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A characterization of singular graphs

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A CHARACTERIZATION OF SINGULAR GRAPHS*

IRENE SCIRIHA†

Abstract. Characterization of singular graphs can be reduced to the non-trivial solutions of a system of linear homogeneous equations $\mathbf{Ax} = \mathbf{0}$ for the 0-1 adjacency matrix $\mathbf{A}$. A graph G is singular of nullity $\eta(G) \geq 1$, if the dimension of the nullspace $\ker(\mathbf{A})$ of its adjacency matrix $\mathbf{A}$ is $\eta(G)$. Necessary and sufficient conditions are determined for a graph to be singular in terms of admissible induced subgraphs.

Key words. Adjacency matrix, Eigenvalues, Singular graphs, Core, Periphery, Singular configuration, Minimal configuration.

AMS subject classifications. 05C50, 05C60, 05B20.

1. Introduction. A system of linear homogeneous equations $\mathbf{Ax} = \mathbf{0}$ yields non-trivial solutions $\mathbf{x} \neq \mathbf{0}$ when the linear transformation $\mathbf{A}$ is not invertible. Such a matrix $\mathbf{A}$ is said to be singular. The solutions have many direct applications, for instance, to networks in computer science and electrical circuits, to financial models in economics, to biological models in genetics and bioinformatics as well as to the understanding of non-bonding orbitals in carbon unsaturated molecules [2, 11, 14].

Once $\mathbf{A}$ is determined for a particular model, the eigenvectors $\mathbf{x}$ satisfying $\mathbf{Ax} = \lambda\mathbf{x}$ for the eigenvalue $\lambda = 0$ in the spectrum (or set of eigenvalues $\{\lambda\}$) of $\mathbf{A}$ are easily calculated. A more challenging problem, and one which we discuss in this paper, is to determine the properties of the possible linear transformations $\mathbf{A}$ that satisfy $\mathbf{Ax} = \mathbf{0}$ for a feasible non-zero $\mathbf{x}$.

A graph $G(\mathcal{V}, \mathcal{E})$ having a vertex set $\mathcal{V}(G) = \{1, 2, \ldots, n\}$ and a set $\mathcal{E}$ of $m(G)$ edges, joining distinct pairs of vertices, is said to be of order $n(G)(= n)$ and size $m(G)(= m)$. The complete graph, the empty graph (with no edges), the cycle and the path on n vertices are denoted by K_n, $\overline{K_n}$, C_n and P_n respectively. The linear transformation we choose to encode the structure of a graph G, up to isomorphism, is the $n \times n$ adjacency matrix $\mathbf{A}(G)(= \mathbf{A})$ of G. The (i, j)th entry, a_{ij}, of $\mathbf{A}$ is one if ij is an edge and zero otherwise. Since $\mathbf{A}$ is a 0-1 (real and symmetric) matrix, the $feasible$ non-zero vectors $\mathbf{x}$ that satisfy

$$\mathbf{Ax} = \mathbf{0}, \tag{1.1}$$

lie in $\ker(\mathbf{A})$ and can be *standardized* to have integer entries with *g.c.d.* equal to 1 and the first non-zero entry positive. Because $\mathbf{x} \in \ker(\mathbf{A})$, it is referred to as a **kernel eigenvector**.

Since different labelings of the vertices of G yield similar matrices and hence an invariant spectrum, we use terminology for a graph G and its adjacency matrix (denoted by $\mathbf{A}$ or $\mathbf{G}$) interchangeably. A graph with the eigenvalue zero, of multiplicity

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$\eta \geq 1$, in the spectrum, is said to be **singular** of nullity (or co-rank) η. Equivalently, a graph G is singular if there exists a non-zero vector $\mathbf{x}$ such that $\mathbf{A}\mathbf{x} = \mathbf{0}$.

A useful result for real symmetric matrices, applied to $\mathbf{A}(G)$, is the Interlacing Theorem (see e.g. [3], p. 314).

THEOREM 1.1. *If G is an n-vertex graph with eigenvalues $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n$ and H is a vertex–deleted subgraph of G with eigenvalues $\mu_1 \leq \mu_2 \leq \ldots \leq \mu_{n-1}$, then $\lambda_i \leq \mu_i \leq \lambda_{i+1}$, $i = 1, 2, \ldots, n-1$.*

This means that the multiplicity of an eigenvalue can change by at most one with the addition or deletion of a vertex to a graph.

The problem of characterizing singular graphs is proving to be hard. The structure of certain classes of singular graphs has been studied for the last sixty years, not only as an interesting problem in mathematics but also in connection with non-bonding molecular orbitals in chemistry, coding theory and more recently in networks; see for instance [2, 4, 5, 6, 7, 8, 9, 10, 12, 13].

In searching for the substructures that are found in singular graphs, we found it effective to define a singular configuration (SC) as a singular graph of nullity one with a minimal number of vertices and its spanning minimal configuration (MC). In Section 2, we describe the construction of a SC, built from a core graph by adding a periphery. The concept of a minimal basis, explained in Section 3, is utilized in the following section to establish necessary and sufficient conditions for a graph G to be singular. We present, in Section 5, an algorithm that determines singularity, while constructing SCs sharing a common core in G.

2. Structure. Equation (1.1) is the key to discover why a graph is singular. We identify graphs of nullity one, so that substructures corresponding to linearly independent kernel eigenvectors do not *mask* one another. If $\mathbf{A}$ has nullity one, then the standardized $\mathbf{x}$ is said to be *the kernel eigenvector* of G.

For a graph of nullity one, we label G so that the kernel eigenvector $\mathbf{x}$ is of the form $\begin{bmatrix} \mathbf{x}_F \\ 0 \end{bmatrix}$, where only the top r entries of $\mathbf{x}$, forming $\mathbf{x}_F$, are non-zero. We call $\mathbf{x}_F$ the *non-zero part* of $\mathbf{x}$ and the subgraph F of G induced by the r vertices corresponding to $\mathbf{x}_F$, the **core** of G. Figure 2.1 shows two graphs, of nullity one, with the same non-zero part $\mathbf{x}_F$ of $\mathbf{x}$ but different cores.

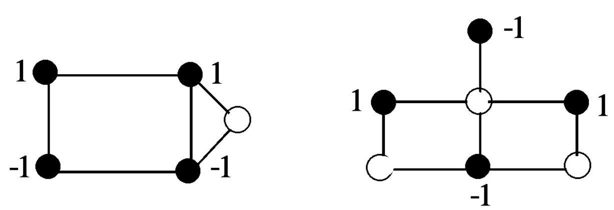

FIG. 2.1. *Two* MC*s with the same feasible non-zero part $(1, 1, -1, -1)^t$ of the kernel eigenvector.*

The set of remaining vertices, $\mathcal{V}(G)\backslash\mathcal{V}(F)$, is said to be the **periphery** $\mathcal{P}$ (with respect to $(F, \mathbf{x}_F)$). Note that if G has nullity one, then the core F and the periphery

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$\mathcal{P}$ are unique.

This prompts us to ask whether there exist graphs where $\mathbf{x} = \mathbf{x}_F$. Indeed such graphs exist and we call them core graphs. A singular graph, on at least two vertices, with a kernel eigenvector having no zero entries, is said to be a **core graph**. The core graphs of nullity one, are called **nut graphs**; the smallest one is of order 7 and size 8 [4]. Note that whereas a core of G is a subgraph associated with a kernel eigenvector of G, a core graph F is itself a core of F.

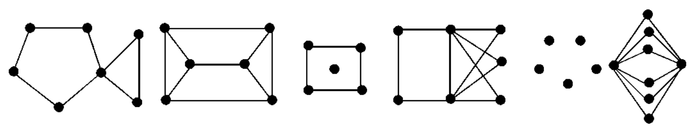

Fig. 2.2. *Core Graphs.*

Examples of six core graphs in order of increasing nullity, $\eta = 1, 2, \ldots, 6$, are shown in Figure 2.2. For molecular graphs in chemistry, where the vertices represent carbon (C) atoms while the edges represent the C-C sigma bonds, core graphs have a special significance. A radical with the C-structure of a core graph has the π electronic charge (proportional to the square of the kernel eigenvector entry associated with a C center) occupying the non-bonding orbitals (for $\lambda = 0$), distributed all over the carbon centers, and therefore would have markedly different reactivity from the more usual type of radical, where the electron density vanishes at some sites.

2.1. Minimal configurations. The underlying idea, that leads to Definition 2.1 of a MC, is its construction. If, in line with the Interlacing Theorem, to a core graph $(F, \mathbf{x}_F)$ of nullity $\eta(F) \geq 1$, $\eta(F) - 1$ independent vertices (forming the periphery), incident only to vertices of F, can be added, reducing the nullity by one with each vertex addition, then the graph N obtained has nullity one. If we also insist on the condition that $\mathbf{x}_F$ remains the non-zero part of the kernel eigenvector of N, then N is a singular graph of nullity one with a minimal number of vertices and edges, having $\mathbf{x}_F$ as the non-zero part of the kernel eigenvector. Figure 2.3 shows three core graphs. The MCs grown from the first two, of order four, have a non-empty periphery; the last core graph, of order seven, is a nut graph and hence also a MC.

Definition 2.1. Let F be a core graph on at least two vertices, with nullity $s \geq 1$ and a kernel eigenvector $\mathbf{x}_F$ having no zero entries. If a graph N, of nullity one, having $\mathbf{x}_F$ as the non-zero part of the kernel eigenvector, is obtained, by adding $s - 1$ independent vertices, whose neighbors are vertices of F, then N is said to be a **minimal configuration** (MC).

Remark 2.2. The allusion to minimality refers to the number of peripheral vertices required to reduce the nullity from $\eta(F)$ to one, in the construction of N, as well as to the number of edges for N to have core $(F, \mathbf{x}_F)$. The necessary and sufficient conditions in the following theorem are often taken as the definition of MC [5, 9].

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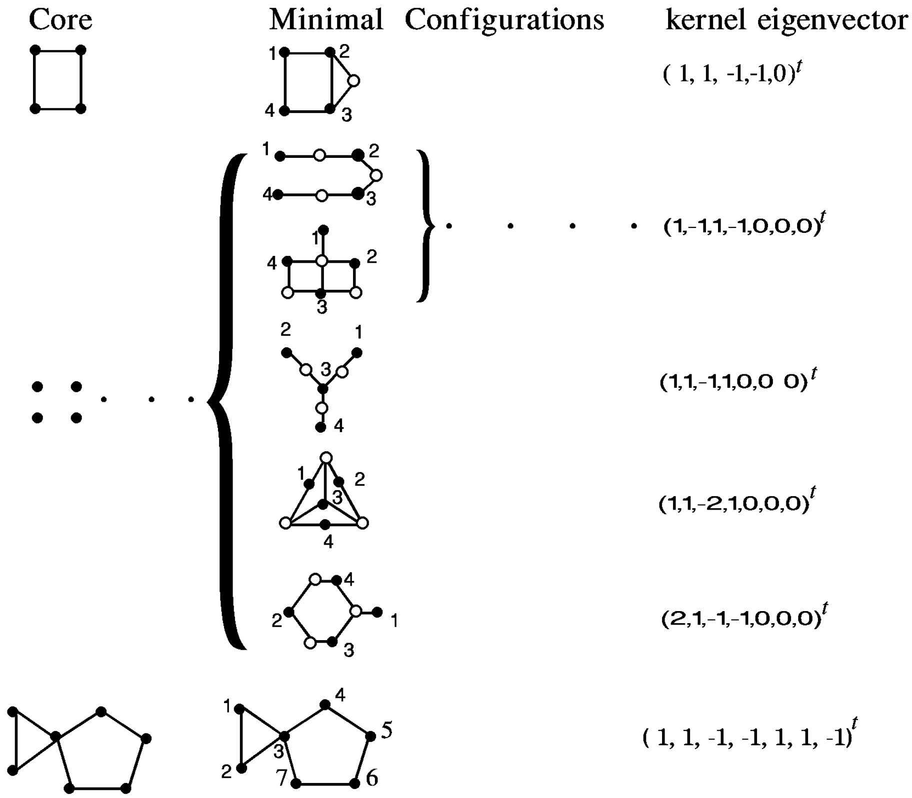

FIG. 2.3. *Cores and MCs 'grown' from them.*

THEOREM 2.3. [9] *Let N be a singular graph of order $n \geq 3$. The graph N is a MC having a core $(F, \mathbf{x}_F)$ and periphery $\mathcal{P} := \mathcal{V}(N) - \mathcal{V}(F)$ if and only if the following conditions are all satisfied:*

(i) $\eta(N) = 1$,

(ii) $\mathcal{P} = \emptyset$ *or* $\mathcal{P}$ *induces a graph consisting of isolated vertices,*

(iii) $\eta(F) = |\mathcal{P}| + 1$.

REMARK 2.4. A MC is connected [9]. In a MC N, a vertex of $\mathcal{P}$ is joined to core-vertices only, N is said to be *extended* from F and the vertex degree of $v \in \mathcal{P}$ is at least two [5]. Note that if $\eta(G) = 1$, then $\mathbf{x_F}$ is uniquely determined (up to a multiplicative constant) and therefore G has a unique core F and a unique periphery $\mathcal{P}$.

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2.2. Singular configurations. For a MC N, if the vertices of F are labeled first, followed by those of $\mathcal{P}$, then for $\mathbf{x} = \begin{bmatrix} \mathbf{x}_F \\ \mathbf{0} \end{bmatrix}$, $\mathbf{N}\mathbf{x} = \mathbf{0}$. The periphery, $\mathcal{P}$, is a set of independent vertices whose defining vectors, given by the last $s-1$ columns of N, determine the edges joining $\mathcal{P}$ to the core vertices. Note that if edges are added joining some or all of the distinct pairs of vertices in $\mathcal{P}$, then the graph, S, produced still satisfies $\mathbf{S} \begin{bmatrix} \mathbf{x}_F \\ \mathbf{0} \end{bmatrix} = \mathbf{0}$.

Definition 2.5. A MC, N, and all such graphs, S, are said to be **singular configurations** (SCs) with underlying spanning MC N.

Proposition 2.6. *A* SC *has nullity one.*

Proof. Let S be a SC with spanning MC N. We note first that the kernel eigenvector of N is also a kernel eigenvector of S.

If $\mathbf{S} = \begin{bmatrix} \mathbf{F} & \mathbf{B}^t \\ \mathbf{B} & \mathbf{P} \end{bmatrix}$, where $\mathbf{F}$ is $r \times r$ and $\mathbf{P}$ is $(n-r)\times(n-r)$, then the spanning MC $\mathbf{N} = \begin{bmatrix} \mathbf{F} & \mathbf{B}^t \\ \mathbf{B} & \mathbf{0} \end{bmatrix}$. Since $\mathbf{P}$ corresponds to the zero part of $\mathbf{x}$, the kernel eigenvector $\mathbf{x} = \begin{bmatrix} \mathbf{x}_F \\ \mathbf{0} \end{bmatrix}$ of N also satisfies $\mathbf{S}\mathbf{x} = \mathbf{0}$.

There remains to show that S does not have a kernel eigenvector linearly independent of $\mathbf{x}$. Indeed, with each addition of a column of $\mathbf{B}^t$ to $\mathbf{F}$, the nullity reduces successively by one. Therefore, there are no linear combinations involving the columns of $\mathbf{B}^t$ that contribute to $\ker([\mathbf{F} \;\; \mathbf{B}^t])$. Since the first r columns of $\mathbf{S}$ and $\mathbf{N}$ are the same, the only non-zero entries in a kernel eigenvector of S correspond to the vertices of F. Thus S and N share the same unique kernel eigenvector. ∎

The number of SCs with a particular underlying MC, N, is finite and equal to the number of distinct possible ways edges can be inserted joining distinct pairs of vertices of the periphery of N.

Lemma 2.7. *Let N be a* MC *with periphery $\mathcal{P}$. There exist 2^k* SC*s having the* MC*, N, as a spanning subgraph, where k is $\begin{bmatrix} |\mathcal{P}| \\ 2 \end{bmatrix}$.*

3. Minimal basis. Let $\mathrm{wt}(\mathbf{u})$ denote the weight (that is the number of non-zero entries) of the vector $\mathbf{u} \in \mathbb{R}^n$. If $\mathbf{u_1}, \mathbf{u_2}, \ldots, \mathbf{u}_\eta$ are the vectors in a basis for the nullspace $\ker(\mathbf{A})$ of a $n \times n$ real matrix $\mathbf{A}$, in non-decreasing weight order, such that $\sum_{i=1}^{\eta} \mathrm{wt}(\mathbf{u}_i)$ is a minimum, then the basis is said to be a minimal basis denoted by B_{min}. Although various B_{min} may be possible, the weight sequence $\{\mathrm{wt}(\mathbf{u}_1), \mathrm{wt}(\mathbf{u}_2), \ldots, \mathrm{wt}(\mathbf{u}_\eta)\}$ is an invariant for $\ker(\mathbf{A})$. Moreover for any basis $B = \{\mathbf{w_1}, \mathbf{w_2}, \ldots, \mathbf{w}_\eta\}$, $\mathrm{wt}(\mathbf{u}_i) \le \mathrm{wt}(\mathbf{w}_i)$ [7].

A basis B for the nullspace can be transformed into another basis B' by linear combinations of the vectors of B. However the union of the collections of the positions of the non-zero entries in the basis vectors is the same for all bases. Thus, if $\mathbf{A}$ is the adjacency matrix of a singular graph, the partition of the vertices into core vertices and core-forbidden vertices is independent of the basis used for the nullspace. Also, the B_{min}-vectors define a fundamental system of cores in G.

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Proposition 3.1. *For all possible bases of the nullspace, the set* CV *of core vertices is an invariant of a graph* G*. The core-forbidden vertices,* $\mathcal{V}(G)\backslash\mathrm{CV}$*, are also an invariant of* G*.*

Remark 3.2. The same result holds for the set of vertices corresponding to the non-zero entries of the vectors in the bases for any eigenspace of G.

This method of constructing MCs by adding a periphery to a core, using the concept that the entries of a kernel eigenvector, corresponding to the periphery, are forced to be zero, was introduced in [5]. A similar idea was also employed in [1], to bound the co-rank of a real symmetric matrix from above.

4. SCs are subgraphs of singular graphs. Henceforth a singular graph without isolated vertices will be denoted by H. We show, in Proposition 4.3, that a singular graph of nullity η necessarily has η SCs as induced subgraphs and therefore the spanning MCs as subgraphs.

Proposition 4.1. *If the core* $(F, \mathbf{x}_F)$ *of* H*, corresponding to* $\mathbf{x} = \begin{bmatrix} \mathbf{x}_F \\ \mathbf{0} \end{bmatrix}$ *in a minimal basis* B_{min} *for the nullspace* $\ker(\mathbf{A})$ *of* $\mathbf{A}(H)$*, is not itself a* SC*, then there is a* SC*, which is a vertex-induced subgraph of* H*, having* $\mathbf{x}_F$ *as the non-zero part of its kernel eigenvector.*

Proof. If the core $(F, \mathbf{x}_F)$ has core-order r, then the first r rows of $\mathbf{A}(H)$ may be partitioned as $[\mathbf{F}|\mathbf{C}]$ and $[\mathbf{F}|\mathbf{C}]^t\mathbf{x_F} = 0$. Moreover the rank of $[\mathbf{F}|\mathbf{C}]$ is $r-1$; otherwise $\mathbf{x}$ in B_{min} is equivalent to the linear combination of at least two linearly independent vectors in the nullspace of $\mathbf{A}(H)$, each of which has a smaller weight than $\mathbf{x}$. This would mean that $\mathbf{x}$ can be reduced, (using linear combinations with other eigenvectors of B_{min}) to another eigenvector of smaller weight that can replace $\mathbf{x}$ in B_{min} to produce another basis B' for $\ker(\mathbf{A})$, lexicographically before B_{min}, a contradiction. If F is not itself a minimal configuration, its nullity μ is more than one. Since row rank and column rank of $(\mathbf{A}(F)|\mathbf{C})$ are equal, there exist $\mu - 1$ column vectors of the associated matrix $\mathbf{C}$ which are linearly independent and form the matrix $\mathbf{C}'$, say, such that $\mathbf{A}' = \left[\begin{array}{c|c} \mathbf{F} & \mathbf{C}' \\ \hline (\mathbf{C}')^{\mathbf{t}} & \mathbf{P} \end{array}\right]$, is a submatrix of $\mathbf{A}(H)$ and defines the SC, S, grown from F. The submatrix $\mathbf{P}$ of $\mathbf{A}$ corresponds to the entries of $\mathbf{A}$ intersecting in the columns of $\mathbf{C}'$ and the rows of $(\mathbf{C}')^{\mathbf{t}}$. Note that the nullity of $\mathbf{A}'$ is one and the MC spanning S has $\mathbf{P} = \mathbf{0}$. If F is itself a MC, then $\mathbf{C}' = \mathbf{0}$ and $\mathcal{P}(F) = \emptyset$; otherwise the successive deletions of the vertices of $\mathcal{P}(S)$, which therefore correspond to the columns of $\mathbf{C}'$, increase the nullity of $\mathbf{A}'$ by one, with each deletion. Thus $\eta(F) = |\mathcal{P}(N)| + 1$. Noting that S is an induced subgraph of H, completes the proof. ∎

Remark 4.2. Since each vector in B_{min} corresponds to a unique core and the choice of $\mathbf{x}$ in B_{min} is arbitrary, we have proved the following result on the structure of singular graphs:

Proposition 4.3. *Let* H *be a singular graph of nullity* η*. There exist* η SC*s as induced subgraphs of* H *whose core-vertices are associated with the non-zero entries of the* η *distinct vectors in a minimal basis of the nullspace of* $\mathbf{A}(H)$*.*

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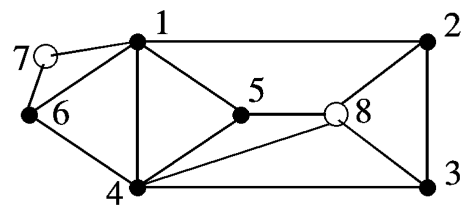

FIG. 4.1. *MCs are subgraphs of a singular graph.*

EXAMPLE 4.4. An example of a singular graph, of nullity one, is shown in Figure 4.1. The core of the graph G, consists of the six black vertices, that induce the core, $G-7-8$, in G. Although G has nullity one, it is not minimal, since the non-isomorphic graphs $G-7$ and $G-8$ are also of nullity one and have the same core as G. These two distinct subgraphs of G satisfy the conditions of Theorem 2.3 and are therefore MCs. Moreover, G has a kernel eigenvector equal to $(1, 1, -1, -1, 1, -1, 0, 0)$ and the vertices 7 and 8, in the periphery, are core-forbidden vertices since they do not lie on any core. For other examples of singular graphs of nullity one where the subgraphs that are possible MCs are neither isomorphic, nor co-spectral, see [11].

REMARK 4.5. The need to use B_{min} as a basis becomes clear when one considers a core graph. For instance, the core graph $C_{4k},\ k \geq 1$, has a kernel eigenvector which is a linear combination of its two B_{min}–vectors but does not have an extension to a MC within C_{4k} itself.

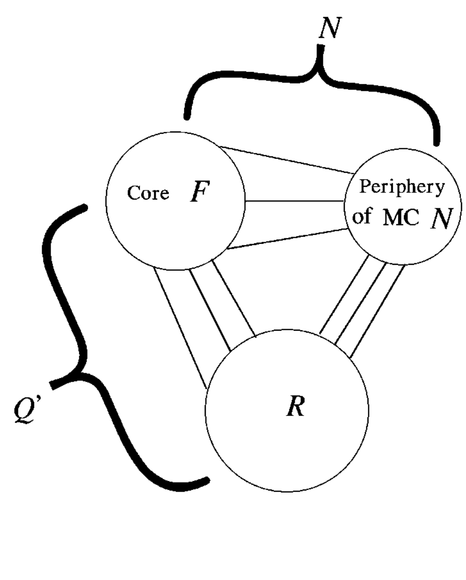

FIG. 4.2. *An edge-decomposition of a singular graph.*

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4.1. Necessary and sufficient conditions for singularity. We have shown that SCs are admissible induced subgraphs of a singular graph G. Indeed, the η SCs (with spanning MCs) corresponding to B_{min} may be thought of as the 'atoms' of G. The graph G may be compared to a 'molecule'. Carrying the analogy to chemical molecular structure further, we may compare the core of a SC to the 'nucleus of the atom' and the periphery to the 'orbiting electrons'. But if η SCs with distinct cores are induced subgraphs of G, is G singular of nullity η? Since the SC P_3 is a subgraph of triangle-free non-singular connected graphs of order three or higher, it is clear that this condition is not sufficient and additional constraints are required.

LEMMA 4.6. *Let S be a* SC *having core F of core-order p and $\mathbf{u} = (\mathbf{x_F}, 0, \ldots, 0)$ be the kernel eigenvector of S (with each of the p entries of $\mathbf{x_F}$ being non-zero). Let S be a subgraph of a graph G, labeled such that the first p rows of $\mathbf{A}(G)$ are $\mathbf{Y} = \left[\begin{array}{c|c|c} \mathbf{A}(F) & \mathbf{C'} & \mathbf{Q} \end{array}\right]$ where $\left[\begin{array}{c|c} \mathbf{A}(F) & \mathbf{C'} \end{array}\right]$ are the first p rows of $\mathbf{A}(S)$. If $\mathbf{x_F} \in (colsp(\mathbf{Q}))^{\perp}$, then G is singular with core F.*

Proof. For the r-vertex SC S, $\mathbf{A}(S) = \left[\begin{array}{c|c} \mathbf{A}(F) & \mathbf{C'} \\ \hline (\mathbf{C'})^{\mathbf{t}} & \mathbf{P} \end{array}\right]$, where $\mathbf{P}$ is the $(r-p)\times(r-p)$ adjacency matrix of the subgraph, induced by $\mathcal{P}$ and where $\mathbf{C'}$, describes the edges between the vertices of the periphery and those of the core. Recall that $\mathbf{A}(S)\mathbf{u} = \mathbf{0}$. Also the first p rows of $\mathbf{A}(G)$ are $\mathbf{Y} = \left[\begin{array}{c|c|c} \mathbf{A}(F) & \mathbf{C'} & \mathbf{Q} \end{array}\right]$, so that the non-zero entries of $\mathbf{Q}$ describe the edges between F and $R = G - \mathcal{V}(S)$ as shown in Figure 4.2. Using the premise $\mathbf{Q^t x_F} = \mathbf{0}$, it follows that $\mathbf{Y^t x_F} = \mathbf{0}$. Thus $\mathbf{A}(G)\begin{bmatrix} \mathbf{x_F} \\ 0 \\ \vdots \\ 0 \end{bmatrix} = 0$ and the result follows. ∎

REMARK 4.7. Whereas Lemma 4.6 may be considered as a characterization of singular graphs using an algebraic test for singular graphs, the following result is a geometrical criterion for a graph to be singular.

PROPOSITION 4.8. *If the* SC *S with core $(F, \mathbf{x}_F)$ and periphery $\mathcal{P}$ is a subgraph of a graph G and the graph $G - \mathcal{P}$, obtained from G by deleting the vertices in $\mathcal{P}$, is also singular with core $(F, \mathbf{x}_F)$, then G is singular with a core $(F, \mathbf{x}_F)$.*

Proof. Let the core-order of S be r. If

$$\mathbf{A}(S) = \left[\begin{array}{c|c} \mathbf{A}(F) & \mathbf{C'} \\ \hline (\mathbf{C'})^{\mathbf{t}} & \mathbf{0} \end{array}\right],$$ and the first p rows of $\mathbf{A}(G)$ are $\mathbf{Y} = \left[\begin{array}{c|c|c} \mathbf{A}(F) & \mathbf{C'} & \mathbf{Q} \end{array}\right]$, then for the same lexicographic ordering of the vertices, $\left[\begin{array}{cc} \mathbf{A}(F) & \mathbf{Q} \end{array}\right]$ are the first p rows of $G-\mathcal{P}$. Since $(F, \mathbf{x}_F)$ is a core of $G-\mathcal{P}$, it follows

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that $\mathbf{Q^t x_F} = \mathbf{0}$. Thus, $\mathbf{Y^t x_F} = \mathbf{0}$, so that $(\mathbf{x}_F, \mathbf{0})$ is a kernel eigenvector of G. □

We have established a geometrical test which may be considered as a characterization of singular graphs.

Proposition 4.9. *A graph G is singular if and only if the following conditions are both satisfied:*
(i) there exists a subgraph of G which is a SC*, S, with core $(F, \mathbf{x}_F)$ and periphery $\mathcal{P} = \mathcal{V}(S) \backslash \mathcal{V}(F)$;*
(ii) the subgraph $G - \mathcal{P}$ is also singular with the same core $(F, \mathbf{x}_F)$.

5. Algorithm. Proposition 4.9 can be utilized iteratively to determine the induced SCs for a particular core $(F, \mathbf{x}_F)$ in a singular graph G $(= G_0)$, perhaps with the use of catalogues of MCs. Lists of the MCs with cores of order less than 6 are found in [5] while in [7], MCs for selected cores of order 6 and 7 are given.

Algorithm:-to determine whether a graph G is singular

-to output SCs with common core $(F, \mathbf{x}_F)$
and disjoint peripheries.

Step 1: Select an induced SC, S_i, with core $(F, \mathbf{x}_F)$
and with a partition $\mathcal{V}(F)\dot{\cup}\mathcal{P}_i$ of its vertices, in G_{i-1},
labelling the vertices of F first.
Step 2: Obtain G_i by deleting $\mathcal{P}_i$ from G_{i-1}.

Step 3: Increment i and repeat steps 1 and 2
until no SCs with core $(F, \mathbf{x}_F)$ remain.

Step4: Output $\mathcal{S} := \{S_i\}$. If $\mathcal{S} \neq \emptyset$, then
(i) G has the set $\mathcal{S}$ of SCs with core $(F, \mathbf{x}_F)$;
(ii) and G is singular with a kernel eigenvector $(\mathbf{x}_F, \mathbf{0})$.

For a large $|\mathcal{P}|$, it becomes easier to notice a SC in the successively smaller $G - \mathcal{P}$, so that implementation of the algorithm becomes progressively less complex. This routine can be repeated for other cores in G.

We conclude with some examples.

Example 5.1. The graph G in Figure 5.1 has nullity two with 6 as a core-forbidden vertex. The kernel eigenvectors $\mathbf{x_1} = (2, 1, -2, -1, 1, 0, 0, 0)^t$ and $\mathbf{x_2} = (-1, -1, 1, 0, 0, 0, -1, 1)^t$ in a minimal basis for the nullspace correspond to the MCs $G - 8$ and $G - 5$ respectively. Note that the non-isomorphic MCs $G - 7$ and $G - 8$ have a kernel eigenvector with the same feasible non-zero part as $\mathbf{x_1}$. Also the non-isomorphic MCs $G - 4$ and $G - 5$ have a kernel eigenvector with the same feasible non-zero part as $\mathbf{x_2}$.

Let us test the graph G of Figure 5.1, for singularity using first the algebraic approach of Lemma 4.6 and secondly the geometrical approach of Proposition 4.8.

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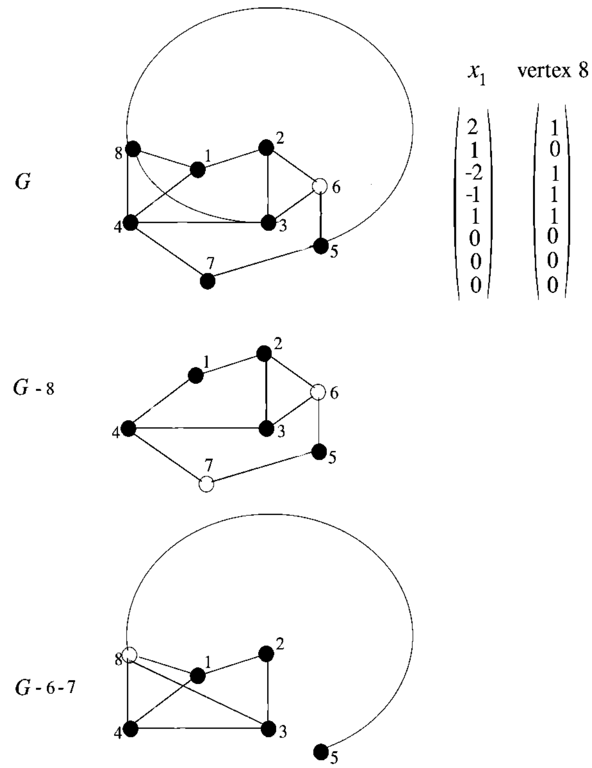

FIG. 5.1. *The singular graph G.*

We recognize (perhaps by using the catalogue in [5]) that $G-8$ is a MC with kernel eigenvector $(2,1,-2,-1,1,0,0)^t$, which is $\mathbf{x_1}$ restricted to $G-8$. Vertex 8 is adjacent to 1, 3, 4 and 5, so that it has a defining vector $v_8 = (1,0,1,1,1,0,0,0)^t$. Since $v_8 \in \mathbf{x_1}^{\perp}$, G is singular with kernel eigenvector $\mathbf{x_1}$, thus completing the algebraic test.

On the other hand, for the geometric test, we identify the MC $G-8$ and delete its periphery $\{6,7\}$ from G. The subgraph $L := G-6-7$ of G, obtained, is singular with core $(F, \mathbf{x_1})$ as required. Indeed L has nullity two, with two linearly independent kernel eigenvectors, whose linear combination gives $\mathbf{x_1}$. A fundamental system of cores for L corresponds to MCs P_3 and P_5 with core-vertices $\{1,3\}$ and $\{2,4,5\}$ respectively.

EXAMPLE 5.2. Let us now apply the same tests to C_6. The 5-vertex path P_5 is a MC with core $(F, \mathbf{x}_F) = (\overline{K_3}, (1,-1,1)^t)$ and is an induced subgraph of the non-singular graph C_6.

For a labeling of the vertices of C_6 in cyclic order, vertex 6 is adjacent to 1 and 5, so that it has a defining vector $v_6 = (1,0,0,0,1,0)^t$. The kernel eigenvector of P_5 is $(1,0,-1,0,1)^t$. If C_6 were to be singular and share the same non-zero part of the kernel

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eigenvector as P_5, then a kernel eigenvector of C_6 would be $\mathbf{y} = (1, 0, -1, 0, 1, 0)^t$. Since $v_6 \notin \mathbf{y}^\perp$, C_6 is not singular with core $(F, \mathbf{x}_F)$. Note that the periphery of P_5 consists of vertices 2 and 4. When these are deleted, the remaining subgraph is $P_3\dot{\cup}K_1$, which does not have a core $(F, \mathbf{x}_F)$. We deduce that C_6 does not have core $(F, \mathbf{x}_F)$.

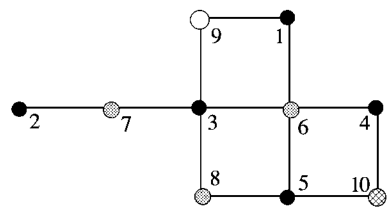

Fig. 5.2. *Two SCs with core $\overline{K_5}$ and overlapping peripheries.*

Example 5.3. The connected graph H in Figure 5.2 has nullity two. The induced subgraphs $N_1 = H - 9$ and $N_2 = H - 10$ are MCs with the same core $(F, \mathbf{x}_F) = (\overline{K_5}, (1, 1, -1, -1, 1)^t)$. Removing the periphery $\{6, 7, 8, 10\}$ of N_1 from H leaves $P_3\dot{\cup}3K_1$ which has core $(F, \mathbf{x}_F)$. Similarly for N_2 which has periphery $\{6, 7, 8, 9\}$. Thus H has two induced SCs, N_1 and N_2, with core $(F, \mathbf{x}_F)$ but in this case, the peripheries are not disjoint. Note that isolated vertices in a core admit any real values as corresponding entries in a kernel eigenvector.

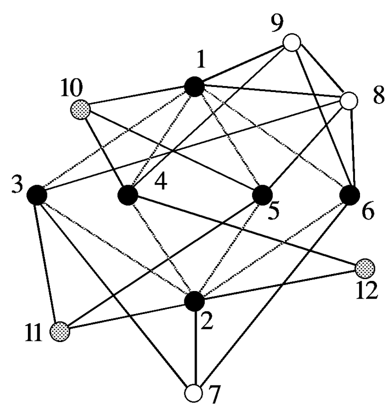

Fig. 5.3. *Two SCs with the same core $K_{2,4}$ and disjoint peripheries.*

Example 5.4. For the connected graph K in Figure 5.3, we apply the above algorithm for a selected core corresponding to a B_{min}-vector. The nullity of K is one. The subgraph $S = K - \{10, 11, 12\}$ is a SC. Its core $(F, \mathbf{x}_F) = (K_{2,4}, (-1, 1, -3, -1, 2, 2)^t)$ induced by the set $\{1, 2, 3, 4, 5, 6\}$ of vertices, has nullity four. Removing the periphery $\mathcal{P}_1 = \{7, 8, 9\}$ of S from K, leaves L, which is a MC with core $(F, \mathbf{x}_F)$

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and periphery $\mathcal{P}_2 = \{10, 11, 12\}$. The algorithm outputs the two SCs of K with core $(F, \mathbf{x}_F)$ and disjoint peripheries $\mathcal{P}_1$ and $\mathcal{P}_2$.

6. Conclusion. We have seen that SCs are the essential elements of singular graphs. Lemma 4.6 tells us that the presence of a SC S with core $(F, \mathbf{x}_F)$ as an induced subgraph must be complemented by another condition on the edges between F and the vertices of the graph not belonging to S, to ensure that the graph is singular with core $(F, \mathbf{x}_F)$. Furthermore, Proposition 4.9 provides a geometrical characterization of singular graphs in terms of admissible induced subgraphs. Having identified a SC with spanning MC N (having core $(F, \mathbf{x}_F)$ and periphery $\mathcal{P} := \mathcal{V}_N \backslash \mathcal{V}_F$) as an induced subgraph of a given graph G, testing the smaller graph $G - \mathcal{P}$ not only determines whether G is singular or otherwise, but also constructs other induced SCs with core $(F, \mathbf{x}_F)$.

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