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COALESCING FIEDLER AND CORE VERTICES

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Dedicated to the memory of Miroslav Fiedler

Abstract. The nullity of a graph G is the multiplicity of zero as an eigenvalue in the spectrum of its adjacency matrix. From the interlacing theorem, derived from Cauchy's inequalities for matrices, a vertex of a graph can be a core vertex if, on deleting the vertex, the nullity decreases, or a Fiedler vertex, otherwise. We adopt a graph theoretical approach to determine conditions required for the identification of a pair of prescribed types of root vertices of two graphs to form a cut-vertex of unique type in the coalescence. Moreover, the nullity of subgraphs obtained by perturbations of the coalescence G is determined relative to the nullity of G. This has direct applications in spectral graph theory as well as in the construction of certain ipso-connected nano-molecular insulators.

Keywords: nullity; core vertex; Fiedler vertex; cut-vertices; coalescence

MSC 2010: 05C50, 15A18, 05B20

1. INTRODUCTION

The *adjacency matrix* $\mathbf{A}(G) = (a_{ij})$ of a labelled simple graph G on n vertices is the $n \times n$ matrix whose entry a_{ij} is 1 if the vertices i and j are adjacent and 0 otherwise. The subgraph of a graph G formed from a subset S of the vertices of G and all the edges connecting pairs of vertices of S in G is a subgraph *induced* by S in G. The graph $G - v$ denotes the subgraph of G obtained by deleting the vertex v (and all the edges incident to it). If G_1 is an induced subgraph of G, $G - G_1$ is obtained from G by deleting all the vertices of G. The graph $G + v$ is obtained from G by adding a vertex v adjacent to a nonempty subset of vertices, which is a prescribed set of neighbours of v in G.

Two nonadjacent vertices i and j of a graph G are *identified* (or *coalesced*) when these two vertices are replaced by a single vertex incident to all the edges which are

incident in G to either i or j. A graph has a root vertex v if one of its vertices, v, is distinguished. Let H_1 and H_2 be two graphs with root vertices v_1 and v_2, respectively. The *coalescence* $H_1 \circ H_2$ of the *component graphs* H_1 and H_2 is a connected graph G obtained by identifying v_1 with v_2 to form the *coalescence vertex* v in G. We note that the coalescence vertex v is a *cut-vertex* of G. The *coalescence* G *of* s ($\geqslant 2$) *component graphs* is obtained by identifying a root vertex of each of the s component graphs to obtain a connected graph.

If $\mathbf{I}$ is the $n \times n$ identity matrix, the *characteristic polynomial of a graph* G, denoted by $\varphi(G)$, is the characteristic polynomial $\det(\lambda \mathbf{I} - \mathbf{A})$ of the $n \times n$ adjacency matrix $\mathbf{A}(= \mathbf{A}(G))$. It is independent of the labelling of the vertices of G. The *eigenvalues of the graph* are the eigenvalues of $\mathbf{A}$ and they form the *spectrum* of G. Since $\mathbf{A}$ is a real symmetric matrix, its eigenvalues are real numbers and the dimension of each eigenspace is equal to the algebraic multiplicity of the respective eigenvalue, that is, the number of times the eigenvalue is repeated as a root of the characteristic equation $\varphi(G) = 0$.

A graph is *singular* if its adjacency matrix $\mathbf{A}$ is not invertible and *nonsingular* otherwise. The multiplicity of zero as an eigenvalue in the spectrum of the graph G is called the *nullity*, denoted by $\eta(G)$. The *nullspace* is the eigenspace associated with the eigenvalue 0. An eigenvector $\mathbf{x}$ ($\neq \mathbf{0}$) in the nullspace of $\mathbf{A}$ is called a *kernel eigenvector* of G and satisfies $\mathbf{A}\mathbf{x} = \mathbf{0}$.

We shall have occasion to use a consequence of Cauchy's Interlacing theorem for real symmetric matrices and Schwenk's Coalescence theorem, stated hereunder as Theorem 1.1 and Theorem 1.2, respectively.

Theorem 1.1 ([13], page 119)**.** *Let u be any vertex of a graph G on $n \geqslant 2$ vertices. Then*
$$\eta(G) - 1 \leqslant \eta(G - u) \leqslant \eta(G) + 1.$$

Theorem 1.2 ([15])**.** *Let $H_1 = G_1 + v_1$ and $H_2 = G_2 + v_2$ be two graphs with root vertices v_1 and v_2, respectively. The characteristic polynomial of the coalescence $H_1 \circ H_2$ is given by*

$$\varphi(H_1 \circ H_2) = \varphi(H_1)\varphi(G_2) + \varphi(G_1)\varphi(H_2) - \lambda\varphi(G_1)\varphi(G_2).$$

According to Theorem 1.1, when a vertex is deleted or added to a graph G, the nullity changes by at most one. We distinguish between a vertex corresponding to a zero entry in each of the kernel eigenvectors and a vertex corresponding to a nonzero entry in some kernel eigenvector.

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Definition 1.3 ([18], [19])**.**   Let **x** be a kernel eigenvector of a singular graph G, of order $n \geqslant 3$. A subgraph of G induced by the vertices corresponding to the nonzero entries of **x** is a *core* with respect to **x**.

Definition 1.4 ([12], [17], [18])**.**   The set of *core vertices* of G consists of those vertices that lie in some core of G. A vertex not lying in any core is said to be a *Fiedler vertex*.

Note that the set of core vertices is an invariant of G in [18]. Fiedler vertices are also referred to as *core-forbidden vertices*. The following result characterises a core vertex in a singular graph.

Proposition 1.5 ([16])**.** *A vertex u is a core vertex in a graph $G + u$ if and only if* $\eta(G + u) = \eta(G) + 1$.

There are three types of vertices, depending on the change in the multiplicity of an eigenvalue allowed by the Interlacing theorem. In [11], [23], a vertex is referred to as *downer*, *neutral* or *Parter* when its deletion decreases, does not change or increases the multiplicity of an eigenvalue, respectively. For the eigenvalue zero, Fiedler vertices and Parter vertices are sometimes referred to as *F-vertices* and *P-vertices*, respectively, see [1]. Following [6], [12], we call a vertex u a *core vertex* (CV), a *middle core-forbidden vertex* (CFV$_{\mathrm{mid}}$) or *an upper core-forbidden vertex* (CFV$_{\mathrm{upp}}$) if the nullity of $G - u$ is $\eta(G) - 1$, $\eta(G)$, or $\eta(G) + 1$, respectively.

In this paper we investigate the nullity of a coalescence and derive some concise formulae. There are areas of graph theory that could benefit directly from the study of the change in nullity on deleting a cut-vertex. The graphs with a cut-vertex form a subclass of the class of forbidden subgraphs of Hamiltonian graphs. The line graphs of a trees can be viewed as the iterative coalescence of complete graphs. The results we obtain here enable the nullity of such graphs to be deduced by determining the types of vertices being identified. Coronas and windmills are also subclasses of graphs with a cut-vertex [8], [20].

A further motivation is the interpretation of the electron energy given by Schrödinger's equation in the quantum theory of molecules [10] and its relation to the nullity of a molecular graph. Collatz and Sinogowitz posed the problem of characterizing all graphs with nonzero nullity (that is, the class of singular graphs), see [3]. Most of the work in this regard was done in [18], [19], where certain subgraphs that force a graph to be singular were identified. However, the problem is hard and research is still ongoing.

In chemical graph theory, a molecular graph, which is a π-system of carbon atoms, is a labelled graph whose vertices correspond to the atoms of the compound and whose edges correspond to chemical sigma bonds. The recent flurry of research on the

conductivity of carbon nano molecules used as components in circuits has spurred the development of the theory to understand the factors that cause a molecule to allow or bar the flow of electricity. For a molecule in a circuit with two leads connected to the same atom (referred to as an ipso connection), the concept of the change in nullity when the connecting vertex is deleted from the underlying graph proved to be crucial to predicting the conductivity or insulation of the molecule [5], [14], [21]. From Theorem 4.5 of [5], our results in this paper predict that a molecule with ipso connection at a cut-vertex is an insulator if it is constructed from component graphs of which at least one has a root vertex which is CFV_{upp}.

Brown et al. [2] proved that a graph G is singular if, and only if, G possesses a nontrivial zero-sum weighting (which is equivalent to the existence of a kernel eigenvector) and asked what causes a graph to be singular. Gutman and Sciriha [9] introduced nut graphs as the graphs of nullity one having a kernel eigenvector with all its entries being nonzero. In [18], [19], Sciriha determined properties of substructures responsible for a graph to be singular, establishing that in a graph of nullity η, there are η induced subgraphs (termed singular configurations) of nullity one from a prescribed list. In [22], Sharaf and Ali proceeded to determine a sharp lower bound and a sharp upper bound for the nullity of the coalescence of two graphs. They showed that the nullity of the coalescence of s component graphs varies by at most $s - 1$ from the sum of the nullities of the component graphs. Other results on the nullity of a graph with a cut-vertex are given in [7].

The rest of this paper is structured as follows. In Sections 2 and 3, we start from the component graphs with a root vertex of prescribed type and determine the type of the coalescence vertex as well as the nullity of the coalescence. The inverse problem is then studied in Section 4. Starting from a given type of a cut-vertex in the coalescence, we determine the possible types of vertices in the component graphs. The subgraphs of G that we consider in the sequel are $R = G - v$, $U_i = (G_i + v_i) \cup (R - G_i)$, $G - G_i$, $W_i = (G_i + v_i) \cup (G - G_i)$, $S_i = G_i \cup (G - G_i)$ and $Y = \bigcup_{j=1}^{s} (G_j + v_j)$ shown in Figure 1 for the case when $i = 1$.

2. Determining the type of the coalescence vertex

In this section we determine the type of the coalescence vertex starting from the type of the root vertex in one or more of the component graphs. We show that the type of a vertex v_i (that is, CV, CFV_{mid} or CFV_{upp}) in $H_i = G_i + v_i$, for $i \in \{1, 2, \ldots, s\}$, determines the possible type of the cut-vertex v in G or of u in W_1 or in S_1. Furthermore, we study the change in nullity when the coalescence G of the component graphs $H_1, H_2, \ldots, H_s$ is perturbed.
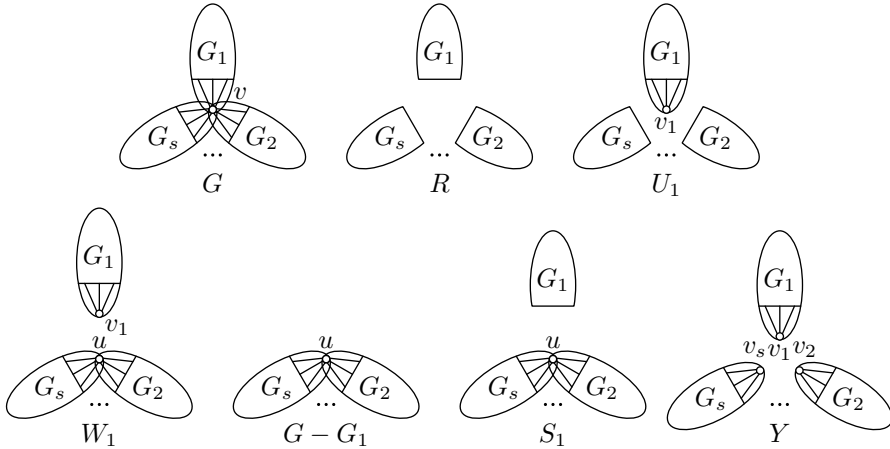
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Figure 1. The graphs G, R, U_1, W_1, $G - G_1$, S_1 and Y.

The statements of all the results that follow refer to Figure 1. The following theorem gives the nullity of U_1.

Theorem 2.1. *Let G be a graph with a cut-vertex v and let $G_1, G_2, \ldots, G_s$ be the components of $G - v$. If v_i is a $\mathrm{CFV}_{\mathrm{upp}}$ in $H_i = G_i + v_i$, then $\eta(U_i) = \eta(G)$.*

P r o o f. Without loss of generality, let $i = 1$ so that v_1 is a $\mathrm{CFV}_{\mathrm{upp}}$ in H_1 (refer to Figure 1). Since v_1 is a $\mathrm{CFV}_{\mathrm{upp}}$ in $H_1 = G_1 + v_1$, hence, by definition, $\eta(G_1) = \eta(H_1) + 1$.

The nullity of a disconnected graph is equal to the sum of the nullities of its components. Thus,

$$(2.1) \qquad \eta(R) - \eta(U_1) = \eta(G_1) - \eta(H_1) = 1.$$

Let $\eta(G) = \eta$. By Theorem 1.1, $\eta - 1 \leqslant \eta(R) \leqslant \eta + 1$, and hence $\eta - 2 \leqslant \eta(U_1) \leqslant \eta$.

We use a result given in [4] for the n-vertex graph $G = R + v$. For an orthonormal set of eigenvectors $\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \ldots, \mathbf{x}^{(n-1)}$ corresponding to the $n - 1$ eigenvalues of R, if $x_k^{(i)}$ is the kth entry of $\mathbf{x}^{(i)}$, then

$$\varphi(G) = \varphi(R)\left(\lambda - \sum_{i=1}^{n-1} \frac{\sum_{k \in \mathcal{N}} \left(x_k^{(i)}\right)^2}{\lambda - \lambda_i}\right),$$

where $\mathcal{N} = N_G(v) = \bigcup_{i=1}^{s} N_{G_i}(v_i)$, $N_{G_i}(v_i)$ is the neighbourhood of v_i in G_i, and $\lambda_1, \lambda_2, \ldots, \lambda_{n-1}$ are the eigenvalues of R. Now from (2.1), $\eta(R) > \eta(U_1) \geqslant 0$, and thus R is singular. Since the adjacency matrix $\mathbf{A}(R)$ of R is diagonalizable, $m_R(\lambda)$

is of the form $\lambda(\lambda - \mu_2)\ldots(\lambda - \mu_t)$, where $\mu_1\ (= 0)$, $\mu_2,\ldots,\mu_t$ are the t ($t \leqslant n-1$) distinct eigenvalues of R.

It follows that $\varphi(G)$ is of the form

$$\varphi(G) = \varphi(R)\left(\lambda - \sum_{i=1}^{t} \frac{\delta_i^2}{\lambda - \mu_i}\right),$$

where $\delta_i \in \mathbb{R}$. Thus,

$$(2.2) \qquad \varphi(G) = \frac{\varphi(R)}{m_R(\lambda)}\left(\lambda m_R(\lambda) - \left(\frac{\delta_1^2}{\lambda} + \frac{\delta_2^2}{\lambda - \mu_2} + \ldots + \frac{\delta_t^2}{\lambda - \mu_t}\right)m_R(\lambda)\right).$$

Note that $\lambda^{\eta(R)}$ divides $\varphi(R)$, and thus the rational quotient $\varphi(R)/m_R(\lambda)$ has $\lambda^{\eta(R)-1}$ as a factor (because both the numerator and the denominator in the quotient have a common factor of λ). Also, $\delta_1^2 m_R(\lambda)/\lambda$ has a nonzero constant term, and hence the right hand side of equation (2.2) has $\lambda^{\eta(R)-1}$ as a factor but it is not divided by $\lambda^{\eta(R)}$. Thus, $\eta(G) = \eta(R) - 1$. From (2.1), $\eta(G) = \eta(U_1)$. $\qquad\square$

We shall also use the following result which gives a sufficient condition for the coalescence vertex to be $\mathrm{CFV}_{\mathrm{upp}}$ in G. We explore the cases for the coalescence vertex to be CV or $\mathrm{CFV}_{\mathrm{mid}}$ in Theorems 2.5 to 2.8.

Theorem 2.2 ([7])**.** *Let G be a graph with a cut-vertex v and let $G_1, G_2, \ldots, G_s$ be the components of $G - v$. If there exists a component G_i among $G_1, G_2, \ldots, G_s$ such that v_i is a $\mathrm{CFV}_{\mathrm{upp}}$ in $H_i = G_i + v_i$, then v is a $\mathrm{CFV}_{\mathrm{upp}}$ in G.*

We now consider the type of a vertex v_i other than $\mathrm{CFV}_{\mathrm{upp}}$ in $H_i = G_i + v_i$.

Lemma 2.3 ([7])**.** *Let G be a graph with a cut-vertex v and let $G_1, G_2, \ldots, G_s$ be the components of $G - v$. If v_1 is a CV in $H_1 = G_1 + v_1$, then $\eta(S_1) = \eta(G_1) + \eta(G - G_1) = \eta(G)$.*

Since the choice of the component graph H_1 is arbitrary, we have:

Corollary 2.4. *Let G be a graph with a cut-vertex v and let $G_1, G_2, \ldots, G_s$ be the components of $G - v$. If there exists $i \in \{1, 2, \ldots, s\}$ such that v_i is a CV in $G_i + v_i$, then $\eta(S_i) = \eta(G_i) + \eta(G - G_i) = \eta(G)$ and $\eta(W_i) = \eta(S_i) + 1$.*

We now present a sufficient condition for the cut-vertex v in G to be a CV.

Theorem 2.5. *Let G be a graph with a cut-vertex v, and let $G_1, G_2, \ldots, G_s$ be the components of $G - v$. If v_i is a CV in each $H_i = G_i + v_i$ for $i \in \{1, 2, \ldots, s\}$, then v is a CV in G.*

P r o o f. Let v_i be a CV in each H_i for $i \in \{1, 2, \ldots, s\}$. To show that v is a CV in G, by Proposition 1.5 it is sufficient to show that $\eta(G) = \sum_{i=1}^{s} \eta(G_i) + 1 = \eta(G - v) + 1$. We use induction on the number s of components of $G - v$.

For $s = 2$, let G_1 and G_2 be the only two components of $G - v$ such that v_1 is a CV in H_1 and v_2 is a CV in H_2. Then by Lemma 2.3, we have $\eta(G) = \eta(G_1) + \eta(G - G_1)$. Now $G - G_1 = H_2$, and thus $\eta(G) = \eta(G_1) + \eta(H_2)$, implying that $\eta(G) = \eta(G_1) + \eta(G_2) + 1$. Since G_1 and G_2 are the components of $G - v$, we have $\eta(G) = \eta(G - v) + 1$. Hence, v is a CV in G.

Assume that the result is true for $k < s$, that is, if $G_1, G_2, \ldots, G_k$ are the components of G such that v_i is a CV in each H_i for $i \in \{1, 2, \ldots, k\}$, then $\eta(G) = \sum_{i=1}^{k} \eta(G_i) + 1$. We show that the result follows for the case when $G - v$ has $(k+1)$ components $G_1, G_2, \ldots, G_k, G_{k+1}$. Let v_i be a CV in each H_i for $i \in \{1, 2, \ldots, k+1\}$, and let $X = G - G_{k+1}$. Then $S_{k+1} = X \cup G_{k+1}$ and by Corollary 2.4, we have $\eta(G) = \eta(S_{k+1}) = \eta(G_{k+1}) + \eta(G - G_{k+1}) = \eta(G_{k+1}) + \eta(X)$. Now, by the inductive hypothesis, $\eta(X) = \sum_{i=1}^{k} \eta(G_i) + 1$. Thus $\eta(G) = \eta(G_{k+1}) + \sum_{i=1}^{k} \eta(G_i) + 1 = \sum_{i=1}^{k+1} \eta(G_i) + 1$. Finally, since $G - v = \bigcup_{i=1}^{k+1} G_i$, we conclude that $\eta(G - v) = \sum_{i=1}^{k+1} \eta(G_i)$. Thus, $\eta(G) = \eta(G - v) + 1$. The result follows by induction on s. $\qquad\square$

As we shall see below, the occurrence of a CFV_{mid} among the root vertices of the component graphs is nondeterministic. We discuss the case when the number of component graphs is two in Theorems 2.6 and 2.7. For any finite number of component graphs, the instance when the occurrence of a CFV_{mid} among the root vertices determines the type of coalescence vertex uniquely is given in Theorem 2.8.

Theorem 2.6. *Let* $H_1 = G_1 + v_1$ *and* $H_2 = G_2 + v_2$ *be two graphs with root vertices* v_1 *and* v_2, *respectively. If* v_1 *is a CV in* H_1 *and* v_2 *is a* CFV_{mid} *in* H_2, *then* $\eta(G) = \eta(H_1) + \eta(H_2) - 1$ *and the coalescence vertex* v *obtained by identifying* v_1 *and* v_2 *is a* CFV_{mid} *in* $G = H_1 \circ H_2$.

P r o o f. By Lemma 2.3, $\eta(G) = \eta(S_1) = \eta(G_1) + \eta(H_2)$. Since v_1 is a CV in H_1, so $\eta(G_1) = \eta(H_1) - 1$ and thus $\eta(G) = \eta(H_1) + \eta(H_2) - 1$. But v_2 is a CFV_{mid} in H_2, implying that $\eta(R) = \eta(S_1)$. Hence $\eta(G) = \eta(R)$ and, by definition, the coalescence vertex v is a CFV_{mid} in $G = H_1 \circ H_2$. $\qquad\square$

Theorem 2.7. *Let* $H_1 = G_1 + v_1$ *and* $H_2 = G_2 + v_2$ *be two graphs with root vertices* v_1 *and* v_2, *respectively, and let* v *be the coalescence vertex in* $G = H_1 \circ H_2$ *obtained by identifying* v_1 *and* v_2. *If both* v_1 *and* v_2 *are* CFV_{mid} *in* H_1 *and* H_2,

respectively, then either v is a $\mathrm{CFV_{mid}}$ in G and $\eta(G) = \eta(H_1) + \eta(H_2)$, or v is a CV in G and $\eta(G) = \eta(H_1) + \eta(H_2) + 1$.

P r o o f. Since v_1 is a $\mathrm{CFV_{mid}}$ in H_1 and v_2 is a $\mathrm{CFV_{mid}}$ in H_2, we have $\eta(G_1) = \eta(H_1)$ and $\eta(G_2) = \eta(H_2)$. By Theorem 1.2, the characteristic polynomial of the coalescence $G = H_1 \circ H_2$ is given by

$$\varphi(G) = \varphi(H_1)\varphi(G_2) + \varphi(G_1)\varphi(H_2) - \lambda\varphi(G_1)\varphi(G_2).$$

So we obtain

$$\eta(G) \geqslant \eta(H_1) + \eta(H_2) = \eta(G_1) + \eta(G_2) = \eta(R).$$

Thus, on the deletion of the cut-vertex v in G, the nullity does not increase. Thus v cannot be a $\mathrm{CFV_{upp}}$. Hence, either v is a $\mathrm{CFV_{mid}}$ in G and $\eta(G) = \eta(H_1) + \eta(H_2)$, or v is a CV in G and $\eta(G) = \eta(H_1) + \eta(H_2) + 1$. $\qquad\square$

Figure 2 shows that each of the situations described in Theorem 2.7 can occur for the coalescence of component graphs with root vertices of the type $\mathrm{CFV_{mid}}$.
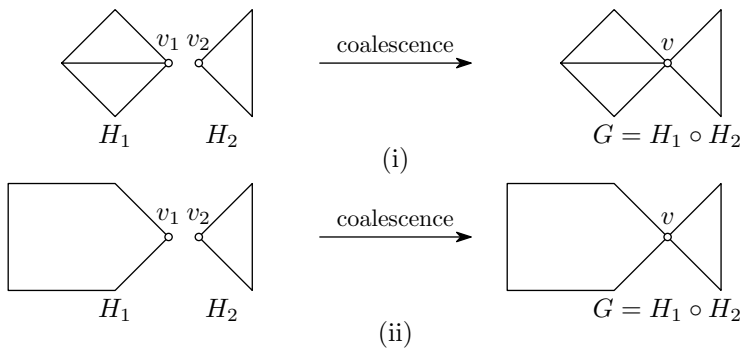

Figure 2. Two graphs illustrating Theorem 2.7 when (i) v is a $\mathrm{CFV_{mid}}$ in G; and (ii) v is a CV in G.

Theorem 2.8. *For each $i \in \{1, 2, \ldots, s\}$, let $H_i = G_i + v_i$ be a graph with root vertex v_i. If no H_i has a $\mathrm{CFV_{upp}}$ and exactly one H_i has a $\mathrm{CFV_{mid}}$, then the coalescence vertex v is a $\mathrm{CFV_{mid}}$ in the coalescence G obtained by identifying all the vertices v_i in H_i.*

P r o o f. Without loss of generality, let H_1 be the only component graph with a $\mathrm{CFV_{mid}}$ root vertex. If no component graph H_i has a $\mathrm{CFV_{upp}}$ root vertex, then the root vertex in each H_i, for $i \in \{2, \ldots, s\}$, is a CV. If we let u be the coalescence vertex in the graph $G - G_1$ obtained by identifying each root vertex v_i, $i \in \{2, \ldots, s\}$, then by Theorem 2.5, u is a CV in $G - G_1$. Since v_1 is a $\mathrm{CFV_{mid}}$ in H_1 and u is a CV in $G - G_1$, by Theorem 2.6, v is a $\mathrm{CFV_{mid}}$ in G, where v is the coalescence vertex in $G = H_1 \circ (G - G_1)$. $\qquad\square$

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3. Determining the nullity of a coalescence

At this stage, using results in Section 2, we can determine the nullity of the coalescence from the nullities of the component graphs. For simplicity we start with the coalescence of exactly two component graphs. This enables us to get the generalization to the coalescence of a finite number $s > 2$ of component graphs, by induction.

In Proposition 3.1 and Theorem 3.2 we consider the case when one or more of the root vertices in the component graphs are CV.

Proposition 3.1. *Let $H_1 = G_1 + v_1$ and $H_2 = G_2 + v_2$ be two graphs with root vertices v_1 and v_2, respectively. If at least one of the root vertices is a CV in the respective component graph, then $\eta(G) = \eta(H_1) + \eta(H_2) - 1$ where $G = H_1 \circ H_2$.*

P r o o f. Without loss of generality, we let v_1 be a CV in H_1. Thus, $\eta(G_1) = \eta(H_1) - 1$, and by Lemma 2.3, $\eta(G) = \eta(G_1) + \eta(G - G_1) = \eta(H_1) - 1 + \eta(G - G_1)$. But $G - G_1 = H_2$ and thus $\eta(G) = \eta(H_1) - 1 + \eta(H_2)$. $\square$

Now we determine the nullity of $G - G_i$ (for $i \in \{1, 2, \ldots, s\}$) and of G in terms of the nullities of their subgraphs.

Theorem 3.2. *Let G be a graph with a cut-vertex v, and let $G_1, G_2, \ldots, G_s$ be all the components of $G - v$. If v_i is a CV in each $H_i = G_i + v_i$ for $i \in \{1, 2, \ldots, s\}$, then*

(i) $\eta(G - G_i) = \sum_{\substack{j=1 \\ j \neq i}}^{s} \eta(G_j) + 1$; *and*

(ii) $\eta(G) = \sum_{i=1}^{s} \eta(H_i) + (1 - s)$.

P r o o f. Since v_i is a CV in each H_i, for $i \in \{1, 2, \ldots, s\}$, by Theorem 2.5, v is a CV in G. Thus,

$$(3.1) \qquad \eta(G) = \eta(G - v) + 1 = \sum_{i=1}^{s} \eta(G_i) + 1.$$

(i) By Corollary 2.4, $\eta(G) = \eta(G_i) + \eta(G - G_i)$ for $i \in \{1, 2, \ldots, s\}$. Thus, $\eta(G - G_i) = \sum_{\substack{j=1 \\ j \neq i}}^{s} \eta(G_j) + 1$ since $\eta(G) = \eta(G_i) + \sum_{\substack{j=1 \\ j \neq i}}^{s} \eta(G_j) + 1$.

(ii) Since v_i is a CV in each H_i, for $i \in \{1, 2, \ldots, s\}$, by definition, $\eta(G_i) = \eta(H_i) - 1$. Thus, from (3.1),

$$\eta(G) = \eta(H_1) - 1 + \eta(H_2) - 1 + \ldots + \eta(H_s) - 1 + 1$$
$$= \eta(H_1) + \eta(H_2) + \ldots + \eta(H_s) + (1 - s)$$
$$= \sum_{i=1}^{s} \eta(H_i) + (1 - s).$$

$\square$

The case when one or more of the root vertices are $\mathrm{CFV_{upp}}$ is treated in Proposition 3.3 and Theorem 3.4.

Proposition 3.3. *Let $H_1 = G_1 + v_1$ and $H_2 = G_2 + v_2$ be two graphs with root vertices v_1 and v_2, respectively.*

(i) *If both the root vertices are $\mathrm{CFV_{upp}}$, then $\eta(H_1 \circ H_2) = \eta(H_1) + \eta(H_2) + 1$.*

(ii) *If v_1 is a $\mathrm{CFV_{upp}}$ in H_1 and v_2 is a $\mathrm{CFV_{mid}}$ in H_2, then $\eta(H_1 \circ H_2) = \eta(H_1) + \eta(H_2)$.*

(iii) *If v_1 is a $\mathrm{CFV_{upp}}$ in H_1 and v_2 is a CV in H_2, then $\eta(H_1 \circ H_2) = \eta(H_1) + \eta(H_2) - 1$.*

P r o o f. In each of the three cases (i), (ii) and (iii), at least one root vertex is a $\mathrm{CFV_{upp}}$ in the respective component graph. Hence by Theorem 2.2, if $G = H_1 \circ H_2$, we have

$$(3.2) \qquad\qquad \eta(R) = \eta(G - v) = \eta(G) + 1.$$

(i) Assume that both the root vertices are $\mathrm{CFV_{upp}}$. As shown in Figure 1, $W_1 = H_1 \cup H_2$. Hence $\eta(S_1) = \eta(W_1) + 1 = \eta(H_1) + \eta(H_2) + 1$ and $\eta(R) = \eta(S_1) + 1 = \eta(H_1) + \eta(H_2) + 2$. Thus, from (3.2) we get $\eta(G) + 1 = \eta(H_1) + \eta(H_2) + 2$. Hence, $\eta(G) = \eta(H_1) + \eta(H_2) + 1$.

(ii) Assume that v_1 is a $\mathrm{CFV_{upp}}$ in H_1 and v_2 is a $\mathrm{CFV_{mid}}$ in H_2. As shown in Figure 1, $\eta(S_1) = \eta(W_1) + 1 = \eta(H_1) + \eta(H_2) + 1$ because v_1 is a $\mathrm{CFV_{upp}}$ in H_1. Since v_2 is a $\mathrm{CFV_{mid}}$ in H_2, we have $\eta(R) = \eta(S_1) = \eta(H_1) + \eta(H_2) + 1$. Thus, from (3.2) we get $\eta(G) = \eta(H_1) + \eta(H_2)$.

(iii) If v_1 is a $\mathrm{CFV_{upp}}$ in H_1 and v_2 is a CV in H_2, then the result follows immediately from Proposition 3.1. $\square$

Generalizing the above result to the case when the number of component graphs is $s \geqslant 2$, we obtain the following.

Theorem 3.4. *Let G be a graph with a cut-vertex v, and let $G_1, G_2, \ldots, G_s$ be the components of $G - v$. If there exists $i \in \{1, 2, \ldots, s\}$ such that v_i is a $\mathrm{CFV_{upp}}$ in $H_i = G_i + v_i$, then $\eta(G) = \sum_{i=1}^{s} \eta(G_i + v_i) + (a - b - 1)$, where a is the number of component graphs which have the root vertex v_i as a $\mathrm{CFV_{upp}}$ in H_i, and b is the number of component graphs which have the root vertex v_i as a CV in H_i.*

P r o o f. Without loss of generality, let G_i be relabelled so that the first a component graphs have v_i as a $\mathrm{CFV_{upp}}$, the next b component graphs have v_i as a CV, and the last c component graphs have v_i as a $\mathrm{CFV_{mid}}$, where $s = a + b + c$. Then we have

$\eta(G_i) = \eta(H_i)+1$ for $i \in \{1, 2, \ldots, a\}$, $\eta(G_i) = \eta(H_i)-1$ for $i \in \{a+1, a+2, \ldots, a+b\}$ and $\eta(G_i) = \eta(H_i)$ for $i \in \{a+b+1, a+b+2, \ldots, a+b+c = s\}$. Since there exists v_i which is a $\mathrm{CFV_{upp}}$ in at least one H_i, for $i \in \{1, 2, \ldots, s\}$, by Theorem 2.2, v is a $\mathrm{CFV_{upp}}$ in G, and thus $\eta(G) = \eta(G-v) - 1$. Hence

$$
\begin{aligned}
\eta(G) &= \sum_{i=1}^{s} \eta(G_i) - 1 \\
&= \left(\sum_{i=1}^{a}(\eta(H_i)+1) + \sum_{i=a+1}^{a+b}(\eta(H_i)-1) + \sum_{i=a+b+1}^{a+b+c} \eta(H_i) \right) - 1 \\
&= \sum_{i=1}^{a} \eta(H_i) + a + \sum_{i=a+1}^{a+b} \eta(H_i) - b + \sum_{i=a+b+1}^{a+b+c} \eta(H_i) - 1 \\
&= \sum_{i=1}^{s} \eta(H_i) + (a-b-1).
\end{aligned}
$$

$\square$

The next result follows immediately.

Corollary 3.5. *Let G be a graph with a cut-vertex v, and let $G_1, G_2, \ldots, G_s$ be the components of $G-v$. If v_i is a $\mathrm{CFV_{upp}}$ in each $H_i = G_i + v_i$, for $i \in \{1, 2, \ldots, s\}$, then we have $\eta(G) = \sum_{i=1}^{s} \eta(H_i) + (s-1)$.*

Theorem 3.2 and Corollary 3.5 give closed formulae for $\eta(G)$ when, for $i \in \{1, 2, \ldots, s\}$, all the v_i are CV and when all the v_i are $\mathrm{CFV_{upp}}$, respectively. The case when all the v_i are $\mathrm{CFV_{mid}}$ will not be considered here. It is more complex and to obtain a closed formula, specific conditions on the component graphs forming the coalescence are required.

4. Determining the type of the root vertex in component graphs

Here we investigate the inverse problem:

Can the type of the cut-vertex v in the coalescence G determine the type of the root vertex in the component graphs?

For the case when the coalescence vertex is $\mathrm{CFV_{upp}}$ in G we give a necessary and sufficient condition for the type of root vertex in at least one of the component graphs.

Theorem 4.1. *Let G be a graph with a cut-vertex v and let $G_1, G_2, \ldots, G_s$ be the components of $G - v$. The coalescence vertex v is a $\mathrm{CFV_{upp}}$ in G if and only*

if there exists at least one component G_i in G, for $i \in \{1, 2, \ldots, s\}$, such that v_i is a $\mathrm{CFV}_{\mathrm{upp}}$ in $H_i = G_i + v_i$.

P r o o f. Sufficiency follows immediately by Theorem 2.2. To prove necessity, let v be a $\mathrm{CFV}_{\mathrm{upp}}$ in G. As shown in Figure 1, W_1 is a disconnected graph with two components $G - G_1$ and H_1 with root vertices u and v_1, respectively. The graph G is obtained by coalescing the two root vertices of the components of W_1. Theorem 2.5, Theorem 2.6 and Theorem 2.7 rule out cases where none of the two root vertices is a $\mathrm{CFV}_{\mathrm{upp}}$. Thus, either the root vertex v_1 is a $\mathrm{CFV}_{\mathrm{upp}}$ in H_1 or the root vertex u is a $\mathrm{CFV}_{\mathrm{upp}}$ in $G - G_1$.

If v_1 is a $\mathrm{CFV}_{\mathrm{upp}}$ in H_1, then the proof is complete. If, on the other hand, v_1 is not a $\mathrm{CFV}_{\mathrm{upp}}$ in H_1, then u is a $\mathrm{CFV}_{\mathrm{upp}}$ in $G - G_1$. We repeat the same argument used above with $G - G_1$ taking the role of G. This iterative argument is repeated as many times as is necessary until we obtain that:

▷ either there exists a vertex v_j which is a $\mathrm{CFV}_{\mathrm{upp}}$ in H_j, for some $j \in \{2, \ldots, s-2\}$;

▷ or the root vertex u of $G - \bigcup_{i=1}^{s-2} G_i = H_{s-1} \circ H_s$ is a $\mathrm{CFV}_{\mathrm{upp}}$. In this case, either v_{s-1} or v_s is a $\mathrm{CFV}_{\mathrm{upp}}$ in the respective component graph.

The result follows. □

The cases when the coalescence vertex is either a $\mathrm{CFV}_{\mathrm{mid}}$ or a CV in G are considered in Theorems 4.2 and 4.3, respectively.

Theorem 4.2. *Let G be a graph with a cut-vertex v and let $G_1, G_2, \ldots, G_s$ be the components of $G - v$. If v is a $\mathrm{CFV}_{\mathrm{mid}}$ in G, then no v_i is a $\mathrm{CFV}_{\mathrm{upp}}$ in $H_i = G_i + v_i$, for $i \in \{1, 2, \ldots, s\}$, and v_i is a $\mathrm{CFV}_{\mathrm{mid}}$ in at least one component graph H_i.*

P r o o f. Let v be a $\mathrm{CFV}_{\mathrm{mid}}$ in G. By Theorem 4.1, no v_i can be a $\mathrm{CFV}_{\mathrm{upp}}$ in H_i, for $i \in \{1, 2, \ldots, s\}$. Since G is obtained from W_1 by identifying the vertex u in $G - G_1$ with the vertex v_1 in H_1 (refer to Figure 1), then by Theorems 2.2 and 2.5, either u is a $\mathrm{CFV}_{\mathrm{mid}}$ in $G - G_1$ or v_1 is a $\mathrm{CFV}_{\mathrm{mid}}$ in H_1.

If v_1 is a $\mathrm{CFV}_{\mathrm{mid}}$ in H_1, then the result follows. If, on the other hand, v_1 is not a $\mathrm{CFV}_{\mathrm{mid}}$ in H_1, then u is a $\mathrm{CFV}_{\mathrm{mid}}$ in $G - G_1$ and we repeat the same argument used above with $G - G_1$ taking the role of G. This iterative argument is repeated as many times as is necessary to test if there is a component graph H_j for which v_j is a $\mathrm{CFV}_{\mathrm{mid}}$ for $j \in \{2, \ldots, s-2\}$. If there is none, then the coalescence vertex of $H_{s-1} \circ H_s$ is $\mathrm{CFV}_{\mathrm{mid}}$. By Theorems 2.2, 2.5 and 4.1, at least one of the root vertices of H_{s-1} or H_s is a $\mathrm{CFV}_{\mathrm{mid}}$. □

Theorem 4.3. *Let G be a graph with a cut-vertex v and let $G_1, G_2, \ldots, G_s$ be the components of $G - v$. If v is a CV in G, then no v_i is a $\mathrm{CFV_{upp}}$ in $H_i = G_i + v_i$, for $i \in \{1, 2, \ldots, s\}$, and*

(i) *either v_i is a $\mathrm{CFV_{mid}}$ in at least two component graphs H_i for $i \in \{1, 2, \ldots, s\}$;*

(ii) *or v_i is a CV in each of the H_i for $i \in \{1, 2, \ldots, s\}$.*

P r o o f. By Theorem 4.1, Theorem 2.2 and Theorem 2.6, u and v_1 in W_1 can be of the types given in the following two cases:

(i) both u and v_1 are $\mathrm{CFV_{mid}}$ in $G - G_1$ and in H_1, respectively; or

(ii) both u and v_1 are CV in $G - G_1$ and in H_1, respectively.

In case (i), by Theorem 4.2, $G - G_1$ has at least one component G_i, for $i \in \{2, \ldots, s\}$, such that v_i is a $\mathrm{CFV_{mid}}$ in H_i. Thus v_i is a $\mathrm{CFV_{mid}}$ in at least two component graphs.

In case (ii), we consider $G - G_1$ and use the same argument used above with $G - G_1$ taking the role of G. This iterative argument is repeated as follows. If we let $k \in \{2, \ldots, s-1\}$ be the smallest integer (if it exists) such that v_k is not a CV in the component graph H_k, then v_k is a $\mathrm{CFV_{mid}}$. By (i), the coalescence vertex of the coalescence of the remaining component graphs $H_{k+1}, \ldots, H_s$ must also be a $\mathrm{CFV_{mid}}$, and by Theorem 4.2, a root vertex of at least one of the component graphs $H_{k+1}, \ldots, H_s$ is a $\mathrm{CFV_{mid}}$. Thus there are at least two component graphs H_i having a root vertex v_i being a $\mathrm{CFV_{mid}}$. If, on the other hand, there is no k such that the vertex v_k is a $\mathrm{CFV_{mid}}$ in H_k, then each vertex v_i, for $i \in \{2, \ldots, s\}$, is a CV in the component graph H_i. Thus v_i is a CV in all component graphs H_i, for $i \in \{1, 2, \ldots, s\}$, completing the proof. $\square$

Since a vertex can be one of three types, namely CV, $\mathrm{CFV_{upp}}$ and $\mathrm{CFV_{mid}}$, there are 3! different ways of choosing the pairs of root vertices when coalescing two component graphs. Table 1 summarizes the results obtained above. The third column

Type of v_1 in H_1	Type of v_2 in H_2	Type of v in $H_1 \circ H_2$	Reason	$\eta(H_1 \circ H_2)$	Reason
$\mathrm{CFV_{upp}}$	$\mathrm{CFV_{upp}}$	$\mathrm{CFV_{upp}}$	Theorem 2.2	$\eta_1 + \eta_2 + 1$	Proposition 3.3 (i)
$\mathrm{CFV_{upp}}$	$\mathrm{CFV_{mid}}$	$\mathrm{CFV_{upp}}$	Theorem 2.2	$\eta_1 + \eta_2$	Proposition 3.3 (ii)
$\mathrm{CFV_{upp}}$	CV	$\mathrm{CFV_{upp}}$	Theorem 2.2	$\eta_1 + \eta_2 - 1$	Proposition 3.1
CV	CV	CV	Theorem 2.5	$\eta_1 + \eta_2 - 1$	Proposition 3.1
CV	$\mathrm{CFV_{mid}}$	$\mathrm{CFV_{mid}}$	Theorem 2.6	$\eta_1 + \eta_2 - 1$	Proposition 3.1
$\mathrm{CFV_{mid}}$	$\mathrm{CFV_{mid}}$	CV or $\mathrm{CFV_{mid}}$	Theorem 2.7	$\eta_1 + \eta_2 + 1$ or $\eta_1 + \eta_2$	Theorem 2.7

Table 1. The type of the coalescence vertex v and the nullity $\eta(H_1 \circ H_2)$ of the coalescence of two graphs $H_1 = G_1 + v_1$ and $H_2 = G_2 + v_2$ with root vertices v_1 and v_2, respectively.

gives the type of coalescence vertex v in $H_1 \circ H_2$ obtained when identifying the root vertices v_1 and v_2 in $H_1 = G_1 + v_1$ and $H_2 = G_2 + v_2$, respectively. The nullity $\eta(H_1 \circ H_2)$ of the coalescence of H_1 and H_2 in terms of the nullity $\eta(H_1) = \eta_1$ and $\eta(H_2) = \eta_2$ is given in the fifth column, for the distinct pairs of types of root vertices. The appropriate link to the respective result in the previous sections is presented for ease of reference.

Generalizing to cases when the number s of component graphs $H_i = G_i + v_i$ is greater than two and G is obtained by identifying the root vertices v_i in each H_i, for $i \in \{1, 2, \ldots, s\}$, we conclude that

(i) if v_i is a CV in each H_i, then the coalescence vertex v is a CV in G;

(ii) if v_i is a CFV_{upp} in each H_i, then the coalescence vertex v is a CFV_{upp} in G;

(iii) if v_i is a CFV_{mid} in each H_i, then the coalescence vertex v cannot be a CFV_{upp} in G.

Also,

(iv) if v_i is a CFV_{mid} in exactly one H_i and each H_j, for $j \neq i$, have a CV, then the coalescence vertex v is a CFV_{mid} in G;

(v) if v_i is a CFV_{upp} in at least one H_i, then the coalescence vertex v is a CFV_{upp} in G.

References

[1] *M. Andelić, C. M. Da Fonseca, R. Mamede*: On the number of P-vertices of some graphs. Linear Algebra Appl. *434* (2011), 514–525.

[2] *M. Brown, J. W. Kennedy, B. Servatius*: Graph singularity. Graph Theory Notes N. Y. *25* (1993), 23–32.

[3] *L. Collatz, U. Sinogowitz*: Spektren endlicher Grafen. Abh. Math. Semin. Univ. Hamb. *21* (1957), 63–77. (In German.)

[4] *D. Cvetković, M. Doob*: Developments in the theory of graph spectra. Linear Multilinear Algebra *18* (1985), 153–181.

[5] *P. W. Fowler, B. T. Pickup, T. Z. Todorova, M. Borg, I. Sciriha*: Omni-conducting and omni-insulating molecules. J. Chem. Phys. *140* (2014), no. 054115, 12 pages.

[6] *P. W. Fowler, B. T. Pickup, T. Z. Todorova, R. De Los Reyes, I. Sciriha*: Omni-conducting fullerenes. Chem. Phys. Lett. *568/569* (2013), 33–35.

[7] *S. C. Gong, G. H. Xu*: On the nullity of a graph with cut-points. Linear Algebra Appl. *436* (2012), 135–142.

[8] *I. Gutman, I. Sciriha*: Spectral properties of windmills. Graph Theory Notes N. Y. *38* (2000), 20–24.

[9] *I. Gutman, I. Sciriha*: Graphs with maximum singularity. Graph Theory Notes N. Y. *30* (1996), 17–20.

[10] *E. Hückel*: Quantentheoretische Beiträge zum Benzolproblem I. Die Elektronenkonfiguration des Benzols und verwandter Verbindungen. Z. Phys. *70* (1931), 204–286. (In German.)

[11] *C. R. Johnson, B. D. Sutton*: Hermitian matrices, eigenvalue multiplicities, and eigenvector components. SIAM J. Matrix Anal. Appl. *26* (2004), 390–399.

[12] *I.-J. Kim, B. L. Shader*: On Fiedler- and Parter-vertices of acyclic matrices. Linear Algebra Appl. *428* (2008), 2601–2613.

[13] *M. Marcus, H. Minc*: A Survey of Matrix Theory and Matrix Inequalities. Allyn and Bacon, Boston, 1964.

[14] *B. T. Pickup, P. W. Fowler, M. Borg, I. Sciriha*: A new approach to the method of source-sink potentials for molecular conduction. J. Chem. Phys. *143* (2015), #194105, 20 pages.

[15] *A. J. Schwenk*: Computing the characteristic polynomial of a graph (R. A. Bari, F. Harary, eds.). Graphs and Combin., Proc. Capital Conf., Washington, Lect. Notes Math. 406, Springer, Berlin, 1974, pp. 153–172.

[16] *I. Sciriha*: Maximal core size in singular graphs. Ars Math. Contemp. *2* (2009), 217–229.

[17] *I. Sciriha*: Coalesced and embedded nut graphs in singular graphs. Ars Math. Contemp. *1* (2008), 20–31.

[18] *I. Sciriha*: A characterization of singular graphs. Electron. J. Linear Algebra *16* (2007), 451–462.

[19] *I. Sciriha*: On the construction of graphs of nullity one. Discrete Math. *181* (1998), 193–211.

[20] *I. Sciriha*: The characteristic polynomials of windmills with an application to the line graphs of trees. Graph Theory Notes N. Y. *35* (1998), 16–21.

[21] *I. Sciriha, M. Debono, M. Borg, P. W. Fowler, B. T. Pickup*: Interlacing-extremal graphs. Ars Math. Contemp. *6* (2013), 261–278.

[22] *K. R. Sharaf, D. A. Ali*: Nullity and bounds to the nullity of dendrimer graphs. Raf. J. of Comp. & Math's *10* (2013), 71–86.

[23] *S. K. Simić, M. Andelić, C. M. Da Fonseca, D. Živković*: On the multiplicities of eigenvalues of graphs and their vertex deleted subgraphs: old and new results. Electron. J. Linear Algebra (electronic only) *30* (2015), 85–105.

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