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Interlacing–extremal graphs*

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Abstract

A graph G is *singular* if the zero-one adjacency matrix has the eigenvalue zero. The multiplicity of the eigenvalue zero is called the *nullity* of G. For two vertices y and z of G, we call (G, y, z) a *device* with respect to y and z. The nullities of G, $G-y$, $G-z$ and $G-y-z$ classify devices into different *kinds*. We identify two particular classes of graphs that correspond to distinct kinds. In the first, the devices have the minimum allowed value for the nullity of $G-y-z$ relative to that of G for all pairs of distinct vertices y and z of G. In the second, the nullity of $G-y$ reaches the maximum possible for all vertices y in a graph G. We focus on the non–singular devices of the second kind.

Keywords: Adjacency matrix, singular graphs, nut graphs, uniform–core graphs, nuciferous graphs, interlacing.

Math. Subj. Class.: 05C50,05C35, 05C60, 05B20, 92E10, 74E40

1 Introduction

A graph $G = G(\mathcal{V}, \mathcal{E})$ of *order* n has a labelled vertex set $\mathcal{V} = \{1, 2, ..., n\}$. The set $\mathcal{E}$ of m edges consists of unordered pairs of adjacent vertices. We write $\mathcal{V}(G)$ for a graph G when the graph G needs to be specified. A subset of $\mathcal{V}$ is said to be *independent* if no two of its vertices are adjacent, i.e., no two are connected by an edge. For a subset $\mathcal{V}_1$ of $\mathcal{V}$, $G - \mathcal{V}_1$ denotes the subgraph of G induced by $\mathcal{V}\backslash\mathcal{V}_1$. The subgraph of G obtained by deleting a particular vertex y is denoted by $G - y$ and that obtained by deleting two distinct vertices

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y and z is denoted by $G - y - z$. A graph is said to be *bipartite* if its vertex set $\mathcal{V}$ may be partitioned into two independent subsets $\mathcal{V}_1$ and $\mathcal{V}_2$. The *cycle* and the *complete graph* on n vertices are denoted by C_n and K_n, respectively. The complete bipartite graph K_{n_1,n_2} has a vertex partition into two subsets $\mathcal{V}_1$ and $\mathcal{V}_2$ of independent vertices of sizes n_1 and n_2, respectively, and has edges between each member of $\mathcal{V}_1$ and each member of $\mathcal{V}_2$.

1.1 The adjacency matrix

The graphs we consider are *simple*, that is, without loops or multiple edges. We use $\mathbf{A}(G)$ (or just $\mathbf{A}$ when the context is clear) to denote the 0-1 *adjacency matrix* of a graph G, where the entry a_{ik} of the symmetric matrix $\mathbf{A}$ is 1 if $\{i, k\} \in \mathcal{E}$ and 0 otherwise. We note that the graph G is determined, up to isomorphism, by $\mathbf{A}$. The adjacency matrix $\mathbf{A}^C$ of the *complement* G^C of G is $\mathbf{J} - \mathbf{I} - \mathbf{A}$, where each entry of $\mathbf{J}$ is one and $\mathbf{I}$ is the identity matrix. The *degree* of a vertex i is the number of non–zero entries in the i^{th} row of $\mathbf{A}$. If the adjacency matrix $\mathbf{A}$ of a n-vertex graph G satisfies $\mathbf{Ax} = \lambda\mathbf{x}$ for some non-zero vector $\mathbf{x}$ then $\mathbf{x}$ is said to be an *eigenvector* belonging to the *eigenvalue* λ. There are n linearly independent eigenvectors. The eigenvalues of $\mathbf{A}$ are said to be *the eigenvalues of* G and to form the *spectrum* of G. They are obtained as the roots of the *characteristic polynomial* $\phi(G, \lambda)$ of the adjacency matrix of G, defined as the polynomial $\det(\lambda\mathbf{I} - \mathbf{A})$ in λ.

Cauchy's inequalities for a Hermitian matrix M (also collectively known as the *Interlacing Theorem*) place restrictions on the multiplicity of the eigenvalues of principal submatrices relative to those of $\mathbf{M}$ (See [6] for instance). When they are applied to graphs we have:

Theorem 1.1. Interlacing Theorem: *Let G be an n-vertex graph and $w \in \mathcal{V}$. If the eigenvalues of G are $\lambda_1, \lambda_2, \ldots, \lambda_n$ and those of $G - w$ are $\xi_1, \xi_2, \ldots, \xi_{n-1}$, both in non-increasing order, then $\lambda_1 \geq \xi_1 \geq \lambda_2 \geq \xi_2 \geq \ldots \geq \xi_{n-1} \geq \lambda_n$.*

1.2 Cores of singular graphs

For the linear transformation $\mathbf{A}$, the *kernel*, $\ker(\mathbf{A})$, of $\mathbf{A}$ is defined as the subspace of $\mathbb{R}^n$ mapped to zero by $\mathbf{A}$. It is also referred to as the *nullspace* of $\mathbf{A}$. A graph G is said to be *singular* of nullity η_G if the dimension of the nullspace $\ker(\mathbf{A})$ of $\mathbf{A}$ is η_G and $\eta_G > 0$. If there exists a non-zero vector $\mathbf{x}$ in the nullspace of the adjacency matrix $\mathbf{A}$, then $\mathbf{x}$ is said to be a *kernel eigenvector* of the singular graph G and satisfies $\mathbf{Ax} = \mathbf{0}$. It is therefore an eigenvector of $\mathbf{A}$ for the eigenvalue zero whose multiplicity η_G is also the number of roots of $\phi(G, \lambda)$ equal to zero. A vertex corresponding to a non-zero entry of $\mathbf{x}$ is said to be a *core vertex* CV of G. The core vertices corresponding to $\mathbf{x}$ *induce* a subgraph of G termed the *core* of G with respect to $\mathbf{x}$. The core structure of a singular graph will be the basis of our classification of all graphs relative to η_G.

A *core graph* is a singular graph in which every vertex is a core vertex. The empty graph $(K_4)^C$ and the four cycle C_4 are examples of 4–vertex core graphs of nullity four and two, respectively. A core graph of order at least three and nullity one is known as a *nut graph*. It is connected and non–bipartite [12].

For singular graphs, the vertices can be partitioned into core and core-forbidden vertices. The set $\mathcal{CV}$ of *core vertices* consists of those vertices lying on some core of G. A *core-forbidden vertex* (CFV) corresponds to a zero entry in *every* kernel eigenvector. The set $\mathcal{V} \backslash \mathcal{CV}$ is the set of CFVs. It follows that, in a core graph, the set of CFVs is empty.

Let y and z be two distinct vertices of a graph G. By interlacing, when a vertex y or z is deleted from G, the nullity η_{G-y} or η_{G-z}, that is the multiplicity of the eigenvalue zero of $G-y$ or $G-z$, respectively, may take one of three values from $\eta_G - 1$ to $\eta_G + 1$. If the two distinct vertices y and z are deleted, then the nullity η_{G-y-z} of $G-y-z$ may take values in the range from $\eta_G - 2$ to $\eta_G + 2$. Let us call the graph having two particular distinct vertices y and z a *device* (G, y, z). The set of devices can be partitioned into three main *varieties*, namely *variety* 1 when both vertices are CVs, *variety* 2 when one vertex is a CFV and one a CV and *variety* 3 when both vertices are CFVs. A device (G, y, z) is said to be of *kind* $(\eta_G, \eta_{G-y}, \eta_{G-z}, \eta_{G-y-z})$. Since η_{G-y} and η_{G-z} can take three values each and η_{G-y-z} can take five values, there are potentially 45 *kinds* of graphs relative to η_G. Interlacing further restricts the values of η_{G-y-z}. Moreover, there are *kinds* of graphs that exclude certain combinatorial properties, such as that of being bipartite, as we shall see in Section 5. In Section 2, we express the characteristic polynomial of $\phi(G-y, \lambda)$ as the sum of two terms in λ^{η_G} and $\lambda^{\eta_G} - 1$ with coefficients $f_a(\lambda)$ and $f_b(\lambda)$, respectively, each of which is a polynomial expanded in terms of the entries of the eigenvectors of $\mathbf{A}$ forming an orthonormal basis for $\mathbb{R}^n$. By comparing the diagonal entries of the adjugate of $(\lambda\mathbf{I} - \mathbf{A})$ and of the spectral decomposition of $(\lambda\mathbf{I} - \mathbf{A})^{-1}$ we obtain, in Section 3, an expression for $\phi(G-y-z)$ as the sum of three terms in λ^{η_G}, $\lambda^{\eta_G} - 1$, $\lambda^{\eta_G} - 2$, respectively, with polynomial coefficients. Moreover, the well known *Jacobi's identity* (see, for instance, [4]), relating the entries of the adjugate of $(\lambda\mathbf{I} - \mathbf{A})$ with the characteristic polynomials of a graph G and those of particular subgraphs of G, is used to determine which *kinds* are not realized by any graph G.

In Section 4, the vertices of a graph are partitioned into three subsets of *type lower, middle or upper*, respectively, according to the vanishing or otherwise of $f_a(0)$ and $f_b(0)$. The Interlacing Theorem and Jacobi's identity impose restrictions on the 45 *kinds*, so that not all are possible. In Sections 5 and 6, we show why there exist exactly twelve *kinds* of device (G, y, z) and how they are partitioned into the three main *varieties*. In Section 7, we identify two interesting classes of graphs that in a certain sense have extremal nullities. The first one has the minimum possible nullity η_{G-y-z}, that is $\eta_G - 2$, for all pairs of distinct vertices y and z in a graph G. A graph G in the second class has the maximum possible nullity η_{G-y}, that is $\eta_G + 1$, for all vertices y of G. We show that devices within the second class can reach the maximum allowed $\eta_G + 2$ for the nullity η_{G-y-z} for some but *not* for *all* pairs of distinct vertices y and z in a graph G. A characterization is given of the non–singular devices within the second class having the inverse $\mathbf{A}^{-1}$ of the adjacency matrix $\mathbf{A}$ with zero entries only on the diagonal.

2 Characteristic polynomials

We first need to define some necessary notation.

Associated with the $n \times n$ adjacency matrix $\mathbf{A}$ of a n–vertex graph of nullity η_G, there is an *ordered orthonormal basis* $\mathbf{x}^r$, $1 \leq r \leq n$, for $\mathbb{R}^n$, consisting of eigenvectors of $\mathbf{A}$, with the η_G eigenvectors in the nullspace being labelled first. Let the $n \times 1$ column vector

$\mathbf{x}^r$ be (x_y^r), where for vertex y, $1 \leq y \leq n$. If

$$\mathbf{P} = \begin{pmatrix} x_1^1 & x_1^2 & \cdots & x_1^n \\ x_2^1 & x_2^2 & \cdots & x_2^n \\ \vdots & \vdots & \vdots & \vdots \\ x_n^1 & x_n^2 & \cdots & x_n^n \end{pmatrix},$$

where the i^{th} column of $\mathbf{P}$ is the eigenvector $\mathbf{x}^i$ belonging to the eigenvalue λ_i in the spectrum of $\mathbf{A}$, diagonalization of $\mathbf{A}$ is given by $\mathbf{P}^{-1}\mathbf{AP} = \mathbf{D}[\lambda_i]$, where $\mathbf{D}[\lambda_i]$ is the diagonal matrix having λ_i as the i^{th} entry on the main diagonal. Expressing $\mathbf{A}$ in terms of $\mathbf{D}$ and $\mathbf{P}$ leads to the spectral decomposition theorem, which can also be applied to $(\lambda\mathbf{I} - \mathbf{A})^{-1}$. This leads to an expression for the characteristic polynomial of the adjacency matrix $\phi(G - y, \lambda)$ of $G - y$ which is given explicitly in terms of the eigenvector entries $\{x_y^i\}$. Together with Jacobi's identity, it will serve as a basis for the characterization of graphs according to those *kinds* that can exist.

Lemma 2.1.

$$\phi(G - y, \lambda) = \sum_{i=1}^{n} \frac{(x_y^i)^2}{(\lambda - \lambda_i)} \phi(G, \lambda).$$

Proof. The characteristic polynomial of the adjacency matrix $\phi(G - y, \lambda)$ of $G - y$ is the y^{th} diagonal entry $(\mathrm{adj}(\lambda\mathbf{I} - \mathbf{A}))_{yy}$ of the adjugate of $(\lambda\mathbf{I} - \mathbf{A})$. For arbitrary λ, the matrix $(\lambda\mathbf{I} - \mathbf{A})$ is invertible and $\phi(G - y, \lambda) = ((\lambda\mathbf{I} - \mathbf{A})^{-1})_{yy}\phi(G, \lambda)$. Since $\mathbf{P}^{-1}\mathbf{AP} = \mathbf{D}[\lambda_i]$, it follows that $\dfrac{\mathrm{adj}(\lambda\mathbf{I} - \mathbf{A})}{\phi(G, \lambda)} = (\lambda\mathbf{I} - \mathbf{A})^{-1} = \mathbf{PD}[\dfrac{1}{\lambda - \lambda_i}]\mathbf{P}^{-1}$.

Taking the y^{th} diagonal entry,

$$\begin{aligned} \frac{\phi(G - y, \lambda)}{\phi(G, \lambda)} &= (x_y^1\ x_y^2 \cdots x_y^n)\mathbf{D}[\frac{1}{\lambda - \lambda_i}] \begin{pmatrix} x_y^1 \\ x_y^2 \\ \vdots \\ x_y^n \end{pmatrix} \\ &= \sum_{i=1}^{n} \frac{(x_y^i)^2}{(\lambda - \lambda_i)}. \end{aligned} \tag{2.1}$$

□

For a graph G with adjacency matrix $\mathbf{A}$ of nullity η_G, let $s(\lambda)$ denote $\phi(G, \lambda)$. If the spectrum of $\mathbf{A}$ is $\lambda_1, \lambda_2, \cdots, \lambda_n$, starting with the zero eigenvalues (if any), we write

$$s(\lambda) = \prod_{\ell=1}^{n} (\lambda - \lambda_\ell) = \lambda^{\eta_G} s_0(\lambda) \quad \text{with} \quad s_0(0) \neq 0. \tag{2.2}$$

Partitioning the range of summation in Equation (2.1),

$$\frac{\phi(G - y, \lambda)}{\phi(G, \lambda)} = \sum_{i=1}^{\eta_G} \frac{(x_y^i)^2}{\lambda} + \sum_{i=\eta_G+1}^{n} \frac{(x_y^i)^2}{\lambda - \lambda_i}$$

Hence

$$\phi(G-y,\lambda) = \sum_{k=1}^{\eta_G} (x_y^k)^2 s_0(\lambda)\lambda^{\eta_G - 1} + \sum_{k=\eta_G+1}^{n} \frac{(x_y^k)^2 s_0(\lambda)\lambda^{\eta_G}}{\lambda - \lambda_k} \tag{2.3}$$

which we shall express as

$$\phi(G-y,\lambda) = f_b\lambda^{\eta_G-1} + f_a\lambda^{\eta_G}. \tag{2.4}$$

3 Jacobi's Identity

Relative to (G, y, z), let us denote by $j(\lambda)$, or j, the entry of the adjugate adj$(\lambda\mathbf{I} - \mathbf{A})$ in the yz position, obtained by taking the determinant of the submatrix of $(\lambda\mathbf{I} - \mathbf{A})$ after deleting row y and column z and multiplying it by $(-1)^{y+z}$. We use the convention that $\eta_{G-y} \geq \eta_{G-z}$. Throughout the paper, where the context is clear, we may write s_0 for $s_0(\lambda)$, j for $j(\lambda)$, etc.

Let $s(\lambda), t(\lambda), u(\lambda), v(\lambda)$, often referred to simply as s, t, u and v respectively, be the characteristic polynomials $\phi(G,\lambda)$, $\phi((G-y),\lambda)$, $\phi((G-z),\lambda)$, $\phi((G-y-z),\lambda)$ of the graphs G, $G-y$, $G-z$ and $G-y-z$, respectively, that is, the determinants

$$\begin{aligned} s(\lambda) &= \det(\lambda\mathbf{I} - \mathbf{A}(G)) \\ t(\lambda) &= \det(\lambda\mathbf{I} - \mathbf{A}(G-y)) \\ u(\lambda) &= \det(\lambda\mathbf{I} - \mathbf{A}(G-z)) \\ v(\lambda) &= \det(\lambda\mathbf{I} - \mathbf{A}(G-y-z)). \end{aligned} \tag{3.1}$$

From Lemma 2.1,

$$t(\lambda) = \sum_{k=1}^{n} (x_y^k)^2 \prod_{\ell\neq k} (\lambda - \lambda_\ell) \tag{3.2}$$

and

$$u(\lambda) = \sum_{k=1}^{n} (x_z^k)^2 \prod_{\ell\neq k} (\lambda - \lambda_\ell). \tag{3.3}$$

We shall see that the characteristic polynomial $v(\lambda)$ of $G-y-z$ can also be expressed in terms of the eigenvector entries $\{x_y^r\}$ and $\{x_z^r\}$ associated with distinct vertices y and z.

Lemma 3.1. *For $y \neq z$, Jacobi's identity expresses the entry j of the adjugate of $\lambda\mathbf{I} - \mathbf{A}$ in the yz position, for a symmetric matrix $\mathbf{A}$, in terms of the characteristic polynomials s, u, t and v:*

$$j^2 = ut - sv$$

Expressing Equations (3.2) and (3.3) as in (2.4),

$$t(\lambda) = \sum_{k=1}^{\eta_G} (x_y^k)^2 s_0(\lambda)\lambda^{\eta_G-1} + \sum_{k=\eta_G+1}^{n} \frac{(x_y^k)^2 s_0(\lambda)\lambda^{\eta_G}}{\lambda-\lambda_k} = t_b\lambda^{\eta_G-1} + t_a\lambda^{\eta_G}, \tag{3.4}$$

and

$$u(\lambda) = \sum_{k=1}^{\eta_G} (x_z^k)^2 s_0(\lambda)\lambda^{\eta_G-1} + \sum_{k=\eta_G+1}^{n} \frac{(x_z^k)^2 s_0(\lambda)\lambda^{\eta_G}}{\lambda-\lambda_k} \tag{3.5}$$

$$= u_b\lambda^{\eta_G - 1} + u_a\lambda^{\eta_G}$$

Now we consider pairs of vertices of G.

Since $\dfrac{\mathrm{adj}(\lambda I - A)}{\phi(G,\lambda)} = (\lambda I - A)^{-1} = PD[\dfrac{1}{\lambda - \lambda_i}]P^{-1}$,

$$j(\lambda) = \sum_{k=1}^{n}(x_y^k x_z^k)\prod_{\ell \neq k}(\lambda - \lambda_\ell.) \tag{3.6}$$

We can write

$$j(\lambda) = \sum_{k=1}^{\eta_G} x_y^k x_z^k s_0(\lambda)\lambda^{\eta_G - 1} + \sum_{k=\eta_G+1}^{n} \frac{x_y^k x_z^k s_0(\lambda)\lambda^{\eta_G}}{\lambda - \lambda_k} \tag{3.7}$$

$$= j_b\lambda^{\eta_G - 1} + j_a\lambda^{\eta_G}$$

The characteristic polynomial $v(\lambda)$ can be written as $v(\lambda) = \dfrac{u(\lambda)t(\lambda) - j^2(\lambda)}{s(\lambda)}$, that is $v(\lambda) = v_a\lambda^{\eta_G} + v_b\lambda^{\eta_G - 1} + v_c\lambda^{\eta_G - 2}$, where

$$v_c = \frac{1}{s_0}(u_b t_b - j_b^2) = \frac{1}{2}s_0\sum_{i=1}^{\eta_G}\sum_{\ell=1}^{\eta_G}(x_z^i x_y^\ell - x_z^\ell x_y^i)^2$$

$$v_b = \frac{1}{s_0}(u_a t_b + u_b t_a - 2j_a j_b) = s_0\sum_{i=1}^{\eta_G}\sum_{\ell=\eta_G+1}^{n}\frac{(x_z^i x_y^\ell - x_y^i x_z^\ell)^2}{\lambda - \lambda_\ell}$$

$$v_a = \frac{1}{s_0}(u_a t_a - j_a^2) = \frac{1}{2}s_0\sum_{i=\eta_G+1}^{n}\sum_{\ell=\eta_G+1}^{n}\frac{(x_y^i x_z^\ell - x_y^\ell x_z^i)^2}{(\lambda - \lambda_i)(\lambda - \lambda_\ell)} \tag{3.8}$$

4 Three types of vertex

By interlacing, we can identify three types of vertex according to the effect on the nullity on deletion. We call a vertex y *lower*, *middle* or *upper* if the nullity of $G - y$ is $\eta_G - 1$, η_G or $\eta_G + 1$, respectively. We shall distinguish among these three types of vertex according to the values of the functions f_a and f_b in Equation (2.4).

In Table 1 we show the entries of the orthonormal eigenvectors $\{\mathbf{x}^r\}$ in an ordered basis for $\mathbb{R}^n$ as presented in Section 2. We choose a vertex labelling such that the core vertices are labelled first. Note the zero submatrix corresponding to the CFVs.

We consider $\dfrac{\phi(G - y,\lambda)}{s_0\lambda^{\eta_G}}$ from Equation 2.3. It has poles at $\lambda = \mu_i$, $1 \leq i \leq h$, where, for $1 \leq i \leq h$, the μ_i are the h distinct non-zero eigenvalues of G. Moreover, the gradient of $\displaystyle\sum_{k=\eta_G+1}^{n}\frac{(x_y^k)^2}{\lambda - \lambda_k}$ is less than 0 for all $\lambda \neq \mu_i$. It follows that $\dfrac{\phi(G - y,\lambda)}{s_0\lambda^{\eta_G}}$ has at most $(h-1)$ roots strictly interlacing the h distinct eigenvalues of $\mathbf{A}$. Note that $\displaystyle\sum_{k=1}^{\eta_G}(x_y^k)^2 \geq 0$ with equality if and only if y is a CFV. Thus at $\lambda = 0$, f_b is non–zero if y is a CV and zero

eigenvector / vertex-entries	x^1	$\dots$	x^{η_G}	x^{η_G+1}	$\dots$	x^n
x_1	$*$	$\dots$	$*$	$*$	$\dots$	$*$
x_2	$*$	$\dots$	$*$	$*$	$\dots$	$*$
$\vdots$	$*$	$\dots$	$*$	$*$	$\dots$	$*$
$x_{\vert CV\vert}$	$*$	$\dots$	$*$	$*$	$\dots$	$*$
$x_{\vert CV\vert+1}$	0	$\dots$	0	$*$	$\dots$	$*$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
x_n	0	$\dots$	0	$*$	$\dots$	$*$

Table 1: Ordered orthonormal basis of eigenvectors of $\mathbf{A}$ with * representing a possibly non–zero entry.

if it is a CFV. For a CFV y, $\sum_{k=\eta_G+1}^{n} \frac{(x_y^k)^2}{\lambda-\lambda_k}$ vanishes at $\lambda = 0$ when y is upper, and does not vanish when y is middle. Note that when $\sum_{k=1}^{\eta_G}(x_y^k)^2 = 0$, one of the $(h-1)$ interlacing roots may be zero. (†)

Different cases occur depending on the vanishing or otherwise of the real constant $\sum_{k=1}^{\eta_G}(x_y^k)^2$ and $\sum_{k=\eta_G+1}^{n} \frac{(x_y^k)^2}{\lambda-\lambda_k}$ at $\lambda = 0$. Equation (2.3) and the analysis in the previous paragraph (marked (†)) lead to the result that $\eta_G - 1 \leq \eta_{G-y} \leq \eta_G + 1$. This can be generalized for the multiplicity of any eigenvalue of G other than zero by replacing the cores and the nullspace of G by the μ_i–cores and μ_i–eigenspace of G (concepts introduced in [10]), thus giving another proof of the Interlacing Theorem.

Proposition 4.1. *The values of f_b and f_a of Expression (2.4) for $\phi(G-y,\lambda)$ at $\lambda = 0$ distinguish the three types of vertex as follows:*

Vertex y	*Status of y*	*The values of f_b and f_a*
Lower	CV	$f_b(0) \neq 0$
Middle	CF	$f_b(0) = 0$ *and* $f_a(0) \neq 0$
Upper	CFV	$f_b(0) = 0$ *and* $f_a(0) = 0$

Proof. Let y be a core vertex of a graph of nullity $\eta_G > 0$. There exists $x_y^k \neq 0$ for some k, $1 \leq k \leq \eta_G$. Then $f_b(0) \neq 0$, which is a necessary and sufficient condition for the multiplicity of the eigenvalue zero to be $\eta_G - 1$ for $G-y$. It follows that a vertex is *lower* if and only if it is a CV.

If y is a CFV, then $f_b(0) = 0$. For $G-y$, the multiplicity of the eigenvalue zero is at least η_G. If one of the roots of $\sum_{k=\eta_G+1}^{n} \frac{(x_y^k)^2}{\lambda-\lambda_k}$ is zero, then λ divides $\sum_{k=\eta_G+1}^{n} \frac{(x_y^k)^2}{\lambda-\lambda_k}$, the multiplicity of the eigenvalue zero is exactly $\eta_G + 1$ for $G-y$ and the vertex y is upper. Otherwise the multiplicity of the eigenvalue zero remains η_G for $G-y$ and the vertex y is middle. □

We consider three *varieties* of devices $\{(G, y, z)\}$ with pairs (y, z) of vertices, namely *variety* 1 with both y and z being CVs, *variety* 2 with z being a CV and y a CFV and *variety* 3 with both y and z being CFVs. Since a CFV can be upper or middle, *varieties* 2 and 3 are subdivided further, as seen in Table 3.

From Proposition 4.1,

for *variety* 1, $u_b \neq 0$; $t_b \neq 0$;
for *variety* 2, $u_b \neq 0$; $j_b = t_b = v_c = 0$;
for *variety* 3: $u_b = j_b = t_b = v_b = v_c = 0$.

Some of these *varieties* can be further subdivided according to the values at $\lambda = 0$ of v_c, v_b and v_a or j_a. From Proposition 4.1, $t_b(0) \neq 0$ if and only if y is a core vertex. Similarly $u_b \neq 0$ if and only if z is a core vertex. If at least one of z or y is core forbidden, then $j_b(0) = 0$. However, there are 'accidental' cases where $j_b(0)$ vanishes when both z and y are CVs, for example in C_4 and $K_{2,3}$ if the vertices y and z are connected by an edge. Indeed this is true for all bipartite core graphs of nullity at least two, since each of u and t has zero as a root. It follows that $E^{2\eta}$ is a factor of $j^2 = ut - sv = (j_b E^{\eta-1} + j_a E^{\eta})^2$ and therefore $j_b(0) = 0$.

5 Restrictions on the nullity of $G - y - z$

It is our aim to classify all graphs according to their *kind* defined by the quadruple

$$(\eta_G, \eta_{G-y}, \eta_{G-z}, \eta_{G-y-z}).$$

Not all the 45 *kinds* mentioned in Section 1 exist, as we shall discover. The classification will be given in Table 3 on Page 272. It is best possible since each kind is realized by some graph.

5.1 Restrictions arising from interlacing

In a device (G, y, z) of *kind* $(\eta_G, \eta_{G-y}, \eta_{G-z}, \eta_{G-y-z})$, interlacing restricts the values that η_{G-y-z} can take. The following result shows an instance when η_{G-y-z} is determined by interlacing alone.

Lemma 5.1. *For* $(\eta_G, \eta_{G-y}, \eta_{G-z}, \eta_{G-y-z}) = (\eta_G, \eta_G + 1, \eta_G - 1, \eta_{G-y-z})$*, the nullity* η_{G-y-z} *of* $G - y - z$ *is* η_G.

Hence, $(\eta_G, \eta_G + 1, \eta_G - 1, \eta_G)$ is the only *kind* where the nullities η_{G-y} and η_{G-z} differ by two. We say that it belongs to *variety* 2a.

In *kinds* where the nullities η_{G-y} and η_{G-z} differ by one, interlacing allows η_{G-y-z} to take either the value η_{G-y} or η_{G-z}. All three possible values of η_{G-y-z} are allowed by interlacing when $\eta_{G-y} = \eta_{G-z}$.

The symmetry about zero of the spectrum of a bipartite graph G (See for instance [8]) requires that the number of zero eigenvalues is $2k$, if G has an even number of vertices and $2k+1$ if G has an odd number of vertices, for some $k \geq 0$. This implies that on deleting a vertex from a bipartite graph, the nullity changes parity. Therefore if the nullity of a graph G and of its vertex–deleted subgraph $G - y$ are the same, then G is not bipartite. Since on deleting a vertex a bipartite graph remains bipartite, it follows that a graph G of a *kind* where $\eta_G = \eta_{G-y}$ or $\eta_{G-y} = \eta_{G-y-z}$ cannot be bipartite.

Lemma 5.2. *If a vertex of a graph is middle, then the graph is not bipartite.*

Figure 1 shows a device (G, y, z) with a middle vertex z which becomes upper in $G-y$.

Figure 1: A graph with two middle vertices y and z.

5.2 Restrictions arising from Jacobi's Identity

Lemma 3.1 requires that $ut - sv$ which is j^2 has $2k,\ k \geq 0$, zero roots. Let g_f denote the number of zero roots of the real function f. Therefore, for kinds of graph that imply
(i) $g_{ut} = g_{sv} - 1$ and $g_u \neq g_t$
or (ii) $g_{ut} = g_{sv} + 1$ and $g_u = g_t$,
there is a contradiction and those *kinds* of graphs do not exist.

Lemma 5.3. *The following kinds of graphs do not exist:*
(i) $(\eta_G, \eta_G, \eta_G - 1, \eta_G)$*;*
(ii) $(\eta_G, \eta_G + 1, \eta_G + 1, \eta_G + 1)$*;*
(iii) $(\eta_G, \eta_G, \eta_G, \eta_G - 1)$.

Furthermore, if $g_{ut} = g_{sv}$ and g_{ut} is odd, then a graph of that *kind* exists if $ut - sv$ is zero at $\lambda = 0$, otherwise j^2 would have an odd number of zeros. Therefore, if $g_{ut} = g_{sv}$ and g_{ut} is odd, $j_b = 0$ at $\lambda = 0$.

Lemma 5.4. *Graphs with* $g_{ut} = g_{sv}$ *and* g_{ut} *odd exist provided* $j_b = 0$ *at* $\lambda = 0$*. They are non–bipartite and of one of the following kinds:*
(i) $(\eta_G, \eta_G, \eta_G - 1, \eta_G - 1)$*;*
(ii) $(\eta_G, \eta_G + 1, \eta_G, \eta_G + 1)$.

We shall call *kinds* (i) and (ii), in Lemma 5.4 above, *variety* 2b and 3b(i), respectively (See Table 3).

Lemma 5.5. *If* (G, y, z) *is a singular graph with* $g_{ut} < g_{sv}$ *and* g_{sv} *odd, then* (G, y, z) *is non–bipartite and of kind* $(\eta_G, \eta_G - 1, \eta_G - 1, \eta_G - 1)$.

Proof. If y and z are CVs, $g_{ut} < g_{sv}$, then $(\eta_G, \eta_{G-y}, \eta_{G-z}, \eta_{G-y-z})$ is
(i) $(\eta_G, \eta_G - 1, \eta_G - 1, \eta_G)$ or
(ii) $(\eta_G, \eta_G - 1, \eta_G - 1, \eta_G - 1)$.
Now if furthermore, g_{sv} is given to be odd, then $\eta_{G-y-z} = \eta_G - 1$. It follows that $\eta_{G-y} = \eta_{G-y-z}$ Therefore, G is not bipartite. □

We shall call the graphs in Lemma 5.5 above, *variety* 1(iii) (See Table 3).

6 Kinds of graphs

In this section we determine the properties of a *kind* $(\eta_G, \eta_{G-y}, \eta_{G-z}, \eta_{G-y-z})$ within each of the three *varieties*.

6.1 Graphs of variety 1

Graphs of *variety* 1, are necessarily singular and therefore have at least one core. There are at least two vertices in a core.

Lemma 6.1. *For a device* (G, y, z) *of variety 1 and nullity one,* $j_b(0) \neq 0$ *for core vertices* y *and* z.

Proof. For $\eta_G = 1$, a non-zero column of the adjugate $\mathrm{adj}(\mathbf{A})$ is a kernel eigenvector of G [9]. The non–zero entries occur only at core vertices. Therefore, $j_b(0) \neq 0$. □

There are three types of pairs of vertices (CV,CV) for graphs of *variety* 1, depending on the nullity of $G - y - z$. Since $\eta_G \geq 1$ and $g_u = g_t = \eta_G - 1$, then the nullity g_v of $G - y - z$ can take any of the three values $\eta_G - 2, \eta_G$ and $\eta_G - 1$, corresponding to *variety* 1(i), 1(ii) and 1(iii), respectively.

Theorem 6.2. *For a device* (G, y, z) *of variety 1(iii),* $j(0) \neq 0$ *for core vertices* y *and* z.

Proof. For nullity one the result follows from Lemma 6.1. Now consider a graph with $\eta_G > 1$ of *variety* 1(iii), that is when $g_v = \eta_G - 1$. The number of zeros g_{ut} of ut is $2\eta_G - 2$ and less than that of sv which is odd. If j^2, which is $ut - sv$, is not to have an odd number of zeros, it follows, from $j = j_b\lambda^{\eta_G - 1} + j_a\lambda^{\eta_G}$, that $j_b \neq 0$ at $\lambda = 0$. □

For *variety* 1(i), the vertices y and z are CVs. Moreover, without loss of generality, the vertex z is a CV of the subgraph $G - y$. Only for *variety* 1(i) is $v_c \neq 0$.

Definition 6.3. The connected graphs G in the devices $\{(G, y, z)\}$ with all pairs of vertices $(y, z) \in \mathcal{V} \times \mathcal{V}$ being of *variety* 1(i) are said to form the class of *uniform–core graphs*.

Equivalently, $\eta_{G-y-z} = \eta_G - 2$, that is z is a CV of $G - y$ for all vertex pairs (y, z). It is clear that all vertices of a uniform–core graph are CVs, and that they remain so even in a vertex–deleted subgraph $G - y$ for any vertex y of G. Note that this is not the case in general; if y and z are two distinct core vertices of a graph G, then z need not remain a core vertex of $G - y$. We shall consider uniform–core graphs in more detail in Section 7.

6.2 Graphs of variety 2

In a device (G, y, z) of *variety* 2, (y, z) is a mixed vertex pair, that is exactly one vertex z of the pair (y, z) is a CV.

From Lemmas 5.1 and 5.3, the following result follows immediately.

Proposition 6.4. *In a device* (G, y, z) *of variety 2,*
(i) there is only one kind when y *is upper, namely kind* $(\eta_G, \eta_G + 1, \eta_G - 1, \eta_G)$ *in variety 2a*
and (ii) only one kind when y *is middle, namely kind* $(\eta_G, \eta_G, \eta_G - 1, \eta_G - 1)$ *in variety 2b.*

From Lemma 5.2, the graphs of *variety* 2b are non-bipartite.

Theorem 6.5. *In a device* (G, y, z) *of variety 2b, the term in* $\lambda^{2\eta_G - 1}$ *of* j^2 *is identically equal to zero.*

Proof. In *variety* 2b, a graph is of *kind* $(\eta_G, \eta_G, \eta_G - 1, \eta_G - 1)$. The parameter v_c vanishes and $v_b(\lambda) = \dfrac{u_b t_a}{s_0} \neq 0$. The number of zeros of ut is the same as that of sv. Therefore, $j^2 = ut - sv$ has at least $2\eta_G - 1$ zeros. In *variety* 2b, the term in $\lambda^{2\eta_G - 1}$ in its expansion is $u_b t_a - s_0 v_b$. Also v_c vanishes and $v_b(\lambda) = \dfrac{u_b t_a}{s_0} \neq 0$. Hence, $s_0 v_b = u_b t_a$ and the term in $\lambda^{2\eta_G - 1}$ in the expansion of j^2 is identically equal to zero, as expected from the fact that j^2 is a perfect square. □

The parameter v_b distinguishes between a graph in *variety* 2a and one in *variety* 2b.

Theorem 6.6. *For a graph in variety 2a, v_b vanishes at $\lambda = 0$. For a graph in variety 2b, $v_b \neq 0$ at $\lambda = 0$.*

Proof. For both *kinds* in *variety* 2, $u_b \neq 0$. For an upper vertex, $t_a = 0$ at $\lambda = 0$ and for a middle vertex $t_a \neq 0$ at $\lambda = 0$. Since $s_0 \neq 0$, it follows that for a graph in *variety* 2a $v_b = 0$ at $\lambda = 0$ and, for a graph in *variety* 2b, $v_b \neq 0$ at $\lambda = 0$.

□

6.3 Graphs of variety 3

We now consider *variety* 3 for (CFV,CFV) pairs, when t_b, u_b, j_b, v_b and v_c all vanish.

Interlacing provides three types of vertex pairs depending on whether a CFV in the pair (y, z) is upper or middle. When both vertices are upper (*variety* 3a), by Lemma 5.3 only *variety* 3a(i) for $g_v = \eta_G$ and *variety* 3a(ii), when $g_v = \eta_G + 2$ are allowed. The values at $\lambda = 0$ of v_a or j_a suffice to distinguish between graphs of *variety* 3(i) and 3(ii).

Theorem 6.7. *For variety 3a(i), both v_a and j_a are non–zero at $\lambda = 0$. For variety 3a(ii), both v_a and j_a vanish at $\lambda = 0$.*

Proof. For *variety* 3, $v_b = 0$. *Variety* 3a(i) is $(\eta_G, \eta_G + 1, \eta_G + 1, \eta_G)$. Since $v = v_a \lambda^{\eta_G}$ and $\eta_{G-y-z} = \eta_G$, $v_a \neq 0$ at $\lambda = 0$. Also $g_{j^2} = 2\eta_G$ so that $j_a \neq 0$ at $\lambda = 0$. *Variety* 3a(ii) is $(\eta_G, \eta_G +, \eta_G - 1, \eta_G - 1)$. Since $g_v = \eta_G + 2$, λ^2 divides v_a and λ divides all of the functions $t_a,\ u_a$ and j_a. □

For *variety* 3b, one vertex is upper and one is middle. Interlacing allows only $g_v = \eta_G + 1$ and η_G, corresponding to *variety* 3b(i) and *variety* 3b(ii), respectively. Both v_b and j_b vanish at $\lambda = 0$. The value of j_a at $\lambda = 0$ distinguishes between *variety* 3b(i) and *variety* 3b(ii).

Theorem 6.8. *For variety 3b(i), j_a vanishes at $\lambda = 0$. For variety 3a(ii), j_a is non–zero at $\lambda = 0$.*

Proof. For *variety* 3b(i), λ divides j_a, as otherwise $ut - sv$ is not the perfect square j^2. *variety* 3b(ii) $g_v = \eta_G$ requires $j_a \neq 0$ at $\lambda = 0$. □

For *variety* 3c, both vertices are middle. The values at $\lambda = 0$ of t_a and u_a are non–zero. By Lemma 5.3, $g_v = \eta_G + 1$ or η_G, corresponding to *variety* 3c(i) and *variety* 3c(ii), respectively.

For *variety* 3c(ii), when $g_v = \eta_G$, v_a is non–zero at $\lambda = 0$. Two cases may occur. Either $j_a \neq 0$ at $\lambda = 0$ or the number of zeros of j_a is at least one. The former case is

Vertex y	Vertex z	*variety*
1	7	*variety* 1(i)
1	4	*variety* 1(ii)
1	2	*variety* 1(iii)
1	15	*variety* 2a
1	5	*variety* 2b
17	18	*variety* 3a(i)
15	17	*variety* 3a(ii)
5	15	*variety* 3b(i)
15	16	*variety* 3b(ii)
11	16	*variety* 3c(i)
5	6	*variety* 3c(iiA)
5	17	*variety* 3c(iiB)

Table 2: All *varieties* and *kinds* for the same graph G illustrated in Figure 2.

denoted by *variety* 3c(iiA). The latter case is *variety* 3c(iiB) for which the terms in $\lambda^{2\eta_G - 2}$ and in $\lambda^{2\eta_G - 1}$ of j^2 vanish.

The remaining case is for *variety* 3c(i) when $g_v = \eta_G + 1$ and λ divides v_a.

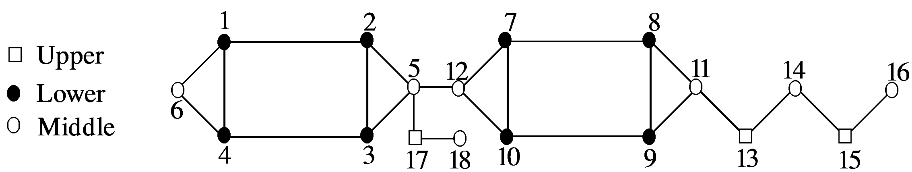

Figure 2: A device (G, y, z) of all possible *kinds* for various (y, z).

The graph in Figure 2 exhibits a device (G, y, z) of all *varieties* and *kinds* for different choices of (y, z).

The classification of devices into *kinds* and *varieties* has an application in chemistry in the identification of molecules (with carbon atoms in particular) that conduct or else bar conduction at the Fermi level. In the chemistry paper [3], conductors and insulators are classified into eleven cases that are essentially the twelve kinds of Table 3, with case 7 in [3] corresponding to the kinds $(\eta_G, \eta_G, \eta_G, \eta_G)$ in variety 3c(iiA) and $(\eta_G, \eta_G, \eta_G, \eta_G)$ in variety 3c(iiB). The latter two varieties are distinguishable by the non–vanishing or otherwise of $j_a(0)$.

7 Graphs with analogous vertex pairs

In general, vertex pairs in a graph may be of different varieties and kinds. We shall explore two interesting classes of graphs with the same extremal nullity (allowed by interlacing) for all vertex–deleted subgraphs. These emerge in the classification of devices $\{(G, y, z)\}$ according to their *kind* $(\eta_G, \eta_{G-y}, \eta_{G-z}, \eta_{G-y-z})$. A pair of vertices y and z for which $\eta_{G-y} = \eta_{G-z}$ is said to be an *analogous vertex pair*.

Kind	Characterization	*Variety*	G bipartite
Two CVs		1	
$(g_s, g_t, g_u) = (\eta_G, \eta_G - 1, \eta_G - 1)$			
$g_v = \eta_G - 2$	$v_c \neq 0$ & $t_b \neq 0$ & $u_b \neq 0$ & $\eta_G \geq 2$	1(i)	Allowed
$g_v = \eta_G$	$v_c = 0$ & $t_b \neq 0$ & $u_b \neq 0$ & $v_b(0) = 0$ & $\eta_G \geq 1$	1(ii)	Allowed
$g_v = \eta_G - 1$	$v_c = 0$ & $t_b \neq 0$ & $u_b \neq 0$ & $v_b(0) \neq 0$ & $\eta_G \geq 1$	1(iii)	Forbidden
CV and CFV		2	
$(g_s, g_t, g_u) = (\eta_G, \eta_G + 1, \eta_G - 1)$ $g_v = \eta_G$	$v_c = 0$ & $t_b = 0$ & $u_b \neq 0$ & $v_b(0) = 0$ & $\eta_G \geq 1$	2a	Allowed
$(g_s, g_t, g_u, g_v) = (\eta_G, \eta_G, \eta_G - 1)$ $g_v = \eta_G - 1$	$v_c = 0$ & $t_b = 0$ & $u_b \neq 0$ & $v_b(0) \neq 0$ & $\eta_G \geq 1$	2b	Forbidden
Two CFVs		3	
$(g_s, g_t, g_u) = (\eta_G, \eta_G + 1, \eta_G + 1)$		3a	
$g_v = \eta_G$	$v_c = 0$ & $t_b = 0$ & $u_b = 0$ & $v_b(0) = 0$ & $t_a(0) = 0$ & $u_a(0) = 0$ & $v_a(0) \neq 0$	3a(i)	Allowed
$g_v = \eta_G + 2$	$v_c = 0$ & $t_b = 0$ & $u_b = 0$ & $v_b(0) = 0$ & $t_a(0) = 0$ & $u_a(0) = 0$ & $v_a(0) = 0$	3a(ii)	Allowed
$(g_s, g_t, g_u) = (\eta_G, \eta_G + 1, \eta_G)$		3b	
$g_v = \eta_G + 1$	$v_c = 0$ & $t_b = 0$ & $u_b = 0$ & $v_b(0) = 0$ & $t_a(0) = 0$ & $u_a(0) \neq 0$ & $v_a(0) = 0$	3b(i)	Forbidden
$g_v = \eta_G$	$v_c = 0$ & $t_b = 0$ & $u_b = 0$ & $v_b(0) = 0$ & $t_a(0) = 0$ & $u_a(0) \neq 0$ & $v_a(0) \neq 0$	3b(ii)	Forbidden
$(g_s, g_t, g_u) = (\eta_G, \eta_G, \eta_G)$		3c	
$g_v = \eta_G + 1$	$v_c = 0$ & $t_b = 0$ & $u_b = 0$ & $v_b(0) = 0$ & $t_a(0) \neq 0$ & $u_a(0) \neq 0$ & $v_a(0) = 0$	3c(i)	Forbidden
$g_v = \eta_G$	$v_c = 0$ & $t_b = 0$ & $u_b = 0$ & $v_b(0) = 0$ & $t_a(0) \neq 0$ & $u_a(0) \neq 0$ & $v_a(0) \neq 0$	3c(ii)	Forbidden
$g_v = \eta_G$ &$j_a(0) \neq 0$	$v_c = 0$ & $t_b = 0$ & $u_b = 0$ & $v_b(0) = 0$ & $t_a(0) \neq 0$ & $u_a(0) \neq 0$ & $v_a(0) \neq 0$ & $j_a(0) \neq 0$	3c(iiA)	Forbidden
$g_v = \eta_G$& $j_a(0) = 0$	$v_c = 0$ & $t_b = 0$ & $u_b = 0$ & $v_b(0) = 0$ & $t_a(0) \neq 0$ & $u_a(0) \neq 0$ & $v_a(0) \neq 0$ & $j_a(0) = 0$	3c(iiB)	Forbidden

Table 3: A characterization of all devices (G, y, z) according to their *variety* and *kind*.

The first of these two classes consists of graphs G with the minimum possible nullity η_{G-y-z} for *all* pairs of distinct vertices y and z, (i.e., $\eta_G - 2$) and therefore also the minimum possible nullities η_{G-y} and η_{G-z} (i.e., $\eta_G - 1$). By Definition 6.3, these graphs form precisely the class of uniform–core graphs. On the other hand, the second of the two classes consists of graphs with the maximum possible nullity η_{G-y-z}, that is $\eta_G + 2$, for *some* pair of distinct vertices y and z, and therefore also the maximum possible nullities η_{G-y} and η_{G-z} (i.e., $\eta_G + 1$).

7.1 Uniform–core graphs

By Definition 6.3, each vertex pair in a uniform–core graph corresponds to a graph of variety (1i). Since the nullity of a graph is non–negative, and $\eta_{G-y-z} = \eta_G - 2$ for all vertex pairs $y,\ z$ of a uniform–core graph G, then the nullity of G is at least two. To understand better the core–structure of uniform–core graphs and be able to characterize them as a subclass of singular graphs, it is necessary to use their core structure with respect to a basis for their nullspace.

Let B be a basis for the η–dimensional nullspace of $\mathbf{A}$ of a singular graph G (with no isolated vertices) of nullity $\eta \geq 1$. As seen in [11], *Hall's Marriage* problem for sets, or the *Rado–Hall* Theorem for matroids, guarantees a vertex–subset S of distinct vertex representatives [1, 11], to represent a system $\mathcal{S}_{Cores}$ of cores corresponding to the vectors of B. This implies that deleting a vertex v representing a core F eliminates the core F from $G - v$, which will now have a new system of $\eta - 1$ cores. Also any $k \geq 1$ cores in a system $\mathcal{S}_{Cores}$ of η_G cores cover at least $k + 1$ vertices.

Theorem 7.1. *A device (G, y, z) is of variety 1(i) if and only if the two vertices y and z do not lie in one core only, i.e. at least two cores are needed to cover the vertices y and z.*

Proof. Consider a basis B for the nullspace of $\mathbf{A}$. The vertices y and z lie on at least one core of G. There are two possibilities. Firstly, B has exactly one vector with non–zero entries at positions associated with y and z. In this case $\eta_{G-y-z} = \eta_{G-y} = \eta_G - 1$, which does not correspond to *variety* 1(i). Secondly, B has at least two vectors with non–zero entries at positions associated with y or z, when $\eta_{G-y-z} = \eta_{G-y} - 1 = \eta_G - 2$, which corresponds to *variety* 1(i). The two core vertices must represent two distinct cores in a system $\mathcal{S}_{Cores}$ of η_G cores corresponding to a basis B for the nullspace [11]. □

A subclass $\mathcal{U}$ of uniform–core graphs can be constructed from nut graphs. A graph $G \in \mathcal{U}$ is obtained from a nut graph H on n vertices and m edges by duplicating each of the n vertices of H. Then G has $2n$ vertices and $4m$ edges. Figure 3 shows the uniform–core graph $G \in \mathcal{U}$ obtained from the smallest nut graph H. The nullity of G is $\frac{|\mathcal{V}(G)|}{2} + 1$. Deletion of any $\frac{|\mathcal{V}(G)|}{2} + 1$ vertices reduces the graph to a non–singular graph.

Let the vertices of G be labelled $1, 2, ..., n, 1', 2', ...n'$ where $\{1, 2, ...\}$ are the vertices of the nut graph H and $\{1', 2', ...\}$ are the duplicate vertices of $\{1, 2, ...\}$ in that order in G. Note that a vertex labelled r for $1 \leq r \leq n$ is adjacent to the original neighbours in H and also to precisely those primed vertices with the same numeric label. For instance, vertex 1 is adjacent to 2 and 7 in H and to 2, 2', 7 and 7' in G. The following result, expressing the adjacency matrix of $G \in \mathcal{U}$ in terms of the adjacency matrix of H, is immediate.

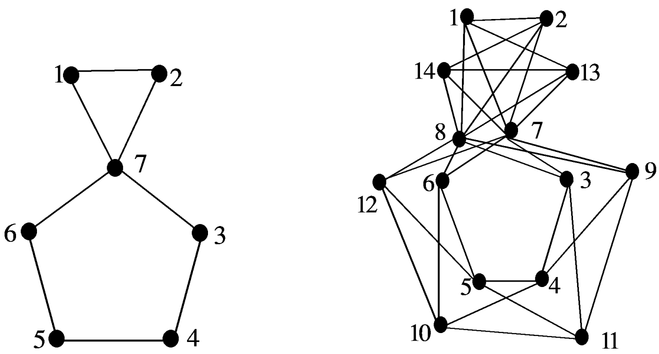

Figure 3: The smallest nut graph H and the uniform–core graph G derived from H.

Theorem 7.2. *If* $\mathbf{H}$ *is the adjacency matrix of the nut graph* H*, then the adjacency matrix of the uniform–core graph* $G \in \mathcal{U}$ *is* $\begin{pmatrix} \mathbf{H} & \mathbf{H} \\ \mathbf{H} & \mathbf{H} \end{pmatrix}$. *The spectrum of* G *consists of* n *eigenvalues equal in value to double the eigenvalues of* H *and an additional* n *zero eigenvalues corresponding to the* n *duplicate vertex pairs. If* $(x_1, x_2, \cdots, x_n)^t$ *is an eigenvector of* H *for an eigenvalue* μ*, then* $(x_1, x_2, \cdots, x_n, x_1, x_2, \cdots, x_n)^t$ *is an eigenvector of* G *for an eigenvalue* 2μ*.*

We shall now characterize uniform–core graphs by requiring that a set of vertex representatives of a system $\mathcal{S}_{Cores}$ of cores be an arbitrary subset of the vertices for all systems of cores.

Theorem 7.3. *A graph of nullity* η_G *is a uniform–core graph if and only if it is a singular graph such that the deletion of any subset of* η_G *vertices produces a non–singular graph.*

Proof. Let us relate the nullspace of $\mathbf{A}$ to the vertices of a uniform–core graph G of nullity η_G. Let S be any subset of η_G vertices of G labelled $\{1, 2, \cdots, \eta_G\}$ and let B be an ordered basis for the nullspace of $\mathbf{A}$. If all pairs of vertices give a graph of *variety* 1(i), then no two vertices lie in only one core of $\mathcal{S}_{Cores}$. Therefore, it is possible to obtain a new ordered basis B' for the nullspace of $\mathbf{A}$, by linear combination of the vectors in B, such that, for $1 \leq i \leq \eta_G$, only the vector i of B' has a non–zero entry at position i [11]. Removal of any vertex in S destroys precisely one eigenvector of B' reducing the nullity by one. Deletion of all the vertices in S destroys all the kernel eigenvectors and leaves a non–singular graph. □

A characterization of the subclass $G \in \mathcal{U}$ of uniform–core graphs uses the operation NEPS (*non–complete extended p-sum*) of a nut graph and K_2. The graph product NEPS is described for instance in [2].

Definition 7.4. Given a collection $\{G_1, G_2, \cdots, G_k, \cdots, G_n\}$ of graphs and a corresponding set $\mathcal{B} \subseteq \{0,1\}^n \backslash \{(0,0,...,0)\}$, called the *basis*, of non–zero binary n-tuples, the NEPS of $G_1, G_2, ..., G_n$ is the graph with vertex set $\mathcal{V}(G_1) \times \mathcal{V}(G_2) \times \cdots \times \mathcal{V}(G_n)$ in which two vertices $\{w_1, w_2, \cdots, w_n\}$ and $\{y_1, y_2, \cdots, y_n\}$ are adjacent if and only if there exists $(\beta_1, \beta_2, \cdots, \beta_n) \in \mathcal{B}$ such that $w_i = y_i$ whenever $\beta_i = 0$ and w_i is adjacent to y_i whenever $\beta_i = 1$.

Lemma 7.5. [2] *If for* $1 \le i \le n$*,* $\lambda_{i1}, \lambda_{i2}, \cdots, \lambda_{in_i}$ *is the spectrum of* G_i*, of order* n_i *for* $1 \le i \le n$*, then the spectrum of the NEPS of* $G_1, G_2, \cdots, G_n$ *with respect to basis* $\mathcal{B}$ *is* $\{\sum_{\beta \in \mathcal{B}} \lambda_{1i_1}^{\beta_1}, \lambda_{2i_2}^{\beta_2}, \cdots, \lambda_{ni_n}^{\beta_n} : i_k = 1, 2, ..., n_k \quad \& \quad k = 1, 2, ..., n\}$*.*

The following result follows from the construction of a uniform–core graph $G \in \mathcal{U}$.

Theorem 7.6. *A uniform–core graph* $G \in \mathcal{U}$ *is the NEPS of a nut graph* G_1 *and* K_2 *with basis* $\{(1,0),(1,1)\}$*.*

From Lemma 7.5 and Theorem 7.6, the spectrum of the uniform–core graph $G \in \mathcal{U}$ is $\lambda_i + \lambda_i\lambda_j$ where $\{\lambda_i\}$ is the spectrum of the nut graph H and $\{\lambda_j\} = \{1, -1\}$ is the spectrum of K_2. This agrees with the result in Theorem 7.2.

7.2 Non-singular graphs with a complete weighted inverse

We shall now look into the second class of devices. Such a graph G is a device (G, y, z), of variety 3a(ii), for some pair of distinct vertices y and z. Graphs which are devices (G, y, z), of variety 3a(ii), for a particular pair of vertices y and z exist, as shown in the example of Figure 2 for vertex connections 15 and 17. Can a graph G be a device (G, y, z), of variety 3a(ii), for *all* vertex pairs $\{y, z\}$? The question amounts to determining whether it is possible to have $\eta(G - y - z)$ equal to the maximum allowed nullity relative to $\eta(G)$, that is $\eta(G) + 2$, for all vertex pairs $\{y, z\}$. The answer is in the negative.

Lemma 7.7. *It is impossible that a graph* G *is a device* (G, y, z) *of variety 3a(ii) for all pairs of distinct vertices* y *and* z*.*

Proof. Suppose G is a graph which is a device (G, y, z) of *variety* 3a(ii) for all pairs of distinct vertices y and z. This requires that each of the graphs $G - y$ and $G - z$ is singular and therefore has CVs. Deletion of a CV from $G - y$, restores the nullity back to $\eta(G)$. Hence it is impossible to achieve $\eta(G - y - z) = \eta(G) + 2$, for *all* vertex pairs $\{y, z\}$. □

By Lemma 5.3(ii), the kind $(\eta_G, \eta_{G-y}, \eta_{G-z}, \eta_{G-y-z})$=$(\eta_G, \eta_G+1, \eta_G, \eta_G+1)$ is impossible. Hence the only devices (G, y, z) within the second class that have the maximum value of $\eta(G - y)$ relative to η_G, for all vertices y, are of kind $(\eta_G, \eta_G + 1, \eta_G + 1, \eta_G)$. Our focus is on the non–singular graphs of this kind having the inverse $\mathbf{A}^{-1}$ equal to the adjacency matrix of the complete graph with real non–zero weighted edges and no loops.

The smallest candidate is K_2. Indeed $\mathbf{A}(K_2) = \mathbf{A}(K_2))^{-1} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$.

Definition 7.8. Let G be a non–singular graph G with the off–diagonal entries of the inverse $\mathbf{A}^{-1}$ of its adjacency matrix $\mathbf{A}$ being non–zero and real, and all the diagonal entries of $\mathbf{A}^{-1}$ being zero. Then G is said to be a *nuciferous graph*.

The motivation for the name nuciferous graph (meaning nut–producing graph) will become clear from Theorem 7.9. To characterize this class of graphs, let us consider the deck $\{G - v : v \in \mathcal{V}\}$ of subgraphs, as in the investigation of the polynomial reconstruction problem [10].

Theorem 7.9. *Let* G *be a nuciferous graph. Then* G *is either* K_2 *or each vertex–deleted subgraph* $G - v$ *is a nut graph.*

Proof. Let $\mathbf{Q}$ be the $n-1 \times n$ matrix obtained from $\mathbf{A}^{-1}$ by suppressing the diagonal entry from each column. Therefore each entry of $\mathbf{Q}$ is non–zero.

Let the i^{th} column of $\mathbf{Q}$ be $\mathbf{q}_i := (q_{(1)i}, q_{(2)i}, ..., q_{(i-1)i}, q_{(i+1)i}, q_{(i+2)i}, ..., q_{(n)i})^t$ for $2 \leq i \leq n-1$. The first and last columns are $\mathbf{q}_1 := (q_{(2)1}, q_{(3)1}, ..., q_{(n)1})^t$ and $\mathbf{q}_n := (q_{(1)n}, q_{(2)n}, ..., q_{(n-1)n})^t$, respectively.

Since $\mathbf{A}\mathbf{A}^{-1}$ is the identity matrix $\mathbf{I}$, then $\mathbf{A}(G-i)\mathbf{q}_i = \mathbf{0}$ for all $1 \leq i \leq n$. Therefore $\mathbf{q}_i$ is a kernel eigenvector (with non–zero entries) of $G-i$ for all the vertices i. Hence $G-i$ is a core graph. By interlacing, it has nullity one. It follows that each vertex–deleted subgraph is a nut graph. □

From Lemma 7.7, nuciferous devices (G, y, z) are not of type of *variety* 3a(ii) for all pairs of distinct vertices y and z. Moreover, from Theorem 7.9, for $G \neq K_2$, each vertex–deleted subgraph is a nut graph and therefore has nullity one. On deleting a vertex from a nut graph, the nullity becomes zero. Hence a candidate graph G cannot be of *variety* 3a(ii) for *any* pair of vertices y and z.

Theorem 7.10. *Let G be a nuciferous graph G. If G is not K_2, then*
(i) it has order at least eight;
(ii) the device (G, y, z) is of variety 3a(i) for **all** *pairs of distinct vertices y and z;*
(iii) the graph G is not bipartite.

Proof. (i) Since nut graphs exist for order at least seven [12], it follows, from Theorem 7.9, that a nuciferous graph G, of order at least three, has at least eight vertices.

(ii) From the proof of Lemma 7.7, a nuciferous graph G is of *kind* $(\eta_G, \eta_G + 1, \eta_G + 1, \eta_G)$. Thus G is a device (G, y, z) of *variety* 3a(i) for all pairs of distinct vertices y and z.

(iii) From Theorem 7.9, $G-y$ and $G-z$ are nut graphs and therefore cannot be bipartite [12]. Hence G has odd cycles and cannot be bipartite. □

To date, no graph (except K_2) has been found to satisfy the condition of Theorem 7.9. An exhaustive search on all graphs on up to 10 vertices and all chemical graphs on up to 16 vertices reveals no counter example. We conjecture the following result.

Conjecture 7.11. *There are no graphs for which* every *vertex–deleted subgraph is a nut graph.*

8 Chemical implications

Graph theory has strong connections with the study of physical and chemical properties of all-carbon frameworks such as those in benzenoids, fullerenes and carbon nanotubes. The eigenvalues and eigenvectors of the adjacency matrix of the molecular graph (the graph of the carbon skeleton) are used in qualitative models of the energies and spatial distributions of the mobile π electrons of such systems. Specifically, graphs and their nullities figure in simple theories of ballistic conduction of electrons by conjugated systems. In the simplest formulation [3] of the SSP (Source and Sink Potential) [5] approach to molecular conduction, the variation of electron transmission with energy is qualitatively modelled in terms of the characteristic polynomials of G, $G-y$, $G-z$, $G-y-z$, where G is the molecular graph and vertices y and z are in contact with wires. (This is the motivation for the definition of a *device* in the present paper.) As a consequence, the transmission at the Fermi level (corresponding here to $\lambda = 0$) obeys selection rules couched in terms of the nullities η_G, η_{G-y}, η_{G-z}, and η_{G-y-z} [7], motivating the definition of *kinds here. In terms of the* varieties defined here, the SSP theory predicts conduction at the Fermi level for connection across the vertex pair (y, z) for $1(ii)$, $1(iii)$, $3a(i)$, $3b(ii)$, $3c(i)$ and $3c(iiA)$, and, conversely, insulation at the Fermi level for $1(i)$, $2a$, $2b$, $3a(ii)$, $3b(i)$ and $3c(iiB)$.

The two classes of graphs with analogous vertex pairs and certain extremal conditions on the nullity of their vertex-deleted subgraphs, explored in Section 7 are envisaged to have interesting developments in spectral graph theory. Moreover, the classification of graphs into *varieties* and *kinds* has an application in chemistry in the identification of molecules (with carbon atoms in particular) that conduct or else bar conduction at the Fermi level that has already been investigated in [3]. According to the SSP theory, the first class, the *uniform–core graphs*, corresponds to insulation at the Fermi–level for all two vertex connections and the second class, the nuciferous graphs, to Fermi–level conducting devices (G, y, z) for all pairs of distinct vertices y and z. The latter class has the additional properties that it consists of devices corresponding to non-singular graphs that are Fermi–level insulators when $y = z$. Therefore nuciferous graphs have no non–bonding orbital and are conductors for all distinct vertex connection pairs and insulators for all one vertex connections. We conjecture that the only nuciferous graph is K_2.

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