbf{G}$ is $\pm\sqrt{\|\mathbf{G}\|}\sqrt{\|\mathbf{L}_{xy}\|}$. $\square$

We remark that Proposition 3.7 could also be deduced from $\mathbf{G}^{-1}$ given in Theorem 4.3 above.

Empirical evidence suggests that the order of NSSDs is even; however, this is still open.

Conjecture 4.4. *There are no NSSDs with an odd number of vertices.*

5 Conclusion

In the search for ipso omni–insulators among non–singular chemical graphs, the SSP model points to real symmetric matrices with each entry on the diagonal equal to zero for the inverse of the 0–1 adjacency matrix. There is a dearth of occurrences of ipso non–singular omni–insulators. Motivated by this, and by the techniques used in the recognition of a conducting or insulating distinct vertex pair of circuit terminals from the entries in the inverse of the adjacency matrix $\mathbf{G}$, we applied the properties of NSSDs developed in [1] to complete graphs. For an adjacency matrix $\mathbf{G}$ belonging to the complete NSSD K_n, the inverse $\mathbf{G}^{-1}$ turns out to be $\mathbf{G}$–nutful. Conversely, for an adjacency matrix $\mathbf{H}$ associated with a $\mathbf{H}$–nutful graph H of order n belonging to the class of NSSDs, the inverse $\mathbf{H}^{-1}$ relates to K_n. Nuciferous graphs are a subclass of the nutful graphs and according to the SSP model, they turn out to be distinct omni–conductors which are also ipso omni–insulators. To date, the only nuciferous graph known is K_2. In [2, 11], it is conjectured that there are no others. Moreover, if in fact others exist, they must be of order at least eight [12].

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