Necessary and Sufficient Conditions for a Hamiltonian Graph

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Dedicated to the memory of Ralph Stanton

Abstract

A graph is singular if the zero eigenvalue is in the spectrum of its 0-1 adjacency matrix **A**. If an eigenvector belonging to the zero eigenspace of **A** has no zero entries, then the singular graph is said to be a core graph. A (κ, τ)-regular set is a subset of the vertices inducing a κ-regular subgraph such that every vertex not in the subset has τ neighbours in it. We consider the case when $\kappa = \tau$ which relates to the eigenvalue zero under certain conditions. We show that if a regular graph has a (κ, κ)-regular set, then it is a core graph. By considering the walk matrix we develop an algorithm to extract (κ, κ)-regular sets and formulate a necessary and sufficient condition for a graph to be Hamiltonian.

1 Introduction

A graph $G = G(\mathcal{V}, \mathcal{E})$ of order n has an n-vertex set $\mathcal{V} = \{1, 2, ..., n\}$ and a set $\mathcal{E}$ of m edges consisting of pairs of vertices. The graphs we consider are

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simple, without loops or multiple edges.

A *subdivision* of a graph G, denoted by G^*, is the graph obtained from G by inserting a vertex in each edge of G. A subdivision produces a bipartite graph with the inserted vertices in one part, and the original vertices of G in the other part. Figure 1 shows the inserted vertices as 'x' in the subdivision G^* of the graph G. Unless a Hamiltonian graph is a cycle, its subdivision loses the property of Hamiltonicity.

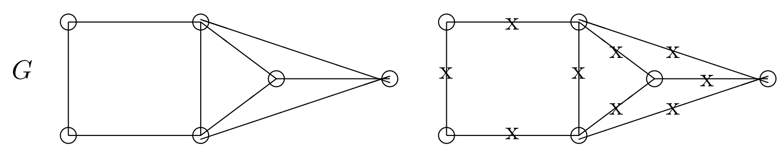

Figure 1: Subdivision G^* of the graph G

We use terminology for a graph G and its adjacency matrix $\mathbf{A}(G)$ (or simply $\mathbf{A}$) interchangeably , since G is determined, up to isomorphism, by $\mathbf{A}$ [13]. The ijth entry a_{ij} of the symmetric matrix $\mathbf{A}$ is 1 if $ij \in \mathcal{E}$ and 0 otherwise.

A graph G is said to be *singular* of nullity η if the dimension of the nullspace $\ker(\mathbf{A})$ of $\mathbf{A}$ is η. The non-zero vectors, $\mathbf{x} \in \mathbb{R}^n$, in the nullspace, termed *kernel eigenvectors* of G, satisfy $\mathbf{Ax} = \mathbf{0}$. We note that the multiplicity of the eigenvalue zero is η. If there exists a kernel eigenvector of G with no zero entries, then G is said to be a *core graph*[12]. The graph G_6 shown in Figure 2 is a core graph of nullity two with a kernel eigenvector $(1, 1, 1, 1, -2, -2)$.

The entry $a_{ij}^{(k)}$ of the symmetric matrix $\mathbf{A}^k$ is the number of walks of length k, starting from i to j. If $\mathbf{j}$ is the all-one $(n\times 1)$ vector, then the ith entry of the $(n\times 1)$ vector $\mathbf{A}^k\mathbf{j}$ is the the number of walks of length k from the vertex labelled i. The $n\times k$ matrix whose k columns are $\mathbf{A}^i\mathbf{j}$ for $i = 0, 1, 2, \ldots, k-1$ is denoted by $\mathbf{W}_k$.

The eigenvalues $\mu_1, \mu_2, ..., \mu_p$, $1 \leq p \leq n$, which have an associated eigenvector *not* orthogonal to $\mathbf{j}$ are said to be *main*. We denote the remaining distinct eigenvalues by $\mu_{p+1}, \ldots, \mu_s$, $s \leq n$, and refer to them as *non-main*. Walks and main eigenvalues are closely related. For $k \geq p$, the rank of $\mathbf{W}_k$ is the number p of main eigenvalues [8]. In section 2, we note that there exists an orthonormal basis for $\mathbb{R}^n$ consisting of eigenvectors of $\mathbf{A}$, of which exactly p are not orthogonal to $\mathbf{j}$. If these p eigenvectors, unique up to sign, generate the subspace $Main(G)$, then $\mathbb{R}^n = Main(G) \oplus (Main(G))^{\perp}$. We show that both $Main(G)$ and $(Main(G))^{\perp}$ are $\mathbf{A}$–invariant.

We relate main eigenvalues with regularity constraints in a graph.

Definition 1 *A (κ, τ)-regular set S is a non-empty subset of the vertex set of a connected graph G inducing a κ-regular subgraph, such that every vertex not in S has τ neighbours in S.*

We focus on the case when $\kappa = \tau$, mentioned in [4] for a class of graphs. In section 3, we show that the vector space generated by the columns $\{\mathbf{A}^h j, h \in \mathbb{Z} \cup \{0\}\}$ of $\mathbf{W}_p$ is $Main(G)$. The $\mathbf{A}$–invariance of the spaces $Main(G)$ and $(Main(G))^\perp$ is crucial to enable us to develop, in section 4, a formula that determines the vertices of (κ, κ)-regular sets, when they occur in a graph. We define a graph parameter, $\mathbf{g}$, referred to as the *discriminating vector*, that determines, whether or not, zero is a main eigenvalue. An algorithm (CHAR-VEC) that extracts (κ, κ)-regular sets is presented. We give examples of different categories of graphs with (κ, κ)-regular sets.

A graph G is *Hamiltonian* if it has a Hamiltonian cycle, that is, if the cycle C_n is a spanning subgraph of G. In section 6, the algorithm CHAR-VEC applied on the subdivision of G gives a necessary and sufficient condition, based on $\mathbf{g}$, for a graph to be Hamiltonian. It is well known that the problem to determine whether a graph is Hamiltonian or not is NP-hard. Many problems that are hard to solve for general graphs might become polynomial-time solvable when restricted to a particular family of graphs. The algorithm CHAR-VEC is adapted to ALG-HAM providing a fixed–parameter tractable solution to the problem of determining whether a graph is Hamiltonian or not, using non-conventional techniques.

2 The Main Subspace

The polynomial $M(G, x) := \prod_{i=1}^{p}(x - \mu_i)$ whose roots are the main eigenvalues of the adjacency matrix of a graph G is termed the *main characteristic polynomial*.

Lemma 2 [7, 10] *The main characteristic polynomial* $M(G, x) = x^p - c_0 x^{p-1} - c_1 x^{p-2} - \ldots.. - c_{p-2} x - c_{p-1}$ *has integer coefficients* c_i*, for all* i*,* $0 \le i \le p - 1$.

Remark 3 Let $\mathbf{I}$ be the identity matrix and let $\{\mathbf{y}_1^i, \mathbf{y}_2^i, \ldots, \mathbf{y}_{k_i}^i\}$ be a basis for the eigenspace $\mathcal{E}_G(\mu_i) = \ker(\mu_i \mathbf{I} - \mathbf{A})$ associated with the main eigenvalue μ_i of multiplicity k_i of G, such that $\mathbf{y}_1^i$ is not orthogonal to $\mathbf{j}$. Writing $\mathbf{y}_\ell^i = \alpha_\ell \mathbf{j} + \mathbf{z}_\ell^i$, where $\mathbf{j}^t \mathbf{z}_\ell^i = 0$, for $2 \le \ell \le k_i$, set $\mathbf{w}_\ell^i = \alpha_\ell \mathbf{y}_1^i - \alpha_1 \mathbf{y}_\ell^i$. Note that the vectors $\mathbf{w}_\ell^i$ are orthogonal to $\mathbf{j}$. Gram Schmidt orthogonalization process on the ordered basis $\mathbf{w}_2^i, \mathbf{w}_3^i, \ldots, \mathbf{w}_{k_i}^i, \mathbf{y}_1^i$ yields an orthonormal basis $B_i = \{\mathbf{x}_1^i, \mathbf{x}_2^i, \ldots, \mathbf{x}_{k_i}^i\}$ with only one vector $\mathbf{x}_1^i$ not orthogonal to $\mathbf{j}$. We note that the vector $\mathbf{x}_1^i$ lies in the k_i–dimensional eigenspace of μ_i and is orthogonal to the subspace generated by the $k_i - 1$ eigenvectors orthogonal to $\mathbf{j}$. Therefore it is an invariant of $\mathcal{E}_G(\mu_i)$, up to sign, independent of the basis $\{\mathbf{y}_\ell^i\}$.

Definition 4 *Let $mv(G) := \{\mathbf{x}_1^1, \mathbf{x}_1^2, \ldots, \mathbf{x}_1^p\}$ be the set of the uniquely determined p eigenvectors, not orthogonal to $\mathbf{j}$, associated with the p distinct main eigenvalues $\mu_1, \mu_2, \ldots, \mu_p$ of $\mathbf{A}$ for a graph G, in that order. The subspace $\mathcal{L}(mv)$ of $\mathbb{R}^n$ generated by mv is denoted by $Main(G)$ and is said to be the* **main subspace** *of G.*

The eigenvectors in mv are orthogonal as they belong to distinct eigenvalues. It follows that they are linearly independent and can be extended to an ordered basis for $\mathbb{R}^n$. The Primary Decomposition Theorem states that $\mathbb{R}^n$ is the direct sum of the eigenspaces of a square real matrix. Therefore the disjoint union of the bases for the distinct eigenspaces forms a basis for $\mathbb{R}^n$.

Definition 5 *An ordered orthonormal basis B_0, for $\mathbb{R}^n$, is obtained by starting with mv, then including the eigenvectors $\mathbf{x}_2^i, \ldots, \mathbf{x}_{k_i}^i$ in B_i from $i = 1$ to p for each of the main eigenvalues in turn when $k_i > 1$, followed by an orthonormal full set of eigenvectors associated with the non-main eigenvalues of $\mathbf{A}$.*

Remark 6 We denote by $\mathbf{P}$ the matrix whose columns are the vectors of B_0.Then $\mathbf{P}$ diagonalizes $\mathbf{A}$ and $\mathbf{P}^{-1}\mathbf{A}\mathbf{P}$ is the diagonal matrix $\mathbf{D}$ whose first p diagonal entries are the main eigenvalues of $\mathbf{A}$.

We note that $\mathbf{P}^{-1}$ is the transpose $\mathbf{P}^t$ of $\mathbf{P}$.

Lemma 7 *If G be a graph with $mv(G) = \{\mathbf{x}_1^1, \mathbf{x}_1^2, \ldots, \mathbf{x}_1^p\}$. Then $\mathbf{j} = \sum_{i=1}^{p} \beta_i \mathbf{x}_i^1$ where each $\beta_i \in \mathbb{R}$ is non-zero.*

Proof: By definition of mv in B_0, out of all the vectors in B_0, only those in mv have a component along $\mathbf{j}$. It follows that the vectors in mv span $\mathbf{j}$.

Thus $\mathbf{j} = \sum_{i=1}^{p} \beta_i \mathbf{x}_1^i$ for some $\beta_i \in \mathbb{R}$. Since the vectors in mv are mutually orthogonal and each has a component along $\mathbf{j}$, then $\beta_i \neq 0$ for all i. ∎

There is an interesting result regarding the main characteristic polynomial $M(G,x)$, analogous to the Cayley-Hamilton Theorem on the characteristic polynomial $\phi(G,\lambda)$. The latter states that $\phi(G,\mathbf{A})$ is the zero operator.

Lemma 8 [14] *Let the main characteristic polynomial of G be $M(G,x)$. The vector $\mathbf{j}$ is in the kernel of the operator $M(G;\mathbf{A})$.*

Proof: Let $\mu_1, \mu_2, \ldots, \mu_p$ be the main eigenvalues of G with corresponding uniquely determined eigenvectors $\mathbf{x}_1^1, \mathbf{x}_1^2, \ldots, \mathbf{x}_1^p$ in mv. For $1 \leq i \leq p$, the vector $\mathbf{x}_1^i$ is in the nullspace of $(\mathbf{A} - \mu_i \mathbf{I})$. Thus $\prod_{i=1}^{p} (\mathbf{A} - \mu_i \mathbf{I}) \mathbf{x}_1^\ell = \mathbf{0}$, for $1 \leq \ell \leq p$, and therefore, by Lemma 7, expressing $\mathbf{j}$ in terms of the vectors in mv, it follows that $\mathbf{j}$ is in the kernel of $\prod_{i=1}^{p} (\mathbf{A} - \mu_i \mathbf{I})$, which is $M(G;\mathbf{A})$. ∎

If the degree of $M(G,x)$ is less than that of the minimum polynomial of $\mathbf{A}$, then $M(G,\mathbf{A})$ is not the zero operator. However by Lemma 8, it maps $\mathbf{j}$ to zero.

3 The Walk matrix

The properties of the walk matrix are central to the underlying theory that leads to the rationale of the definition of the discriminating vector introduced in section 4.

3.1 The Walk Matrix

The entries of $\mathbf{A}^{r-1}\mathbf{j}$ give the number of walks of length $r-1$ from each vertex v of G. The dimension of the subspace $ColSp(\mathbf{W}_k)$ generated by the columns of $\mathbf{W}_k$ is the rank of $\mathbf{W}_k$.

Theorem 9 [8] *For a graph with p main eigenvalues, the rank, $dim(ColSp(\mathbf{W}_k))$, of the $n \times k$ matrix $\mathbf{W}_k = \big(\mathbf{j}, \mathbf{A}\mathbf{j}, \mathbf{A}^2\mathbf{j}, ..., \mathbf{A}^{k-1}\mathbf{j}\big)$ is p, for $k \geq p$.*

Proof: Since for $mv(G) := \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_p\}$, $\mathbf{j} = \sum_{i=1}^{p} \beta_i \mathbf{x}_i$, where $\beta_i \neq 0$ for all i, then for $0 \leq h \leq k$, a column of $\mathbf{W}_k$, which is of the form $\mathbf{A}^h j = \sum_{i=1}^{p} \beta_i \mu_i^h \mathbf{x}_i$, is in the linear span $\mathcal{L}(mv(G))$ of $mv(G)$. Thus $ColSp(\mathbf{W}_k) \subseteq \mathcal{L}(mv(G))$, so that $\operatorname{rank}(\mathbf{W}_k) \leq p$.

We now show that $\mathbf{j}, \mathbf{Aj}, \mathbf{A}^2\mathbf{j}, ..., \mathbf{A}^{p-1}\mathbf{j}$ are a maximal set of linearly independent vectors in $ColSp(\mathbf{W}_k)$.

Suppose that $\sum_{h=0}^{p-1} \gamma_h \mathbf{A}^h \mathbf{j} = \mathbf{0}$. Then $\mathbf{0} = \sum_{i=1}^{p} \mathbf{x}_i \beta_i \sum_{h=0}^{p-1} \gamma_h \mu_i^h$.

Since the vectors in $mv(G)$ are orthogonal, they are linearly independent. Hence, for $1 \leq i \leq p$, $\beta_i \sum_{h=0}^{p-1} \gamma_h \mu_i^h = 0$. Since $\beta_i \neq 0$ for all i, if $\mathbf{V} = \begin{pmatrix} 1 & \mu_1 & \mu_1^2 & \ldots & \mu_1^{p-1} \\ 1 & \mu_2 & \mu_2^2 & \ldots & \mu_2^{p-1} \\ \vdots & \vdots & \vdots & \vdots & \\ 1 & \mu_p & \mu_p^2 & \ldots & \mu_p^{p-1} \end{pmatrix}$ and $\mathbf{y} = \begin{pmatrix} \gamma_0 \\ \gamma_1 \\ \vdots \\ \gamma_{p-1} \end{pmatrix}$, then we can write this system of equations as $\mathbf{Vy} = \mathbf{0}$.

Note that the determinant of matrix $\mathbf{V}$ is the well known Vandermonde determinant which is not zero for distinct values of μ_i. Hence $\gamma_i = 0$, for all i, whence $\operatorname{rank}(\mathbf{W}_k) \geq p$. We deduce that $\operatorname{rank}(\mathbf{W}_k) = p$ as required. ■

Definition 10 *The matrix* $\mathbf{W} = \mathbf{W}_p = \left(\mathbf{j}, \mathbf{Aj}, \mathbf{A}^2\mathbf{j}, \ldots, \mathbf{A}^{p-1}\mathbf{j}\right)$ *is said to be the* **walk matrix** *of* G.

Proposition 11 *If* $\mathbf{W}$ *is the walk matrix of a graph* G *and the main characteristic polynomial* $M(G, x)$ *of* G *is* $x^p - c_0 x^{p-1} - c_1 x^{p-2} - ..... - c_{p-2}x - c_{p-1}$, *then the pth column of* $\mathbf{AW}$ *is* $\mathbf{A}^p\mathbf{j} = \mathbf{W} \begin{pmatrix} c_{p-1} \\ \vdots \\ c_1 \\ c_0 \end{pmatrix}$.

Proof: By Lemma 8, $M(G, \mathbf{A})\mathbf{j} = 0$. Hence $\mathbf{A}^p\mathbf{j} - c_0\mathbf{A}^{p-1}\mathbf{j} - c_1\mathbf{A}^{p-2}\mathbf{j} - ..... - c_{p-2}\mathbf{Aj} - c_{p-1}\mathbf{j} = 0$. Since the first p columns $\mathbf{j}$, $\mathbf{Aj}, ..., \mathbf{A}^{p-2}\mathbf{j}, \mathbf{A}^{p-1}\mathbf{j}$ of $\mathbf{W}_k$ form a basis B' for $ColSp(\mathbf{W}_k)$ for all finite k, then $\mathbf{A}^p\mathbf{j}$ has a unique expression in terms of the vectors in B'. ■

We denote by $\mathbf{e}_k$ the column vector with all its entries equal to zero except for the kth which is equal to one.

Proposition 12 *Let* $\mathbf{C}$ *be the companion matrix* $\begin{pmatrix} 0 & 0 & \dots & 0 & c_{p-1} \\ 1 & 0 & \ddots & \vdots & \vdots \\ 0 & 1 & \ddots & \vdots & \vdots \\ 0 & 0 & \ddots & 0 & c_1 \\ 0 & 0 & \dots & 1 & c_0 \end{pmatrix}$, *with the entries* c_i *being the coefficients of* $M(G,x)$. *The walk matrix of a graph* G *with adjacency matrix* $\mathbf{A}$ *is* $\mathbf{W}$ $(= W_p)$ *if and only if* $\mathbf{AW} = \mathbf{WC}$.

Proof: By Proposition 11,
$\mathbf{AW} = (\mathbf{Aj}, \mathbf{A}^2\mathbf{j}, \dots, \mathbf{A}^{p-1}\mathbf{j}, \mathbf{A}^p\mathbf{j}) = (\mathbf{We}_2, \mathbf{We}_3, \dots, \mathbf{We}_p, \mathbf{A}^p\mathbf{j}) = \mathbf{WC}$. ■

Proposition 13 *If* $\mathbf{W}$ *is the walk matrix of a graph* G*, then the spectrum of* $\mathbf{C}$ *is the main spectrum of* G.

Proof: Note that the characteristic polynomial $f(p,\lambda) = (\lambda\mathbf{I} - \mathbf{C})$ of the $p \times p$ matrix $\mathbf{C}$ satisfies the recurrence relation $f(p,\lambda) = \lambda f(p-1,\lambda) + (-1)^{2p-1}c_{p-1}$, so that $f(p,\lambda) = \lambda^p - c_0\lambda^{p-1} - c_1\lambda^{p-2} - \dots.. - c_{p-2}\lambda - c_{p-1}$. Since this is $M(G,\lambda)$, the spectrum of C is the main spectrum of G. ■

Since C has p columns we obtain:

Lemma 14 $\mathbf{C}^k\mathbf{e}_1 = \mathbf{C}^{k-p+1}\mathbf{e}_p$.

Remark 15 From Lemma 14, we can obtain an independent proof of Proposition 11. Indeed, since $\mathbf{C}^p\mathbf{e}_1 = \mathbf{Ce}_p$ and $\mathbf{A}^p\mathbf{We}_1 = \mathbf{WC}^p\mathbf{e}_1$, then $\mathbf{A}^p\mathbf{j} = \mathbf{WCe}_p = \mathbf{W}\left(c_{p-1}, c_{p-2}, \dots, c_0 \right)^t$.

The number of walks of length k can be expressed in terms of the main eigenvalues [5, p46].

Theorem 16 *The number* w_k *of walks of length* k *starting from any vertex of* G *is given by*

$$w_k = \sum_{i=1}^{p} c_i'\mu_i^k$$

where $c_i' \in \mathbb{R}$ *and* $\mu_1, \mu_2, \dots, \mu_p$ *are the main eigenvalues of* $\mathbf{A}$.

Since w_k is the sum of all the entries of $\mathbf{A}^k$ which can be expressed as $\mathbf{PD}^k\mathbf{P}^t$, the real coefficients $\{c'_i\}$ turn out to be the square of the projection $\{(\mathbf{j}^t\mathbf{x}_1^i)^2\}$, onto $\mathbf{j}$, of the vectors of B_0 (of Definition 5). Therefore, only the coefficients $\{c'_i\}$ for $1 \le i \le p$, in $w_k = \sum_{i=1}^{n} c'_i \mu_i^k$ are not zero.

We shall be using the representation of the number of walks in a graph given in Theorem 16. We have proved the following formulae for w_k:

Corollary 17

$$\begin{aligned} w_k &= \mathbf{j}^t\mathbf{A}^k\mathbf{j} \\ &= \mathbf{j}^t\mathbf{A}^k\mathbf{W}\mathbf{e}_1 \\ &= \mathbf{j}^t\mathbf{W}\mathbf{C}^k\mathbf{e}_1 \\ &= \mathbf{j}^t\mathbf{W}\mathbf{C}^{k-p+1}\mathbf{e}_p \quad \text{by Lemma 14} \\ &= \sum_{i=1}^{p} c'_i\mu_i^k, \quad c'_i \neq 0, \forall i. \end{aligned}$$

3.2 The Main Eigenspace

We now show that $ColSp(\mathbf{W})$ of $\mathbf{W}$ is precisely $Main(G)$. The theory is based on the $\mathbf{A}$-invariance of $Main(G)$.

Lemma 18 *The subspace $ColSp(\mathbf{W})$ is $\mathbf{A}$–invariant.*

Proof: Since $\mathbf{A}(\mathbf{W}\mathbf{e}_k) = \mathbf{W}(\mathbf{C}\mathbf{e}_k) = \sum_{\ell=1}^{p} c_{\ell k}\mathbf{W}\mathbf{e}_k$, for $1 \le k \le p$, it follows that $ColSp(\mathbf{AW}) \subseteq ColSp(\mathbf{W})$. Thus $\mathbf{A}(ColSp(\mathbf{W})) \subseteq ColSp(\mathbf{W})$ and therefore $ColSp(\mathbf{W})$ is $\mathbf{A}$–invariant. ■

Theorem 19 *Let G be a graph with adjacency matrix $\mathbf{A}$ and walk matrix $\mathbf{W}$. The column space $ColSp(\mathbf{W})$ of $\mathbf{W}$ is $Main(G)$.*

Proof: First we transform the ordered column vectors of $\mathbf{W}$ to an orthonormal set, using Gram Schmidt orthogonalization process, thus producing a new basis for $ColSp(\mathbf{W})$. Let $\mathbf{U}$ be the $n \times p$ matrix whose columns are the vectors of this orthonormal set, $\frac{1}{\sqrt{n}}\mathbf{j}$ being the first column. Since $ColSp(\mathbf{U}) = ColSp(\mathbf{W})$, it is also $\mathbf{A}$–invariant and therefore there exists a matrix $\mathbf{Q}$, such that $\mathbf{AU} = \mathbf{UQ}$. Since $\mathbf{U}^t\mathbf{U} = \mathbf{I}$, the matrix $\mathbf{Q}$ is equal to

$\mathbf{U}^t\mathbf{U}\mathbf{Q} = \mathbf{U}^t\mathbf{A}\mathbf{U}$, so that $\mathbf{Q}^t = \mathbf{Q}$. Hence $\mathbf{Q}$ is real and symmetric with p real eigenvalues.

Now let λ be a main eigenvalue of G. Then $\mathbf{A}\mathbf{x} = \lambda\mathbf{x}$, where $\mathbf{j}^t\mathbf{x} \neq 0$. Since $\mathbf{A}\mathbf{U} = \mathbf{U}\mathbf{Q}$, $\lambda\mathbf{x}^t\mathbf{U} = \mathbf{x}^t\mathbf{A}\mathbf{U} = (\mathbf{x}^t\mathbf{U})\mathbf{Q}$ so that $\lambda(\mathbf{U}^t\mathbf{x}) = \mathbf{Q}(\mathbf{U}^t\mathbf{x})$. Thus the eigenvalue λ of G is also an eigenvalue of $\mathbf{Q}$, provided that $\mathbf{U}^t\mathbf{x} \neq \mathbf{0}$. Indeed this is the case when λ is a main eigenvalue, since $\mathbf{x}^t\mathbf{U}\mathbf{e}_1 = \mathbf{x}^t\frac{\mathbf{j}}{\sqrt{n}} \neq 0$. Thus the main part of the spectrum of G contains the spectrum of $\mathbf{Q}$. Therefore the p distinct main eigenvalues of G are precisely the eigenvalues of the $p \times p$ matrix $\mathbf{Q}$.

If $\mathbf{Q}\mathbf{y} = \mu\mathbf{y}$, $\mathbf{y} \neq \mathbf{0}$, then $\mathbf{A}\mathbf{U}\mathbf{y} = \mathbf{U}\mathbf{Q}\mathbf{y} = \mu\mathbf{U}\mathbf{y}$. Since the columns of $\mathbf{U}$ are orthogonal, they are linearly independent, so that $\mathbf{U}\mathbf{y} \neq \mathbf{0}$. It follows that each of the p real eigenvalues of $\mathbf{Q}$ is a main eigenvalue of G, with corresponding eigenvector $\mathbf{U}\mathbf{y}$.

Moreover, the p linearly independent eigenvectors of $\mathbf{G}$ generating $Main(G)$ are in the p–dimensional space $ColSp(\mathbf{U})$, which is equal to $ColSp\mathbf{W}$. ■

Remark 20 Recall that $\mathbb{R}^n = ColSp(\mathbf{W}) \oplus (ColSp(\mathbf{W}))^\perp$. The proofs of the results in section 4 rely on the invariance of $(ColSp(\mathbf{W}))^\perp$.

Lemma 21 *$(ColSp(\mathbf{W}))^\perp$ is A-invariant.*

Proof: Using the same notation as in Proposition 19, (ColSp($\mathbf{W}$))=(ColSp($\mathbf{U}$)). For $u \in ColSp(\mathbf{U})$, $\mathbf{A}\mathbf{u} \in ColSp(\mathbf{W})$ and for $\mathbf{v} \in (ColSp(\mathbf{W}))^\perp$, $0 = \mathbf{v}^t\mathbf{A}\mathbf{u} = (\mathbf{A}\mathbf{v})^t\mathbf{u}$, showing that $\mathbf{A}\mathbf{v}$ is orthogonal to $\mathbf{u}$. We deduce that $\mathbf{A}(ColSp(\mathbf{W}))^\perp \subseteq (ColSp(\mathbf{W}))^\perp$, as required. ■

4 (κ, κ)–Regular Sets

Under particular conditions, a graph with a (κ, τ)–regular set may have $(\kappa - \tau)$ as an eigenvalue [3, 15]. We consider the case when $\kappa = \tau$ and take $0 < \kappa < \rho_{max}$, where ρ_{max} is the maximum vertex degree.

Definition 22 *Let S be a subset of the n labelled vertices of G. The $(n \times 1)$* **characteristic vector** $\mathbf{x}_S$ *of S has the ith-entry $x_i = 1$ if $i \in S$ and $x_i = 0$ otherwise.*

Lemma 23 [15] *If S is a (κ, τ)-regular set with characteristic vector $\mathbf{x}_S$, then $\mathbf{A}\mathbf{x}_S = (\kappa - \tau)\mathbf{x}_S + \tau\mathbf{j}$.*

Proof: By Definition 1,

$$\begin{aligned}\mathbf{A}\mathbf{x}_S &= \kappa\mathbf{x}_S + \tau(\mathbf{j} - \mathbf{x}_S)\\ &= (\kappa - \tau)\mathbf{x}_S + \tau\mathbf{j}.\end{aligned}$$

. ■

4.1 Regular Core Graphs

Theorem 24 [3] *If S_1 is a (κ_1, τ_1)-regular set and $S_2 \neq S_1$ is a distinct (κ_2, τ_2)-regular set in a graph G such that $\lambda = \kappa_1 - \tau_1 = \kappa_2 - \tau_2$, then λ is an eigenvalue of G with associated eigenvector $\mathbf{x}_{S_1} - \frac{\tau_1}{\tau_2}\mathbf{x}_{S_2}$.*

Proof: By definition of the characteristic vectors,

$$\begin{aligned}\mathbf{A}\mathbf{x}_{S_1} &= \kappa_1\mathbf{x}_{S_1} + \tau_1(\mathbf{j} - \mathbf{x}_{S_1}) \quad \text{and}\\ \mathbf{A}\mathbf{x}_{S_2} &= \kappa_2\mathbf{x}_{S_2} + \tau_2(\mathbf{j} - \mathbf{x}_{S_2}).\end{aligned}$$

Thus $\mathbf{A}\mathbf{y} = \lambda\mathbf{y}$ where $\mathbf{y} = \tau_2\mathbf{x}_{S_1} - \tau_1\mathbf{x}_{S_2}$. Since the symmetric difference of S_1 and S_2 is not empty, $\mathbf{y} \neq \mathbf{0}$. The results now follow. ■

Remark 25 If a ρ–regular graph G has a (κ, τ)-regular set, then $\lambda = \kappa - \tau$ is an eigenvalue of G [15]. This result can be viewed as a special case of Theorem 24. A ρ–regular graph G with a (κ, τ)-regular set S has another independent $(\kappa_2, \tau_2) = (\rho - \tau, \rho - \kappa)$-regular set, $\bar{S} = \mathcal{V}\backslash S$, with the same difference $\lambda = \kappa - \tau$. Thus λ is an eigenvalue of G. Note that $\mathbf{y}_S$ and $\mathbf{y}_{\bar{S}}$ are linearly independent.

Corollary 26 *If an n–vertex ρ–regular graph G has a (κ, κ)–regular set of n_1 vertices, then $\frac{n_1}{n} = \frac{\kappa}{\rho}$.*

Proof: The maximum eigenvalue of G is ρ since $\mathbf{A}\mathbf{j} = \rho\mathbf{j}$. By the orthogonality of independent eigenspaces, $(\mathbf{x}_S - \frac{\kappa}{\rho}\mathbf{j}).\mathbf{j}^t = 0$, yielding $n_1 - \frac{\kappa}{\rho}n = 0$. ■

The next result relates (κ, κ)–regular sets to the structure of singular graphs.

Corollary 27 *If a ρ–regular graph G has a (κ, κ)–regular set S, then G is a core graph.*

Proof: Let π be the equitable partition $S \cup \bar{S}$ of the vertices of G. Consider the 2×2 adjacency matrix $\mathbf{B} = \left(\begin{array}{c|c} \kappa & \rho - \kappa \\ \hline \tau & \rho - \tau \end{array}\right)$ of the quotient graph $\frac{G}{\pi}$.

Since $\kappa = \tau$, $\mathbf{A}\mathbf{x}_S = \kappa\mathbf{j}$. The graph G is labelled so that $\mathbf{X} = \begin{pmatrix} 1 & 0 \\ 1 & 0 \\ \vdots & \vdots \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ \vdots & \vdots \\ 0 & 1 \end{pmatrix}$ is the characteristic matrix of π. Therefore $\mathbf{AX} = \mathbf{XB}$. The eigenvalues of $\mathbf{B}$, which are ρ and 0, are also eigenvalues of G. Thus G is singular. Moreover, if $\mathbf{y}_S = \mathbf{x}_S - \frac{\kappa}{\rho}\mathbf{j}$, then $\mathbf{G}\mathbf{y}_S = \mathbf{0}$. Since $0 < \kappa = \tau < \rho$, no entry of $\mathbf{y}_S$ is zero, so that G is a core graph. ■

Proposition 28 *If an n-vertex ρ–regular core graph G has a (κ, κ)–regular set S, of size n_1, then $\frac{n_1}{n} = \frac{\kappa}{\rho}$.*

Proof: If G is ρ–regular, then counting the edges joining the vertices of S and those of $\bar{S}$ gives $n_1(\rho - \kappa) = \kappa(n - n_1)$.

■

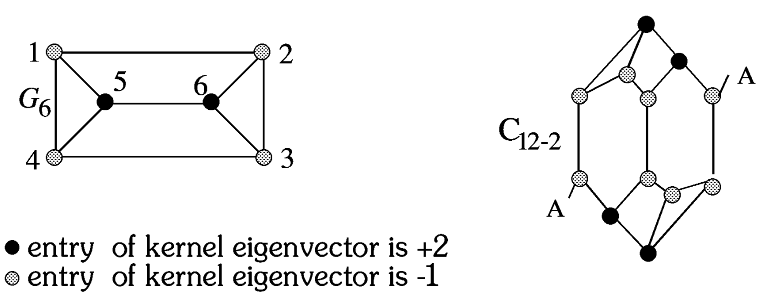

Figure 2: Regular Core Graphs

Remark 29 We give two examples of such regular core graphs, shown in Figure 2. The graph, G_6, is a core graph of nullity two while G_{12} is a nut graph [11], that is a core graph of nullity one. Each graph is 3–regular and has a $(2, 2)$–regular set shown as grey vertices. The next result follows immediately from Lemma 23.

Proposition 30 *Let G have a (κ, τ)-regular set S, $1 \le \tau \le n$.*
Then $\kappa = \tau$ if and only if $\mathbf{A}\mathbf{x}_S = \kappa\mathbf{j}$.

Proof: Since for $S \neq \mathcal{V}$ in G, $\mathbf{j}$ and $\mathbf{x}_S$ are linearly independent, considering the entry of $\mathbf{A}\mathbf{x}_S$ corresponding to a vertex in S and one corresponding to a vertex not in S, we deduce that $\mathbf{A}\mathbf{x}_S = \kappa\mathbf{x}_S + \tau(\mathbf{j} - \mathbf{x}_S) = \kappa\mathbf{j}$ is true if and only if $\kappa - \tau = 0$. ■

Remark 31 The occurrence of one (κ, κ)-regular set is not a conclusive test for the graph to be singular. Graph H_2 of Figure 5 has a $(1, 1)$-regular set but is non-singular.

4.2 Determination of a (κ, κ)-regular set

Remark 32 (i) For $0 < \kappa, \tau < \rho_{max}$, the determination of a (κ, τ)-regular set is a hard problem. Here, we present a formula that, under particular conditions, gives the characteristic vector of a (κ, κ)-regular set.
(ii) From Proposition 24, a non-regular graph, with no integer eigenvalues, does *not* have two (κ_i, τ_i)–regular sets, with the same difference $\kappa_i - \tau_i$, for $i = 1, 2$. The same conclusion can be drawn for a ρ–regular graph with only ρ as an integer eigenvalue.

The ordered basis B_0 generates $Main(G) \oplus Main(G)^{\perp}$. Theorem 19 allows the construction of another basis B_1 for $\mathbb{R}^n$ by replacing the first p vectors of B_0 by the p columns of $\mathbf{W}$ as a basis for $Main(G)$.

Proposition 33 *Let S be a subset of $\mathcal{V}(G)$ and $\mathbf{A}$ be the adjacency matrix of G. Then* $\mathbf{x}_S = \sum_{i=0}^{p-1} \alpha_i \mathbf{A}^i \mathbf{j} + \mathbf{q}, \quad \mathbf{A}(\mathbf{x}_S - \mathbf{q}) \in Main(G)$ *for some* $\alpha_i \in \mathbb{R}$ *and* $\mathbf{A}\mathbf{q} \in (Main(G))^{\perp}$.

Proof: The columns of $\mathbf{W}$ are linearly independent but not mutually orthogonal. Since $\mathbb{R}^n = ColSp(\mathbf{W}) \oplus (ColSp(\mathbf{W}))^{\perp}$ where $\mathbf{j}, \mathbf{A}\mathbf{j}, \ldots, \mathbf{A}^{p-1}\mathbf{j}$ is a basis for $ColSp\mathbf{W}$, any vector, $\mathbf{x}_S$ in particular, can be expressed as $\sum_{i=0}^{p-1} \alpha_i \mathbf{A}^i j + \mathbf{q}$, for some $\alpha_i \in \mathbb{R}$, where $\mathbf{q} \in (ColSp(\mathbf{W}))^{\perp}$.

Now $\mathbf{j}^t.\mathbf{x}_S \neq 0$ and $\mathbf{A}\mathbf{x}_S = \sum_{i=0}^{p-2} \alpha_i \mathbf{A}^{i+1}\mathbf{j} + \alpha_{p-1}\mathbf{A}^p\mathbf{j} + \mathbf{A}\mathbf{q}$.

By Proposition 11, $\mathbf{A}^p\mathbf{j} = c_{p-1}\mathbf{j} + \ldots + c_0\mathbf{A}^{p-1}\mathbf{j}$, where the coefficients $\{c_i\}$ are the same as in the main characteristic polynomial $M(G, x) = x^p - c_0x^{p-1} - c_1x^{p-2} - \ldots.. - c_{p-2}x - c_{p-1}$.

Also by Lemmas 18 and 21, $ColSp(\mathbf{W})$ and $(ColSp(\mathbf{W}))^{\perp}$ are separately $\mathbf{A}$-invariant. Thus $\mathbf{Aq} \in (ColSp(\mathbf{W}))^{\perp}$ and

$$(\mathbf{Ax}_S - \mathbf{Aq}) = \sum_{i=0}^{p-2} (\alpha_i + \alpha_{p-1} c_{p-2-i}) \mathbf{A}^{i+1} \mathbf{j} + \alpha_{p-1} c_{p-1} \mathbf{j} \in ColSp(\mathbf{W}). \quad (1)$$

The result follows since $ColSp(\mathbf{W}) = Main(G)$, by Theorem 19. ■

Remark 34 For $p = 1$, G is ρ–regular. If G has a (κ, κ)-regular set S with $\mathbf{x}_S = \alpha_0 \mathbf{j} + \mathbf{q}$ where $\mathbf{q} \in \mathbf{j}^{\perp}$, $\mathbf{Aq} \in \mathbf{j}^{\perp}$. Also then $\mathbf{Ax}_S = \kappa \mathbf{j}$ and $\mathbf{Aj} = \rho \mathbf{j}$. Hence in this case, $\mathbf{Aq} = \mathbf{0}$ and $\alpha_0 = \frac{\kappa}{\rho}$.

Theorem 35 *Let G have a (κ, κ)-regular set S.*

Then

$$\mathbf{x}_S = \sum_{i=0}^{p-1} \alpha_i \mathbf{A}^i \mathbf{j} + \mathbf{q} \text{ where}$$

i $\mathbf{Aq} = \mathbf{0}$;

ii $\kappa = \alpha_{p-1} c_{p-1}$, *for* $p \geq 1$;

iii *for* $0 \leq i \leq p-2$, $\alpha_i + \alpha_{p-1} c_{p-2-i} = 0$, *for* $p \geq 2$

where the product of the main eigenvalues is $(-1)^{p-1} c_{p-1} = (-1)^p Main(G, 0)$.

Proof: (i) Since a (κ, κ)-regular set S, in G, gives $\mathbf{Ax}_S = \kappa \mathbf{j}$, by Proposition 30 and since $\mathbf{Aq} \in (\mathbf{Main(G)})^{\perp}$, then $\mathbf{Aq} = \mathbf{0}$.
(ii) and (iii) The vectors $\mathbf{j}, \mathbf{Aj}, \ldots, \mathbf{A}^{p-1}\mathbf{j}, \mathbf{q}$ are linearly independent, yielding, from equation (1), the required $(p + 1)$ relations. ■

4.3 Zero as a Main or Non-Main Eigenvalue

The presence of (κ, κ)-regular sets will be shown to preclude $\mathbf{A}$ from having zero as a main eigenvalue.

Proposition 36 *If G is a singular graph with a (κ, κ)-regular set for $\kappa > 0$, then zero is a non-main eigenvalue.*

Proof: Let $\mathbf{v} \neq \mathbf{0}$ satisfy $\mathbf{Av} = \mathbf{0}$. If $\mathbf{x}_S$ is the characteristic vector of the (κ, κ)-regular set, then $\mathbf{Ax}_S = \kappa\mathbf{j}$. Hence $\mathbf{v}^t\mathbf{A}^t\mathbf{x}_S = 0$, so that $\kappa\mathbf{v}^t\mathbf{j} = 0$, whence zero is a non-main eigenvalue, for $\kappa > 0$. ■

As a direct consequence we have:

Corollary 37 *If a singular connected graph G has zero as a main eigenvalue, then G has no (κ, κ)–regular sets, for $0 < \kappa < n$.*

This result can also be deduced from Theorem 35(ii), since for a zero main eigenvalue, $c_{p-1} = 0$.

Proposition 38 *If the singular connected graph G has zero as a main eigenvalue, then $c_{p-2} \neq 0$.*

Proof: The roots of $M(G, x)$ are distinct. Thus at most one root can be zero. Since $c_{p-1} = 0$ for a main eigenvalue, then $c_{p-2} = 0$ would result in a repeated zero main eigenvalue, a contradiction. ■

From the proof of Theorem 35, we can obtain an expression for $\mathbf{x}_S$ in terms of basis B_1, which will lead to the definition of *the discriminating vector* $\mathbf{g}$.

Proposition 39 *Let G have a (κ, κ)–regular set S.*
Then $\mathbf{x}_S = (-\frac{\kappa}{c_{p-1}})\left(c_{p-2}\mathbf{j} + c_{p-3}\mathbf{Aj} + \ldots + c_0\mathbf{A}^{p-2}\mathbf{j} - \mathbf{A}^{p-1}\mathbf{j} + \mathbf{q}'\right)$, where $\mathbf{q}' \in (Main(G))^{\perp}$ and $\mathbf{Aq}' = \mathbf{0}$.

Definition 40 *The graph parameter $c_{p-2}\mathbf{j}+c_{p-3}\mathbf{Aj}+\ldots+c_0\mathbf{A}^{p-2}\mathbf{j}-\mathbf{A}^{p-1}\mathbf{j}$, denoted by $\mathbf{g}$, is said to be the* **discriminating vector***.*

We shall see that $\mathbf{g}$ is in the nullspace of $\mathbf{A}$ if and only if zero is a main eigenvalue of G. Moreover, the formula

$$\mathbf{x}_S = (-\frac{\kappa}{c_{p-1}})\mathbf{g} + \mathbf{q} \tag{2}$$

determines (κ, κ)–regular sets when they occur.

Corollary 41 *If a non–singular graph G has a (κ, κ)-regular set S, then $\mathbf{g}$ is an integral multiple of $\mathbf{x}_S$.*

Proof: As $M(G,x)$ has integral coefficients and the entries of each vector $\mathbf{A}^h\mathbf{j}$ are also integers, the vector $\mathbf{g}$ has integer entries. Since G is non-singular, it follows that $\mathbf{q}' = 0$. Thus $(-\frac{c_{p-1}}{\kappa}) \in \mathbb{Z}\backslash\{0\}$ and the result follows. ∎

This result can be generalized to all graphs where $\mathbf{q} = 0$ yields a 0-1 vector for $\mathbf{x}_S$ as for instance, in the graph of Figure 3.

Corollary 42 *If a graph G has a (κ,κ)-regular set S, and $\mathbf{x}_S$ is obtained by setting $\mathbf{q} = \mathbf{0}$ in equation (2), then κ divides c_{p-1}.*

We now present a criterion, in terms of $\mathbf{g}$, for a graph to have zero as a main eigenvalue.

Proposition 43 *For a non-regular graph G (i.e. $p \geq 2$), $\mathbf{Ag} = \mathbf{0}$, $\mathbf{g} \neq \mathbf{0}$ if and only if zero is a main eigenvalue of G.*

Proof: Zero is a main eigenvalue of $\mathbf{A}$ if and only if $c_{p-1} = 0$.

Let zero be a main eigenvalue of $\mathbf{A}$ with an associated eigenvector $\mathbf{v} \neq \mathbf{0}$. Then both $\mathbf{v}$ and $\mathbf{Av}$ are in $ColSp(\mathbf{W})$. If $\mathbf{v} = \sum_{i=0}^{p-1} \beta_i \mathbf{A}^i\mathbf{j}$, then

$$\mathbf{0} = \mathbf{Av} = \sum_{i=0}^{p-2} (\beta_i + \beta_{p-1}c_{p-2-i})\mathbf{A}^{i+1}\mathbf{j} + \beta_{p-1}c_{p-1}\mathbf{j} \tag{3}$$

Since the columns of $\mathbf{W}$ are linearly independent, then

$\beta_i = -\beta_{p-1}c_{p-2-i}$, so that $\beta_{p-1} \neq 0$.

Thus

$$\begin{aligned} \mathbf{v} &= -\beta_{p-1}\left(\sum_{i=0}^{p-2} c_{p-2-i}\mathbf{A}^i\mathbf{j} \ - \ \mathbf{A}^{p-1}\mathbf{j}\right) \\ &= -\beta_{p-1}(\mathbf{g}) \end{aligned} \tag{4}$$

We deduce that $\mathbf{Ag} = \mathbf{0}$.

Conversely, let $\mathbf{Ag} = \mathbf{0}$. The vector $\mathbf{g}$ is a non-trivial linear combination of the linearly independent columns of $\mathbf{W}$ and therefore non-zero. Since $ColSp(\mathbf{W}) = Main(G)$, if $\mathbf{Ag} = \mathbf{0}$ then zero is a main eigenvalue. ∎

Remark 44 We use a minimal set of parameters that calculates the discriminating vector $\mathbf{g}$.

Corollary 45 *The $p-1$ coefficients $\{c_i : 0 \leq i \leq p-2\}$ of $M(G,x)$ and the walk matrix suffice to determine*
(i) whether, or not, G has zero as a main eigenvalue.
(ii) the (κ,κ)–regular set if G is non-singular and has such a set.

Proof: Result (i) follows immediately from equation (4).

To prove result (ii), we note that if G is non-singular, then $\mathbf{A}\mathbf{x}_S = \kappa\mathbf{j}$ implies that $\mathbf{x}_S = \kappa\mathbf{A}^{-1}\mathbf{j}$, which is well defined, so that there exists at most one value of κ for which G has a (κ,κ)–regular set. In this case, the discriminating vector $\mathbf{g}$ is $(-\frac{c_{p-1}}{\kappa})\mathbf{x}_S = -c_{p-1}\mathbf{A}^{-1}\mathbf{j}$. The result follows from Corollary 41. ■

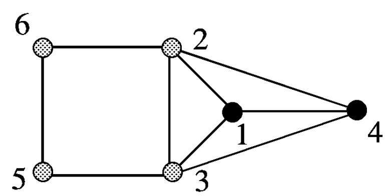

Figure 3: Unique $(2,2)$–regular set with zero as a non-main eigenvalue.

Remark 46 The graph H in Figure 3 has zero as a non-main eigenvalue and a unique $(2,2)$–regular set. The vector $\mathbf{g} = (0,2,2,0,2,2)^t$, $c_{p-1} = -4$, $\kappa = 2$ and $\mathbf{x}_S$ is uniquely determined for $\kappa = 2$ and $\mathbf{q} = 0$. A kernel eigenvector $\mathbf{q}'$ generating the one dimensional nullspace of $\mathbf{A}$ for H is $(1,-1,-1,1,0,0)$. From equation (2), substituting multiples of $\mathbf{q}'$ for $\mathbf{q}$, two other $(1,1)$–regular sets are obtained, namely $\{2,6\}$ and $\{3,5\}$.

To calculate $\mathbf{Ag}$ the paramenters $c_0, c_1, \ldots, c_{p-2}$ and the matrix $\mathbf{W}$ suffice.

Algorithm 47 (CHAR-VEC) *Input: The nullspace ker($\mathbf{A}$) of a singular graph, $\mathbf{W}$, and the first $p-1$ coefficients $c_0, c_1, \ldots, c_{p-2}$ of $M(G,x)$.*

Output: To determine
i)whether, or not zero is a main eigenvalue;
ii) If zero is a non-main eigenvalue, determine the possible values of κ and $\mathbf{x}_S$.

1. Construct the vector $\mathbf{g} := c_{p-2}\mathbf{j} + c_{p-3}\mathbf{A}\mathbf{j} + \ldots + c_0\mathbf{A}^{p-2}\mathbf{j} - \mathbf{A}^{p-1}\mathbf{j}$.

2. If $\mathbf{A}\mathbf{g} \neq \mathbf{0}$, then zero is a non-main eigenvalue and $\mathbf{x}_S = \frac{-\kappa}{c_{p-1}}\mathbf{g} + \mathbf{q}$ where $0 < \kappa < \rho_{max}$ and $\mathbf{q} \in ker(\mathbf{A})$;
else zero is a main eigenvalue.

This algorithm will be adapted to determine if a graph is Hamiltonian.

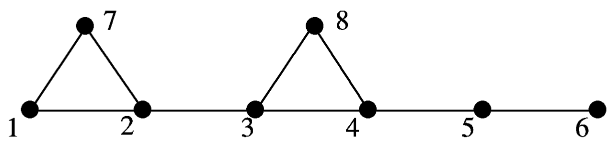

Figure 4: No (κ, κ)-regular sets

5 Examples

5.1 Core Graphs

Non-singular graphs with no (κ, κ)-regular sets are the cycles $C_n,\ n \neq 4k$. The non-singular graph in Figure 4 is another example. This graph has a non-trivial equitable partition which is a refinement of the walk partition. The graph has four main eigenvalues, $c_{p-1} = -3$ and $\mathbf{g} = (1, 2, 1, 2, 3, 1, 1, -1)^t$.

The graphs, in Figure 5, belong to three different categories.

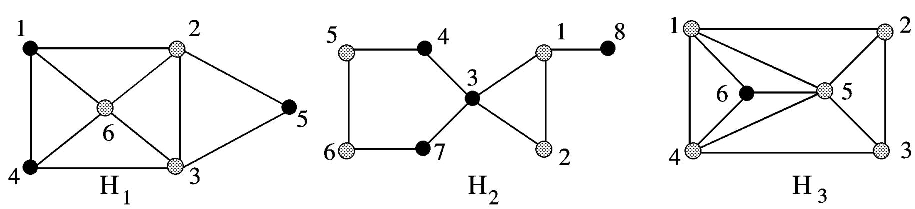

Figure 5: Graphs with (κ, κ)-regular sets.

The graph H_1 has the zero eigenvalue and one (κ, κ)-regular set, with $p = 4,\ \kappa = 2,\ c_{p-1} = -4$ and $\mathbf{g} = (0, 2, 2, 0, 0, 2)^t$. The (2,2)–regular set is $\{2, 3, 6\}$.The non-singular graph H_2 has a (1,1)-regular set, $p = 6$,

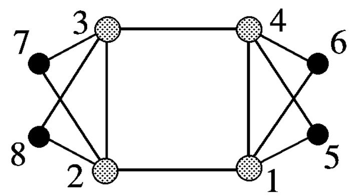

Figure 6: Non-regular core graph with a $(2,2)$-regular set.

$c_{p-1} = 1$ and $\mathbf{g} = (-1,0,0,0,-1,-1,0,-1)^t$. The graph H_3 has the zero eigenvalue, with two (κ,κ)-regular sets, $p = 3$, $c_{p-1} = -4$ and $\kappa = 2$, yielding $\mathbf{g} = (1,1,1,1,2,0)^t$. If $\mathbf{q} = (-1,-1,1,1,0,0)^t$, then $\mathbf{g} - \mathbf{q} = (2,2,0,0,2,0)^t$ and $\mathbf{g} + \mathbf{q} = (0,0,2,2,2,0)^t$, corresponding to $(2,2)$-regular sets $\{1,2,5\}$ and $\{3,4,5\}$, respectively.

There are core graphs with a (κ,κ)-regular set, which are not regular. The core graph of Figure 6 has a zero eigenvalue of multiplicity two. The main characteristic polynomial $M(G,x) = x^2 - 2x - 4$ and $\mathbf{g} = (-2,-2,-2,-2,0,0,0,0)^t$. Taking $\mathbf{q} = \mathbf{0}$ gives $\mathbf{x}_S = -\frac{2}{4}\mathbf{g}$, the $(2,2)$-regular set $\{1,2,3,4\}$, whereas $\mathbf{q} = \{\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, 0,0,0,0\}$ gives $\mathbf{x}_S = -\frac{1}{4}\mathbf{g} + \mathbf{q}$, the $(1,1)$-regular set $\{1,2\}$.

Two-regular graphs with a (κ,κ)-regular set S, satisfy $\kappa = 1$. The only connected graphs in this class are the cycles C_{4k} which are core graphs with a non-main zero eigenvalue of multiplicity two corresponding to independent (κ,κ)-regular sets. For the 2–regular graph C_8, $M(C_8,x) = x - 2$, $c_{p-1} = c_0 = 2$, $\kappa = 1$, $\mathbf{x}_S = \alpha_0\mathbf{j} + \mathbf{q}$ and $\kappa\mathbf{j} = \alpha_0 2\mathbf{j} + \mathbf{A}\mathbf{q}$. So $\alpha_0 = \frac{1}{2}$ and $\mathbf{g} = \alpha_0\mathbf{j}$. Taking $\mathbf{q} = \{\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}\}$ gives the $(1,1)$-regular set $\{1,2\} \cup \{5,6\}$.

The smallest tri-valent polyhedron, which is a nut graph is G_{12} of Figure 2, which has a $(1,1)$-regular set. Families of $\rho+1$–regular graphs with a (κ,κ)-regular set, can be grown from ρ–regular graphs. For instance from C_4, the two graphs G_6 of Figure 2 and the complete bipartite graph $K_{3,3}$ can be obtained. Duplicate vertices correspond to zero as a non-main eigenvalue, as in $K_{3,3}$. Any edge of $K_{3,3}$ is a $(1,1)$-regular set and any induced subgraph C_4 is a $(2,2)$-regular set.

5.2 A Graph with Zero as a Main Eigenvalue

When zero is a main eigenvalue, the graph has no (κ,κ)-regular sets.

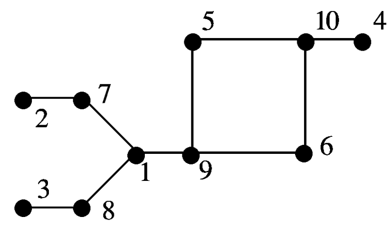

Figure 7: Repeated main zero eigenvalue

The graph on 10 vertices, shown in Figure 7, has zero as a main eigenvalue of multiplicity two. The main characteristic polynomial is $x^7 - 9x^5 + 21x^3 - 9x$ corresponding to the main eigenvalues 0, 2.33, -2.33, 1.73, -1.73, 0.742, -0.742.

A run of CHAR-VEC gives $\mathbf{g} = (-2, 2, 2, -2, 1, 1, 0, 0, 0, 0)^t$. Note that $\mathbf{Ag} = \mathbf{0}$, verifying that zero is a main eigenvalue and therefore $\mathbf{q} = \mathbf{0}$. The vertex set S, corresponding to the value of $\mathbf{x}_S$ obtained from (2), is not defined; that is G does not have a (κ, κ)-regular set, as expected from Corollary 37.

6 Hamiltonian Graphs

The subdivision of a Hamiltonian graph G retains the property of Hamiltonicity if and only if G is a cycle. If a vertex v has degree two, with neighbours u and w, then we can contract the edge uv without affecting Hamiltonicity. We may therefore consider graphs with minimum degree more than two.

6.1 The Spectrum of a Subdivision

We now consider the question: when is a subdivision G^* singular? The answer depends on the value of the dimension of the cycle space, also known as the *cyclomatic number*, $m - n$, of the graph G.

Lemma 48 *The nullity of the subdivision G^* of a graph G is*
$\begin{cases} m-n, & G \text{ non-bipartite;} \\ m-n+2, & G \text{ bipartite.} \end{cases}$

Proof: The subdivision G^* of a graph G is the bipartite graph $(\mathcal{V}_G, \mathcal{E}_G, \mathcal{E}^\star)$ where two vertices of G^* are adjacent if they are a vertex-edge pair in G.

Therefore for an appropriate labelling of the vertices, the adjacency matrix is $\mathbf{G}^*$ is of the form $\begin{pmatrix} \mathbf{0} & \mathbf{B}^t \\ \mathbf{B} & \mathbf{0} \end{pmatrix}$

where $\mathbf{B}$ is the $n \times m$ vertex-edge incidence matrix of G. Thus the

characteristic polynomial of G^* is $\det(\lambda \mathbf{I}_{m+n} - \mathbf{G}^*)$

$= \lambda^{(m-n)} |\lambda^2 \mathbf{I}_n - \mathbf{B}\mathbf{B}^t|$

$= \lambda^{(m-n)} |\lambda^2 \mathbf{I}_n - (\mathbf{D} + \mathbf{G})|$

Now the signless Laplacian $\mathbf{D} + \mathbf{G}$ is singular if and only if G is bipartite and its nullity is the number of bipartite components of G [1].

Therefore the nullity of G^* is $\begin{cases} m-n+2, & \text{if } G \text{ is bipartite;} \\ m-n, & \text{otherwise.} \end{cases}$

■

Corollary 49 *The subdivision G^* of a Hamiltonian graph G is non-singular if and only if G is C_{2k+1}, $k \in \mathbb{Z}^+$.*

Proof: From Lemma 48, the subdivision G^* of a connected graph G is non-singular if and only if G is a non-bipartite unicyclic graph. Since a unicyclic graph is Hamiltonian if and only if it is a cycle (with no pendent edges), and a bipartite graph is odd cycle–free, the result follows. ■

6.2 Recognition of Hamiltonian graphs

The next result is the basis of the $(m-n)$–fixed parameter, polynomial–time, algorithm ALGO-HAM that determines Hamiltonian cycles in a family $\mathcal{F}_{m-n}$ of graphs of fixed cyclomatic number $m-n$.

Theorem 50 *A graph $G \not\cong C_n$ is Hamiltonian if and only if its subdivision G^* has a $(2,2)$-regular set S inducing a connected subgraph.*

Proof: Let G be a graph and G^* its subdivision.

If an n–vertex graph G is a Hamiltonian graph drawn so that all vertices lie on an outer cycle with possibly other edges in the interior, and G^* is obtained from a copy of this drawing of G by inserting a vertex of degree two in each edge of G, then the vertices on the outer cycle of G^* form a $(2,2)$-regular set inducing a connected subgraph.

Conversely, if $S \subseteq \mathcal{V}(G^*)$ is a $(2,2)$-regular set inducing a connected subgraph, then the induced subgraph $G^*[S]$ is a 2-regular connected subgraph, that is, a cycle $C_{|S|}$. By construction, in every cycle of G^*, inserted vertices alternate with the original vertices of $\mathcal{V}(G)$. Every inserted vertex has only two neighbors. Therefore, an inserted vertex of G^* has its two neighbors in S, independently of whether it is in S or not. Furthermore, we claim that all the original vertices must be in S. Otherwise, assuming that there exists an original vertex $v \in \mathcal{V}(G)$ which is not in S, then it has two neighbors $x, y \in S$, by definition of a $(2,2)$-regular set, and both are inserted vertices in S. This is a contradiction as the degree of an inserted vertex is two. Therefore, the 2-regular connected subgraph $G^*[S]$ is C_{2n} and determines a Hamiltonian cycle C_n in G. ∎

Corollary 51 *If zero is a main eigenvalue of the subdivision G^* of a graph G, then G is not Hamiltonian.*

Proof: By Corollary 37, G^* has no (κ, κ)-regular sets. By Proposition 50, G is not Hamiltonian. ∎

As an immediate consequence we have:

Theorem 52 *Let G be a non-regular graph and G^* its subdivision. If G^* is singular and $\mathbf{g}^*$ is the discriminating vector of G^*, then G is Hamiltonian if and only if $\exists \mathbf{q}^* \in \mathcal{E}_{G^*}(0)$ such that $\frac{-\kappa}{c_{p-1}}\mathbf{g}^* + \mathbf{q}^*$ is the characteristic vector of a $(2,2)$-regular set $S \subset \mathcal{V}(G^*)$ inducing a connected subgraph.*

To determine a Hamiltonian cycle in a graph G^*, out of the m edges of G, $m-n$ are chosen for deletion. If there is a cycle on $2n$ vertices with n inserted vertices of degree two in G^*, then out of the the $m+n$ vertices of G^*, $(m+n)-2n = m-n$ are chosen for deletion. From these considerations alone, this approach and that from Theorem 52 seem to be of equal difficulty. However if we partition connected graphs into families $\mathcal{F}_{m-n}$ of fixed cyclomatic number, that is acyclic, unicyclic, bicyclic, etc., we propose an algorithm which when run on a graph in a particular family is polynomial–time. Even if this algorithm is not faster than the ones already used on families of graphs with a fixed cyclomatic number, the algebraic techniques used provide a novel insight into Hamiltonian cycles.

If $m < n$, then G is a tree or disconnected. If $m = n$ and the spectrum of $\mathbf{BB^t} - 2\mathbf{I}$ is that of the cycle C_n, then G is Hamiltonian. We shall propose an algorithm, based on Theorems 35 and 52, to determine if G is Hamiltonian for $m > n + 1$.

Algorithm 53 [ALGO-HAM] *For a graph in the family $\mathcal{F}_{m-n}$ of cyclomatic number $m - n$ at least two:*

Input Incidence Matrix $\mathbf{B}$ of G; $\kappa = 2$.

Step 1: Determine the adjacency matrix $\mathbf{A}$ of G^*. If $\mathbf{j}$ is the all-one vector, determine the least positive integer $p \geq 2$ such that the vectors

$\mathbf{j},\ \mathbf{Aj},\ \mathbf{A}^2\mathbf{j},\ \ldots,\ \mathbf{A}^p\mathbf{j}$ are linearly dependent.

Step 2: The entries $c_{p-1}, c_{p-2}, \ldots, c_0, 1$ of the generator of the one dimensional nullspace of the $n \times (p+1)$ matrix $\mathbf{W}_{p+1}$, obtained by augmenting the walk matrix with column $\mathbf{A}^p\mathbf{j}$, are determined by solving $\mathbf{W}_{p+1}\mathbf{x} = \mathbf{0}$.

Step 3: The discriminating vector $\mathbf{g}$ is $c_{p-2}\mathbf{j} + c_{p-3}\mathbf{Aj} + ... + c_0\mathbf{A}^{p-2}\mathbf{j} - \mathbf{A}^{p-1}\mathbf{j}$.

If $\mathbf{Ag} = \mathbf{0}$ then G^* has no (2,2)–regular sets and G is not Hamiltonian.

If $\mathbf{Ag} \neq \mathbf{0}$, then zero is a non-main eigenvalue of G^*.

Step 4: If $\mathbf{Ag} \neq \mathbf{0}$, and $\mathbf{y} = \left(\frac{-\kappa}{c_{p-1}}\right)\mathbf{g}$ is a $(0,1)$–vector with $2n$ non–zero entries corresponding to a connected induced subgraph of G^*, then G^* has a (2,2)–regular set defined by vector $\mathbf{x}_S$ and G is Hamiltonian.

Step 5: A basis $\mathbf{q}_1,\ \mathbf{q}_2,\ \ldots, \mathbf{q}_s$ where $s = m - n$ or $m - n + 2$ for the nullspace of $\mathbf{A}$ is determined. If $\mathbf{Ag} \neq \mathbf{0}$, and for some $\mathbf{q} \in \ker(\mathbf{A})$, $\left(\frac{-\kappa}{c_{p-1}}\right)\mathbf{g} + \sum_{i=1}^{s} \beta_i \mathbf{q}_i$ is a $(0,1)$–vector with $2n$ non–zero entries corresponding to a connected induced subgraph of G^*, then G has a (2,2)–regular set and G is Hamiltonian.

On analysing the modules of Algorithm 53,

we find that

(i) Step 1 involves multiplication of matrices and is polynomial-time of at most $O(n^4)$;

(ii) Step 2 may be done using Gaussian Elimination and is polynomial-time of at most $O(n^3)$;

(iii) Step 3 involves multiplication of matrices and is polynomial-time of at most $O(n^2)$;

(iv) Step 4 involves obtaining the multiplicity of the maximum eigenvalue of the subgraph $G^*[S]$ associated with $\mathbf{x}_S$, that is $\dim(\ker(\mathbf{G}^*[S]-2\mathbf{I}))$. If the multiplicity of the maximum eigenvalue of $G^*[S]$ is one then $\mathbf{y}$ corresponds to a connected induced subgraph of G^* on $2n$ vertices, and therefore G is Hamiltonian. The number of steps is at most $O(n^4)$;

(v) Step 5 involves determining unique values of the rational numbers β_i, that is solving $\left(\frac{-\kappa}{c_{p-1}}\right)\mathbf{g}^v + \sum_{i=1}^{s} \beta_i {\mathbf{q}^v}_i = \begin{cases} 0, \\ 1, \end{cases}$ obtained by taking the vth entry, for a sufficient number of vertices v.

If the multiplicity of the maximum eigenvalue of the subgraph $G^*[S]$ associated with $\mathbf{x}_S$ is one, then G is Hamiltonian. For a fixed cyclomatic number $m-n$, this module is polynomial-time of at most $O(n^4)$.

The algorithm we have developed contains polynomial-time modules and one module (step 5) which is exponential in s. Although the problem to determine whether a graph is Hamiltonian is NP-hard, it is polynomial-time solvable when restricted to a family of graphs with a fixed cyclomatic number $m-n$.

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