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Non-Singular graphs with a Singular Deck

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ABSTRACT

The n-vertex graph $G(=\Gamma(\mathbf{G}))$ with a non-singular real symmetric adjacency matrix $\mathbf{G}$, having a zero diagonal and singular $(n-1)\times(n-1)$ principal submatrices is termed a NSSD, a Non-Singular graph with a Singular Deck. NSSDs arose in the study of the polynomial reconstruction problem and were later found to characterise non-singular molecular graphs that are distinct omni-conductors and ipso omni-insulators. Since both matrices $\mathbf{G}$ and $\mathbf{G}^{-1}$ represent NSSDs $\Gamma(\mathbf{G})$ and $\Gamma(\mathbf{G}^{-1})$, the value of the nullity of a one-, two- and three-vertex deleted subgraph of G is shown to be determined by the corresponding subgraph in $\Gamma(\mathbf{G}^{-1})$. Constructions of infinite subfamilies of non-NSSDs are presented. NSSDs with all two-vertex deleted subgraphs having a common value of the nullity are referred to as $\mathbf{G}$-nutful graphs. We show that their minimum vertex degree is at least 4.

1. Introduction

All the graphs considered in this paper have weighted edges and no loops. The *adjacency matrix* $\mathbf{G}$ of a (weighted) graph G is a real and symmetric matrix which encodes the adjacencies of the graph by assigning the ijth entry of $\mathbf{G}$ a nonzero value w if and only if the edge $\{i, j\}$ in G connecting the two distinct vertices i and j has weight w. The number of edges incident to a vertex is called the *degree* or, equivalently, the *valency* of the vertex. The $n \times n$ circulant matrix $\mathbf{C} = (a_{k,j} : k, j = 1, 2, \ldots, n)$ where $a_{k,j} = a_{(j-k) \bmod n}$ is denoted by $\mathbf{C} = \langle a_0, a_1, \ldots, a_{n-1}\rangle$.

The *characteristic polynomial* $\phi(\mathbf{M}, \lambda)$ of a square $n \times n$ matrix $\mathbf{M}$, over a field F, is the determinant $\det(\lambda\mathbf{I} - \mathbf{M})$, denoted also by $|\lambda\mathbf{I} - \mathbf{M}|$, which is a polynomial of degree n in λ. The set of *eigenvalues* $\{\lambda\}$ of $\mathbf{M}$ consists of the roots of $\phi(\mathbf{M}, \lambda) = 0$ (in the algebraic closure of F), and the *eigenvectors* $\mathbf{x}$ of $\mathbf{M}$ associated with λ are the nonzero vectors determined by $\mathbf{M}\mathbf{x} = \lambda\mathbf{x}$. If the matrix has an eigenvalue equal to zero, then we say that the matrix is *singular*; otherwise, the matrix is *non-singular*. The multiplicity of the zero eigenvalue of $\mathbf{M}$ is the *nullity* $\eta(\mathbf{M})$ of $\mathbf{M}$. When the matrix $\mathbf{M}$ represents the adjacency matrix of a graph G, we write $G = \Gamma(\mathbf{M})$, and we refer to the characteristic polynomial, eigenvalues and eigenvectors of the matrix $\mathbf{M}$ as the characteristic polynomial, eigenvalues and eigenvectors, respectively, of the graph G. We denote by $\mathbf{G} - \mathbf{x}$ the matrix $\mathbf{G}$ with its xth row and column removed. This is the adjacency matrix of the graph $G - x$, also written as $\Gamma(\mathbf{G} - \mathbf{x})$.

In this paper, we discuss the class of NSSDs, namely the Non-Singular graphs with a Singular Deck, introduced in [1]. The concept arose in the context of the polynomial reconstruction problem, which, from a purely graph-theoretical approach, offers the first motivating factor of this work. This reconstruction problem, posed by Cvetković at the XVIII International Scientific Colloquium in Ilmenau in 1973, asks whether it is true that the characteristic polynomial of a graph G can be uniquely determined from the collection ("polynomial deck" of G) of the characteristic polynomials of all the one-vertex-deleted subgraphs of G. In particular, a variant of this problem seeks to reconstruct the non-singular graph G having a singular deck from the ordered kernel eigenvectors of the deck of G [4,5].

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The second motivating factor for this work is embedded in theoretical chemistry. The Source-and-Sink Potential (SSP) model in chemistry describes the process of ballistic conduction by examining the behaviour of a wave of electron flow through a molecule, and how the wave is reflected and/or transmitted. The graph-theoretical approach to the SSP model predicts that conductivity through a non-singular chemical graph G, with no loops, when the particular molecular energy is zero (referred to as the Fermi energy level) occurs for distinct contacts x and y if and only if the xyth entry of the inverse of the 0–1 adjacency matrix $\mathbf{A}$ associated with G is nonzero [6]. This innate bond between molecular chemistry and graph theory has matured especially since the discovery of fullerenes in 1985 (see, for instance, [3]), and underlies this current work.

The rest of this paper is structured as follows. We first describe the main properties of the family of NSSDs upon which this work is based in Section 2. Motivated by the link with molecular graphs, in Section 3 we consider a subfamily of graphs, termed nutful graphs, and examine their properties. We then show in Section 4 that an infinite family of nutful graphs exists and we describe how to construct this family. In Section 5 we show that there is a strict lower bound on the minimum degree for nutful graphs on at least three vertices to occur.

2. Properties of NSSDs

The focus of our work is a class of graphs, termed NSSD, which were introduced in [1]. A graph in this class corresponds to a non-singular adjacency matrix with zero diagonal and has the property that the adjacency matrix of each of its one-vertex-deleted subgraphs is singular (Definition 2.1).

Definition 2.1 ([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.

2.1. Duality property of $\mathbf{G}$ and $\mathbf{G}^{-1}$

Direct consequences of the Interlacing Theorem are that for a NSSD G, the dimension of the nullspace of $\mathbf{G} - \mathbf{x}$ is one, for any vertex $x \in \mathcal{V}(G)$, and that upon deleting any two vertices of G, the nullity changes by at most one. More precisely, it was shown in [1] that $\eta(\mathbf{G} - \mathbf{x} - \mathbf{y})$ is either zero or two, for any $x, y \in \mathcal{V}(G)$. Furthermore, we can distinguish between the two cases by using the following result.

Theorem 2.2 ([1]). *Let x and y be two vertices of a NSSD G with adjacency matrix $\mathbf{G}$. The nullity of $\mathbf{G} - \mathbf{x} - \mathbf{y}$ and of $\mathbf{G}^{-1} - \mathbf{x} - \mathbf{y}$ is given by*

$$\eta(\mathbf{G} - \mathbf{x} - \mathbf{y}) = \begin{cases} 0 & \text{if and only if } \{x, y\} \text{ is an edge of } \Gamma(\mathbf{G}^{-1}) \\ 2 & \text{if and only if } \{x, y\} \text{ is a non-edge of } \Gamma(\mathbf{G}^{-1}) \end{cases}$$

and

$$\eta(\mathbf{G}^{-1} - \mathbf{x} - \mathbf{y}) = \begin{cases} 0 & \text{if and only if } \{x, y\} \text{ is an edge of } G \\ 2 & \text{if and only if } \{x, y\} \text{ is a non-edge of } G, \end{cases}$$

respectively.

Before providing a more streamlined proof of the above theorem than that provided in [1], we draw the attention of the reader to a very remarkable property of the class of NSSDs, namely that the class of NSSDs is closed under taking the inverse. Stated more formally, we have the following theorem.

Theorem 2.3 ([1]). *For a NSSD G with associated adjacency matrix $\mathbf{G}$, the graph $\Gamma(\mathbf{G}^{-1})$ is also a NSSD.*

This duality property has important implications, in that any one of $\mathbf{G}$ and $\mathbf{G}^{-1}$ can assume a principal role. Furthermore, it yields a necessary and sufficient condition for G and $\Gamma(\mathbf{G}^{-1})$ to be both NSSDs, namely that the matrices $\mathbf{G}$ and $\mathbf{G}^{-1}$ are both real and symmetric with a zero diagonal (Theorem 2.4). The necessity part follows directly from the definition of NSSDs (Definition 2.1), while the sufficiency part is a consequence of the duality property and of the fact that the determinant of each principal submatrix of $\mathbf{G}$ corresponds to a diagonal entry of $\mathbf{G}^{-1}$, and thus has nullity one by the Interlacing Theorem.

Theorem 2.4 ([1]). *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.*

Using the above two theorems, we now prove Theorem 2.2.

Proof of Theorem 2.2. For any two vertices x and y of a NSSD G, we write the adjacency matrix $\mathbf{G}$ and its inverse in block form as follows:

$$\mathbf{G} = \begin{pmatrix} \mathbf{P}_{xy} & \mathbf{R}_x & \mathbf{R}_y \\ \mathbf{R}_x^{\top} & 0 & \beta_{xy} \\ \mathbf{R}_y^{\top} & \beta_{xy} & 0 \end{pmatrix} \quad \text{and} \quad \mathbf{G}^{-1} = \begin{pmatrix} \mathbf{L}_{xy} & \mathbf{S}_x & \mathbf{S}_y \\ \mathbf{S}_x^{\top} & 0 & \alpha_{xy} \\ \mathbf{S}_y^{\top} & \alpha_{xy} & 0 \end{pmatrix},$$