# Graphs with at most one generalized cospectral mate<sup>\*</sup>

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#### Abstract

Let G be an n-vertex graph with adjacency matrix A, and  $W = [e, Ae, ..., A^{n-1}e]$ be the walk matrix of G, where e is the all-one vector. In Wang [J. Combin. Theory, Ser. B, 122 (2017): 438-451], the author showed that any graph G is uniquely determined by its generalized spectrum (DGS) whenever  $2^{-\lfloor n/2 \rfloor}$  det W is odd and square-free. In this paper, we introduce a large family of graphs

 $\mathcal{F}_n = \{n \text{-vertex graphs } G \colon 2^{-\lfloor n/2 \rfloor} \det W = p^2 b \text{ and rank } W = n-1 \text{ over } \mathbb{Z}/p\mathbb{Z}\},\$ 

where b is odd and square-free, p is an odd prime and  $p \nmid b$ . We prove that any graph in  $\mathcal{F}_n$  either is DGS or has exactly one generalized cospectral mate up to isomorphism. Moreover, we show that the problem of finding the generalized cospectral mate for a graph in  $\mathcal{F}_n$  is equivalent to that of generating an appropriate rational orthogonal matrix from a given integral vector. This equivalence essentially depends on a surprising property of graphs in terms of generalized spectra, which states that any symmetric integral matrix generalized cospectral with the adjacency matrix of some graph must be an adjacency matrix. Based on this equivalence, we develop an efficient algorithm to decide whether a given graph in  $\mathcal{F}_n$  is DGS and further to find

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the unique generalized cospectral mate when it is not. We give some experimental results on graphs with at most 20 vertices, which suggest that  $\mathcal{F}_n$  may have a positive density (nearly 3%) and possibly almost all graphs in  $\mathcal{F}_n$  are DGS as  $n \to \infty$ . This gives supporting evidence for Haemers' conjecture that almost all graphs are determined by their spectra.

Mathematics Subject Classifications: 05C50

# 1 Introduction

All graphs considered in this paper are simple and undirected. The spectrum of a graph G, denoted by  $\sigma(G)$ , is the multiset of all eigenvalues of its adjacency matrix. The generalized spectrum of a graph G is defined to be the pair  $(\sigma(G), \sigma(\bar{G}))$ , where  $\bar{G}$  is the complement of G. Two graphs are generalized cospectral if they share the same generalized spectrum. Clearly, isomorphic graphs are generalized cospectral, but the converse is not true in general. Two graphs G and H are called a pair of generalized cospectral mates if they are generalized cospectral but nonisomorphic. A graph G is determined by generalized spectrum (or DGS for short) if it has no generalized cospectral mates, that is, all graphs having the same generalized spectrum as G are isomorphic to G. We remark that in the context of the classical adjacency spectrum, the corresponding notions have received considerable attention. We refer the readers to [1, 2].

We are mainly concerned with the generalized spectra of graphs in this paper. For a given graph G, a natural problem is to determine whether G is DGS or not, or more subtly, to find some or all (if any) generalized cospectral mates of G. The problem turns out to be very difficult in general. Nevertheless, Wang [12, 13] found a strong connection between this problem and the properties of walk matrices of graphs. For a graph G with n vertices, the walk matrix of G, denoted by W(G) or simply W, is the  $n \times n$  matrix  $[e, Ae, \ldots, A^{n-1}e]$ , where A is the adjacency matrix of G and e is the all-one column vector of dimension n. The following simple arithmetic condition on det W for a graph G being DGS was obtained in [13].

**Theorem 1** ([13]). If  $2^{-\lfloor \frac{n}{2} \rfloor} \det W$  (which is always an integer) is odd and square-free, then G is DGS.

The condition of Theorem 1 is the best possible in the sense that if det W has a multiple odd prime factor then G may not be DGS. A small counterexample can be found in [12]. The general idea hidden in that counterexample was revealed by the following theorem. For an integral matrix M and a prime p, we use rank<sub>p</sub>M to denote the rank of M over the finite field  $\mathbb{F}_p = \mathbb{Z}/p\mathbb{Z}$ .

**Theorem 2** ([11]). Let p be an odd prime. Suppose that det  $W \neq 0$  and the following conditions hold: (i)  $p^2 \mid \det W$ ; (ii)  $\operatorname{rank}_p W = n - 1$ ;

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(iii)  $W^{\mathrm{T}}z \equiv 0 \pmod{p}$  has a solution (permuting the entries, or equivalently reordering the vertices, if necessary) of the form

$$(\underbrace{-1,-1,\ldots,-1}_{p},\underbrace{1,1,\ldots,1}_{p},0,0,\ldots,0)^{\mathrm{T}}.$$

Then G is not DGS. Furthermore, G has a generalized cospectral mate whose adjacency matrix is similar to A via a rational orthogonal matrix

$$Q = \begin{pmatrix} \frac{1}{p} \begin{pmatrix} pI_p - J & J \\ J & pI_p - J \end{pmatrix} & \\ & & I_{n-2p} \end{pmatrix},$$
(1)

where I and J are the identity matrix and the all-one matrix, respectively.

The key point of Theorem 2 is that, under the stated assumptions, the matrix  $Q^{T}AQ$  must be a symmetric (0, 1)-matrix with vanishing diagonal, that is, an adjacency matrix. We remark that the established pair of generalized cospectral mates also has a clear meaning from the viewpoint of edge switchings. This kind of switching is referred to as generalized GM-switching, which, as an analogue to the original GM-switching method introduced in [3], can be used to construct some new pairs of generalized cospectral mates; see [6, 7] for some recent application of the generalized GM-switching in constructing cospectral strongly regular graphs.

The main weakness of the above theorem is the third condition. The required solution seems so special that it can rarely be satisfied. A natural question is whether there exist some other kinds of solutions to guarantee the existence of a generalized cospectral mate for G. What is the exact relationship between the DGS-property of G and the solutions to  $W^{T}z \equiv 0 \pmod{p}$ ?

In this paper, we shall introduce a large family of graphs closely related to the first two conditions of Theorem 2. The main discovery is that for this family of graphs, the DGS-property of a graph can be completely determined from any nontrivial solution to the equation  $W^{T}z \equiv 0 \pmod{p}$ . To give the definition, we first recall some basic facts about the Smith normal form of an integral matrix.

Two  $n \times n$  integral matrices  $M_1$  and  $M_2$  are *integrally equivalent* if  $M_2$  can be obtained from  $M_1$  by a sequence of the following operations: row permutation, row negation, addition of an integer multiple of one row to another and the corresponding column operations. Any integral invertible matrix M is integrally equivalent to a diagonal matrix diag  $[d_1, d_2, \ldots, d_n]$ , known as the *Smith normal form* of M, in which  $d_1, d_2, \ldots, d_n$  are positive integers with  $d_i \mid d_{i+1}$  for  $i = 1, \ldots, n-1$ . We are mainly interested in the Smith normal form of an invertible walk matrix. A particularly interesting example is the walk matrix for graphs satisfying the condition of Theorem 1.

**Theorem 3** ([13]). If  $2^{-\lfloor \frac{n}{2} \rfloor} \det W = b$  for some odd and square-free integer b, then the Smith normal form of W is

diag 
$$[\underbrace{1, 1, \dots, 1}_{\lceil \frac{n}{2} \rceil}, \underbrace{2, 2, \dots, 2, 2b}_{\lfloor \frac{n}{2} \rfloor}].$$

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Now we introduce a family of graphs using Smith normal forms of walk matrices.

**Definition 4.** For a positive integer n, we use  $\mathcal{F}_n$  to denote the family of all graphs G of order n such that the Smith normal form of W(G) is

diag 
$$[\underbrace{1,1,\ldots,1}_{\lceil \frac{n}{2}\rceil},\underbrace{2,2,\ldots,2,2p^2b}_{\lfloor \frac{n}{2}\rfloor}],$$

where b is odd and square-free, p is an odd prime and  $p \nmid b$ .

*Remark* 5. The unique odd prime p satisfying  $p^2 \mid \det W$  is a crucial parameter for a graph  $G \in \mathcal{F}_n$ . We shall use the notation  $\mathcal{F}_n^p = \{G \in \mathcal{F}_n : p^2 \mid \det W\}$ .

We note that graphs in  $\mathcal{F}_n$  can also be equivalently defined as graphs satisfying (i)  $2^{-\lfloor n/2 \rfloor} \det W = p^2 b$  and (ii)  $\operatorname{rank}_p W = n - 1$  simultaneously, with the same assumptions on b and p as in Definition 4. In particular, every graph in  $\mathcal{F}_n$  clearly satisfies the first two conditions of Theorem 2. Compared the Smith normal form in Definition 4 with that in Theorem 3, the only difference is the last invariant factor. For graphs in  $\mathcal{F}_n$ , the last invariant contains exactly one square factor. Intuitively, since a graph in  $\mathcal{F}_n$  almost satisfies the condition of Theorem 1, it may be almost determined by its generalized spectrum. Indeed, we shall prove the following theorem.

#### **Theorem 6.** Every graph in $\mathcal{F}_n$ has at most one generalized cospectral mate.

We shall prove Theorem 6 in Section 2.2. We relate any possible generalized cospectral mates of  $G \in \mathcal{F}_n^p$  to a particular kind of orthogonal matrices, which we call *primitive* matrices. We show that for a fixed graph  $G \in \mathcal{F}_n^p$  not being DGS, all possible primitive matrices related to G are unique up to column permutations. In Section 2.3, we further establish the equivalence between the existence of a generalized cospectral mate for a graph and the existence of a primitive matrix.

In order to give a complete criterion to distinguish two different kinds (DGS v.s. non-DGS) of graphs in  $\mathcal{F}_n$ , in Section 3 we develop a procedure to generate all possible primitive matrices from a given vector. When it succeeds, it finds a generalized cospectral mate; when it fails, it indicates that the given graph is DGS. Using the proposed algorithm, we conduct a numerical experiment on graphs with at most 20 vertices, which suggests that, for not too small n, while  $\mathcal{F}_n$  may have a stable positive density (nearly 3%), almost none of  $\mathcal{F}_n$  has a generalized cospectral mate. This gives some evidence for Haemers' conjecture that almost all graphs are determined by their spectra.

### 2 Existence and uniqueness of generalized cospectral mates

#### 2.1 Preliminaries

An orthogonal matrix Q is called *regular* if Qe = e (or equivalently,  $Q^{\mathrm{T}}e = e$ ). An old result of Johnson and Newman [8] states that two graphs G and H are generalized cospectral if and only if there exists a regular orthogonal matrix Q such that  $Q^{\mathrm{T}}A(G)Q = A(H)$ . A graph G is *controllable* if W(G) is invertible. For controllable graphs, the corresponding matrix Q is unique and rational [10].

**Lemma 7** ([8, 10]). Let G be a controllable graph of order n and H be a graph generalized cospectral with G. Then H is controllable and there exists a unique regular rational orthogonal matrix Q such that  $Q^{T}A(G)Q = A(H)$ . Moreover, the unique Q satisfies  $Q = W(G)W^{-1}(H)$  and hence is rational.

For a rational matrix Q, the *level* of Q, denoted by  $\ell(Q)$ , or simply  $\ell$ , is the smallest positive integer k such that kQ is an integral matrix. For a controllable graph G, define  $\mathcal{Q}(G)$  to be the set of all regular rational orthogonal matrices Q such that  $Q^{\mathrm{T}}A(G)Q$  is an adjacency matrix. It is easy to show that for any  $Q \in \mathcal{Q}(G)$ , the level  $\ell(Q)$  must be a factor of  $d_n$ , the last invariant factor of W(G). It turns out that under some mild assumptions on W, some factors of  $d_n$  can never be realized as levels for any  $Q \in \mathcal{Q}(G)$ . For nonzero integers n, m and positive integer k, we use  $m^k \parallel n$  to indicate that  $m^k$ precisely divides n, i.e.,  $m^k \mid n$  but  $m^{k+1} \nmid n$ .

**Lemma 8** ([12]). Let  $Q \in \mathcal{Q}(G)$  with level  $\ell$ , and p be an odd prime. Suppose that  $\operatorname{rank}_p W = n - 1$  and  $p \mid\mid \det W$  (or equivalently,  $p \mid\mid d_n$ ). Then  $p \nmid \ell$  and hence  $\ell \mid \frac{d_n}{n}$ .

**Lemma 9** ([13]). Let  $Q \in \mathcal{Q}(G)$  with level  $\ell$ . Suppose that  $\operatorname{rank}_2 W = \lceil n/2 \rceil$  and  $2^{\lfloor n/2 \rfloor} \parallel$  det W (or equivalently,  $2 \parallel d_n$ ). Then  $2 \nmid \ell$  and hence  $\ell \mid \frac{d_n}{2}$ .

Both of the above lemmas have been strengthened in a recent paper by Qiu et al. [9], using a new and unified approach. We need the following improvement of Lemma 8, which is an easy consequence of [9, Theorem 1.2].

**Lemma 10** ([9]). Let  $Q \in \mathcal{Q}(G)$  with level  $\ell$ , and p be an odd prime. Suppose that  $\operatorname{rank}_p W = n - 1$  and  $p^k \mid\mid \det W$  (or equivalently  $p^k \mid\mid d_n$ ) for some positive integer k. Then  $p^k \nmid \ell$  and hence  $\ell \mid \frac{d_n}{n}$ .

The following corollary is immediate.

**Corollary 11.** Let  $G \in \mathcal{F}_n^p$ . Then  $\ell(Q) = 1$  or  $\ell(Q) = p$  for any matrix  $Q \in \mathcal{Q}(G)$ .

Note that any regular rational orthogonal matrix with level one is a permutation matrix. Since permutation matrices generate isomorphic graphs, we shall be mainly concerned with the case  $\ell(Q) = p$ .

**Lemma 12.** Let  $G \in \mathcal{F}_n^p$  and  $Q \in \mathcal{Q}(G)$ . If  $\ell(Q) = p$  then  $\operatorname{rank}_p(pQ) = 1$ .

Proof. Let H be the graph such that  $Q^{\mathrm{T}}A(G)Q = A(H)$ . Then  $Q^{\mathrm{T}}W(G) = W(H)$ , or equivalently,  $W^{\mathrm{T}}(G)Q = W^{\mathrm{T}}(H)$ . Write  $\hat{Q} = pQ$ . We have  $W^{\mathrm{T}}(G)\hat{Q} = pW^{\mathrm{T}}(H) \equiv 0$ (mod p). As  $G \in \mathcal{F}_n^p$ , we see that  $\operatorname{rank}_p W(G) = n - 1$  and hence  $\operatorname{rank}_p W^{\mathrm{T}}(G) = n - 1$ . Therefore, the solution space of  $W^{\mathrm{T}}(G)z \equiv 0 \pmod{p}$  is one dimensional. Consequently,  $\operatorname{rank}_p \hat{Q} \leq 1$ . On the other hand, since  $\ell(Q) = p$ , the minimality of  $\ell(Q)$  means that  $\hat{Q}$ contains at least one entry which is nonzero over  $\mathbb{F}_p$ . Thus  $\operatorname{rank}_p \hat{Q} \geq 1$ . This proves that  $\operatorname{rank}_p \hat{Q} = 1$ , as desired.

#### 2.2 Primitive matrix and its uniqueness

We always assume that p is an odd prime.

**Definition 13.** A regular rational orthogonal matrix Q of level p is called a *primitive* matrix if rank<sub>p</sub>(pQ) = 1.

**Example 14.** Consider a regular rational orthogonal matrix

$$Q = \frac{1}{3} \begin{pmatrix} -1 & 2 & 0 & 2\\ 0 & 0 & 3 & 0\\ 2 & -1 & 0 & 2\\ 2 & 2 & 0 & -1 \end{pmatrix}.$$
 (2)

One can see that  $\ell(Q) = 3$  and  $\operatorname{rank}_3(3Q) = 1$ . Thus, Q is a primitive matrix.

Removing the second row and the third column from Q, the resulting submatrix is also a primitive matrix, each entry of which is nonintegral. The following lemma summarizes this phenomenon in a slightly different manner.

**Lemma 15.** Let Q be a primitive matrix of order n. If there exists some entry which is integral, then after necessary row permutations and column permutations, Q has the quasi-diagonal form diag  $[Q_0, I]$ , where  $Q_0$  is a primitive matrix containing no integral entries.

Proof. Clearly for any primitive matrix Q, the integral entry of Q can only be 0 or 1. Moreover, we claim that Q contains 0 if and only if Q contains 1. The 'if' part is clear since each row (and column) of Q has length one in  $\mathbb{R}^n$ . Let the (i, j)-entry  $q_{i,j}$  of Qbe zero. Write  $\hat{Q} = pQ$ . Then either the *i*-th row or the *j*-th column of  $\hat{Q}$  is the zero vector over  $\mathbb{F}_p$  since otherwise one would easily find a  $2 \times 2$  invertible submatrix in  $\hat{Q}$ , contradicting the fact that rank<sub>p</sub>( $\hat{Q}$ ) = 1. Clearly, in either case,  $\hat{Q}$  contains p as an entry, i.e., Q contains 1 as an entry.

Suppose that Q has exactly k entries equal to one. Then these k entries clearly lie in different rows and columns in Q, and all other entries in the involved rows and columns are necessarily zero. Thus, by some obvious row and column permutations, we can change Q into a quasi-diagonal form diag  $[Q_0, I_k]$ . Clearly  $Q_0$  is a primitive matrix. Finally, as  $Q_0$  does not contain 1 as an entry, it does not contain 0 as an entry. Thus,  $Q_0$  contains no integral entries.

**Definition 16.** Let v be an n-dimensional integral vector and Q be a primitive matrix. We say Q can be generated from v (or v can generate Q) if each column of pQ is a multiple of v over  $\mathbb{F}_p$ .

Remark 17. If a primitive matrix Q can be generated from v and v' is an integral vector such that  $v' \equiv cv \pmod{p}$  for some  $c \not\equiv 0 \pmod{p}$ , then Q can also be generated from v'.

Now we can give a necessary condition for a graph in  $\mathcal{F}_n$  to have a generalized cospectral mate.

**Proposition 18.** Let  $G \in \mathcal{F}_n^p$ . If G is not DGS then any nontrivial solution to  $W^T z \equiv 0 \pmod{p}$  can generate some primitive matrix.

*Proof.* As G is not DGS, we see that  $\mathcal{Q}(G)$  contains a matrix which is not a permutation matrix. Let Q be such a matrix in  $\mathcal{Q}(G)$ . Then by Corollary 11, we have  $\ell(Q) = p$ . Moreover, by Lemma 12, we see that  $\operatorname{rank}_p(pQ) = 1$  and hence Q is a primitive matrix. From the proof of Lemma 12, we find that the column space of pQ coincides with the (one-dimensional) solution space of  $W^T z \equiv 0 \pmod{p}$ . The proposition follows.

Remark 19. Under the assumption of Proposition 18, each matrix  $Q \in \mathcal{Q}(G)$  that is not a permutation matrix can be generated from a nontrivial solution to  $W^{\mathrm{T}}z \equiv 0 \pmod{p}$ .

Suppose Q is a primitive matrix generated from v. By the very definition, we know that all matrices obtained from Q by column permutations can also be generated from v. A key result of this section is to show the reversed direction: Every primitive matrix generated from v can be obtained from Q by some column permutations.

The following lemma plays a fundamental role in this paper.

**Lemma 20.** Let u and v be two n-dimensional integral column vectors with each entry nonzero modulo p. Suppose that (i) u and v are linearly dependent over  $\mathbb{F}_p$ ; (ii)  $u \neq \pm v$ ; and (iii)  $u^{\mathrm{T}}u = v^{\mathrm{T}}v = p^2$ . Then  $u^{\mathrm{T}}v = 0$ .

*Proof.* Since u and v are linearly dependent over  $\mathbb{F}_p$ , there exist two integers a and b, not both zero in  $\mathbb{F}_p$ , such that

$$au + bv \equiv 0 \pmod{p}.$$
 (3)

We claim that neither a nor b is zero. Actually, if  $a \equiv 0 \pmod{p}$  then  $b \not\equiv 0 \pmod{p}$  and hence we obtain  $v \equiv 0 \pmod{p}$  by (3). This contradicts our assumption on v. Thus  $a \not\equiv 0 \pmod{p}$ . Similarly, we also have  $b \not\equiv 0 \pmod{p}$ . This proves the claim.

By (3) we have  $(au+bv)^{\mathrm{T}}(au+bv) \equiv 0 \pmod{p^2}$ , that is,  $a^2u^{\mathrm{T}}u + 2abu^{\mathrm{T}}v + b^2v^{\mathrm{T}}v \equiv 0 \pmod{p^2}$ , which can be reduced to

$$2abu^{\mathrm{T}}v \equiv 0 \pmod{p^2},\tag{4}$$

as  $u^{\mathrm{T}}u = v^{\mathrm{T}}v = p^2$ . Since  $2ab \not\equiv 0 \pmod{p}$ , Eq. (4) can be further reduced to  $u^{\mathrm{T}}v \equiv 0 \pmod{p^2}$ .

By the Cauchy-Schwarz inequality, we have  $|u^{\mathrm{T}}v| \leq \sqrt{u^{\mathrm{T}}u}\sqrt{v^{\mathrm{T}}v}$  with the equality holding if and only if u and v are linearly dependent over  $\mathbb{R}$ . From the last two conditions of this lemma, one clearly sees that u and v are not linearly dependent over  $\mathbb{R}$ . Therefore, we must have  $|u^{\mathrm{T}}v| < p^2$ , which, together with the established congruence  $u^{\mathrm{T}}v \equiv 0$ (mod  $p^2$ ), implies  $u^{\mathrm{T}}v = 0$ . This completes the proof.  $\Box$ 

**Theorem 21.** Let Q be a primitive matrix generated from v. Then every primitive matrix generated from v can be obtained from Q by some column permutations.

*Proof.* Let Q' be any primitive matrix generated from v. We use  $\alpha_i$  and  $\beta_i$  respectively to denote the *i*-th column of pQ and pQ', for i = 1, 2, ..., n. We first consider the case that each entry of v is nonzero modulo p.

We claim that Q (and similarly Q') contains no integral entries. Suppose to the contrary that Q contains an integral entry. Then Q contains one as an entry, say  $q_{i,j} = 1$ . Let  $\alpha_k$  be the k-th column such that  $\alpha_k \not\equiv 0 \pmod{p}$ . Then we have  $\alpha_k = cv \pmod{p}$  for some integer c. Since  $\alpha_k$  contains at least one entry which is nonzero modulo p, we see that  $c \not\equiv 0 \pmod{p}$ . Consequently, as we assume that each entry of v is nonzero modulo p, we find that each entry of  $\alpha_k$  is nonzero modulo p, that is each entry of  $\alpha_k/p$  is nonintegral. But, as  $q_{i,j} = 1$ , the *i*-th row of Q must be a standard unit vector and hence at least one entry of  $\alpha_k/p$  is integral. This contradiction proves the claim.

We next claim that either  $\alpha_i = \beta_j$  or  $\alpha_i^{\mathrm{T}}\beta_j = 0$  for each pair (possibly equal) *i* and *j*. We may assume  $\alpha_i \neq \beta_j$ . Noting that  $e^{\mathrm{T}}\alpha_i = e^{\mathrm{T}}\beta_j = p$ , it can never happen that  $\alpha_i \neq -\beta_j$ . Thus,  $\alpha_i \neq \pm \beta_j$ . Moreover, as *Q* and *Q'* contains no integral entries, both  $\alpha_i$ and  $\beta_j$  are nonzero multiples of *v* over  $\mathbb{F}_p$ . Thus,  $\alpha_i$  and  $\beta_j$  are linearly dependent over  $\mathbb{F}_p$ , and each entry of  $\alpha_i$  and  $\beta_j$  is nonzero modulo *p*. Of course,  $\alpha_i^{\mathrm{T}}\alpha_i = \beta_j^{\mathrm{T}}\beta_j = p^2$  by the orthogonality of *Q* and *Q'*. Therefore, all conditions of Lemma 20 for  $u = \alpha_i$  and  $v = \beta_j$ are satisfied and we can obtain  $\alpha_i^{\mathrm{T}}\beta_j = 0$ , as claimed. Now we fix  $\beta_j$  and consider all possible  $\alpha_i$ 's. Note that  $\{\alpha_1, \alpha_2, \ldots, \alpha_n\}$  constitutes a basis of  $\mathbb{R}^n$ . Since  $\beta_j$  is a nonzero vector in  $\mathbb{R}^n$ , the equality  $\alpha_i^{\mathrm{T}}\beta_j = 0$  cannot hold for all *i* simultaneously. Thus, by the claim,  $\beta_j = \alpha_i$  for some *i*. That is, the *j*-th column of *pQ'* must appear as a column of *pQ*. Noting that all columns of *pQ'* are pairwise different, we see that *pQ'* can be obtained from *pQ*, or equivalently, *Q'* can be obtained from *Q*, by some column permutations.

It remains to consider that case that v contains at least one entry which is zero modulo p. For convenience, we make a similar assumption on v as in the proof of Lemma 15. Assume all nonzero entries of v appear as the first k entries and write

$$v = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}$$
,

where  $v_1$  is the k-dimensional column vector consisting of the first k entries and  $v_2$  is the (n-k)-dimensional zero vector. We remark that this assumption corresponds to the row permutations in Lemma 15. Next we forbid row permutations and continue to use only column permutations to transform Q and Q' into quasi-diagonal forms. It is not difficult to see that Q and Q' have similar quasi-diagonal forms, say diag  $[Q_0, I]$  and diag  $[Q'_0, I]$ , where both  $Q_0$  and  $Q'_0$  have order k, the number of nonzero entries in v. Moreover, both  $Q_0$  and  $Q'_0$  can be generated from  $v_1$ . Using the conclusion for the first case, we see that  $Q'_0$  can be obtained from  $Q_0$  by some column permutations. Clearly, taking the same column permutations on diag  $[Q_0, I]$  will result in diag  $[Q'_0, I]$ . Since diag  $[Q_0, I]$  and diag  $[Q'_0, I]$  are obtained from Q and Q' by some column permutations, we find that Q' can be obtained from Q by some column permutations.

Before presenting the proof of Theorem 6, we would like to record the following fact from the above proof.

Remark 22. If each entry of v is nonzero (mod p) and Q is a primitive matrix generated from v, then each entry of Q is nonintegral (or equivalently, nonzero).

Proof of Theorem 6. Let  $G \in \mathcal{F}_n^p$ . We may assume that G is not DGS. Let  $H_1$  and  $H_2$  be any two generalized cospectral mates of G. It suffices to show that  $H_1$  and  $H_2$  are isomorphic. Let  $Q_1$  and  $Q_2$  be the corresponding matrices such that  $Q_1^T A(G)Q_1 = A(H_1)$  and  $Q_2^T A(G)Q_2 = A(H_2)$ . Let v be a nontrivial solution to  $W^T(G)z \equiv 0 \pmod{p}$ . Then by Corollary 18 and Remark 19, we see that both matrices  $Q_1$  and  $Q_2$  can be generated from v. It follows from Theorem 21 that  $Q_2 = Q_1P$  for some permutation matrix P. Now, we have  $A(H_2) = Q_2^T A(G)Q_2 = Q_2^T Q_1 A(H_1)Q_1^T Q_2 = P^T A(H_1)P$ , indicating that  $H_1$  and  $H_2$  are isomorphic. This completes the proof of Theorem 6.

### 2.3 0-1 property of $Q^{\mathrm{T}}AQ$

The main aim of this subsection is to show that the converse of Proposition 18 is also true. We need an interesting and somewhat unexpected result on the adjacency matrix of a simple graph, which may have independent interests. Roughly speaking, among all integral symmetric matrices, the subsets of all adjacency matrices are 'closed' under generalized cospectrality. Here, the generalized spectrum of a matrix A naturally refers to the spectrum of A together with the spectrum of J - I - A.

**Lemma 23.** Let A be an adjacency matrix and B be an integral symmetric matrix. If A and B are generalized cospectral then B must also be an adjacency matrix.

Proof. For any  $n \times n$  matrix M and integer  $k \in \{1, \ldots, n\}$ , we use  $c_k(M)$  to denote the coefficient of the term  $x^{n-k}$  in the characteristic polynomial  $\det(xI - M)$  of M. Define  $\xi(M) = c_2(M) + c_2(J - I - M)$ . It is well known that  $(-1)^k c_k(M)$  equals the sum of its principal minors of size k; see e.g. [5, Theorem 1.2.16]. When k = 2 and M is an adjacency matrix,  $c_2(M)$  equals the opposite of the number of edges in the corresponding graph. Since the total number of edges in a graph and its complement is the constant  $\binom{n}{2}$ , we have

$$\xi(A) = -\binom{n}{2}.\tag{5}$$

Write  $B = (b_{i,j})_{n \times n}$ . Note that tr(A) = 0 as each diagonal entry of A is zero. Since A and B are cospectral, we have tr(B) = 0, that is,

$$\sum_{1 \le k \le n} b_{k,k} = 0. \tag{6}$$

Next we estimate  $\xi(B)$ , the sum of  $c_2(B)$  and  $c_2(J-I-B)$ . Noting that B is symmetric, we have

$$c_2(B) = \sum_{1 \le i < j \le n} \begin{vmatrix} b_{i,i} & b_{i,j} \\ b_{j,i} & b_{j,j} \end{vmatrix} = \sum_{1 \le i < j \le n} b_{i,i} b_{j,j} - \sum_{1 \le i < j \le n} b_{i,j}^2,$$
(7)

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and similarly,

$$c_2(J - I - B) = \sum_{1 \le i < j \le n} \begin{vmatrix} -b_{i,i} & 1 - b_{i,j} \\ 1 - b_{j,i} & -b_{j,j} \end{vmatrix} = \sum_{1 \le i < j \le n} b_{i,i} b_{j,j} - \sum_{1 \le i < j \le n} (1 - b_{i,j})^2.$$
(8)

Adding the above two equalities and using (6), we find

$$\xi(B) = 2 \sum_{1 \leq i < j \leq n} b_{i,i} b_{j,j} - \sum_{1 \leq i < j \leq n} \left( b_{i,j}^2 + (1 - b_{i,j})^2 \right)$$
  
$$= \left( \sum_{1 \leq k \leq n} b_{k,k} \right)^2 - \sum_{1 \leq k \leq n} b_{k,k}^2 - \sum_{1 \leq i < j \leq n} \left( 2 \left( b_{i,j} - \frac{1}{2} \right)^2 + \frac{1}{2} \right)$$
  
$$\leq - \sum_{1 \leq i < j \leq n} \left( 2 \left( b_{i,j} - \frac{1}{2} \right)^2 + \frac{1}{2} \right), \qquad (9)$$

where equality holds in (9) if and only if  $\sum_{1 \leq k \leq n} b_{k,k}^2 = 0$ , i.e., all diagonals of *B* are zero. Consider the quadratic function  $f(x) = 2(x - 1/2)^2 + 1/2$ ,  $x \in \mathbb{Z}$ . It is easy to see

Consider the quadratic function  $f(x) = 2(x - 1/2)^2 + 1/2$ ,  $x \in \mathbb{Z}$ . It is easy to see that  $f(x) \ge 1$  for all  $x \in \mathbb{Z}$ , and the equality holds if and only if  $x \in \{0, 1\}$ . Since B is integral, we have

$$-\sum_{1 \le i < j \le n} \left( 2\left(b_{i,j} - \frac{1}{2}\right)^2 + \frac{1}{2} \right) \le -\sum_{1 \le i < j \le n} 1 = -\binom{n}{2},$$
(10)

with equality holding if and only if each non-diagonal entry  $b_{i,j}$  is 0 or 1. Finally, as A and B are generalized cospectral, we must have  $\xi(A) = \xi(B)$  and hence  $\xi(B) = -\binom{n}{2}$  by (5). This means that the equalities must hold in (9) and (10) simultaneously. Using the established conditions for these two equalities, we find that the symmetric matrix B is a (0, 1)-matrix with vanishing diagonal. This completes the proof of this lemma.

**Lemma 24** ([11]). Let G be a controllable graph with n vertices. Let p be an odd prime. Suppose that  $p^2 \mid \det W$  and  $\operatorname{rank}_p W = n - 1$ . Let v be a nontrivial integral solution to  $W^{\mathrm{T}}z \equiv 0 \pmod{p}$ . If there exists a primitive matrix Q generated from v, then  $Q^{\mathrm{T}}AQ$  is an integral matrix.

Now we can show that the necessary condition for G to have a generalized cospectral mate is also sufficient.

**Theorem 25.** Let  $G \in \mathcal{F}_n^p$ . Then G is not DGS if and only if any nontrivial solution to  $W^{\mathrm{T}}z \equiv 0 \pmod{p}$  can generate some primitive matrix.

*Proof.* It suffices to show the sufficiency part. Let v be a nontrivial solution to  $W^{\mathrm{T}}v \equiv 0 \pmod{p}$ . Let Q be a primitive matrix generated from v. Clearly, G satisfies the condition of Lemma 24. Thus,  $Q^{\mathrm{T}}AQ$  is an integral matrix. Note that  $Q^{\mathrm{T}}AQ$  is generalized cospectral with A. It follows from Lemma 23 that  $Q^{\mathrm{T}}AQ$  is the adjacency matrix of some graph, say H. Noting that G is controllable but Q is not a permutation matrix, Lemma 7 implies that G is nonisomorphic to H and hence G is not DGS. This proves the theorem.

# 3 Finding generalized cospectral mates

We shall develop an algorithm to determine whether a given graph  $G \in \mathcal{F}_n^p$  is DGS. And when the graph G is not DGS, the algorithm will find its (unique) generalized cospectral mate. The overall idea is based on Theorem 25. We pick an arbitrary nontrivial solution v of  $W^{\mathrm{T}}(G)z \equiv 0 \pmod{p}$  and try to generate a primitive matrix. By Lemma 15, it suffices to consider the restricted case that every entry of v is nonzero modulo p. Indeed, for general v, we use  $v^*$  to denote the vector obtained from v by deleting the zero entries. Then it is easy to see that v can generate a primitive matrix if and only if  $v^*$  can do so. To generate a primitive matrix Q from v with t zero entries, we first use  $v^*$  to generate a primitive matrix  $Q_0$  of order n - t. Then we can obtain an  $n \times n$  primitive matrix Qfrom  $Q_0$  by adding t 1's and appropriate number of 0's naturally as in Example 14.

### 3.1 Criterion for a vector to generate a primitive matrix

The following lemma gives a simple necessary condition for an integral vector to generate some primitive matrix. It essentially appeared in [10]. We include its short proof here.

**Lemma 26** ([10]). Let v be an n-dimensional integral vector. If v can generate some primitive matrix Q, then  $v^{T}e \equiv 0 \pmod{p}$  and  $v^{T}v \equiv 0 \pmod{p}$ .

Proof. Let  $\hat{Q} = pQ$  and u be a column of  $\hat{Q}$  such that  $u \not\equiv 0 \pmod{p}$ . By the condition of this lemma, there exists an integer c such that  $u \equiv cv \pmod{p}$ . As  $u \not\equiv 0 \pmod{p}$ , we must have  $c \not\equiv 0 \pmod{p}$ . Let d be an integer such that  $cd \equiv 1 \pmod{p}$ . Then we have  $v \equiv du \pmod{p}$ . Noting that  $\hat{Q}^{\mathrm{T}}e = pQ^{\mathrm{T}}e = pe$  and  $\hat{Q}^{\mathrm{T}}\hat{Q} = p^2I$ , we have  $u^{\mathrm{T}}e = p$  and  $u^{\mathrm{T}}u = p^2$ . Thus,  $v^{\mathrm{T}}e \equiv du^{\mathrm{T}}e \equiv 0 \pmod{p}$  and  $v^{\mathrm{T}}v \equiv d^2u^{\mathrm{T}}u \equiv 0 \pmod{p}$ . This proves the lemma.

**Definition 27.** For two integral vectors v and w, we call w a perfect p-representative of v if w satisfies (i)  $w \equiv v \pmod{p}$ , (ii)  $w^{\mathrm{T}}e = p$ , and (iii)  $w^{\mathrm{T}}w = p^2$ .

**Proposition 28.** Let v be an integral vector with each entry nonzero modulo p. Let  $c_1$  and  $c_2$  be two distinct integers in  $\{1, 2, ..., p-1\}$ . Then the followings hold:

(i) Any two distinct perfect p-representatives  $u_1$  and  $u_2$  of  $c_1v$  are orthogonal in  $\mathbb{R}^n$ .

(ii) Any two perfect p-representatives  $w_1$  and  $w_2$  of  $c_1v$  and  $c_2v$  respectively are distinct and orthogonal in  $\mathbb{R}^n$ .

*Proof.* Note that  $u_1 \equiv u_2 \equiv c_1 v \pmod{p}$ . The assumptions on v and  $c_1$  imply that each entry of  $u_1$  and  $u_2$  is nonzero modulo p. As  $u_1 \equiv u_2 \pmod{p}$ , we see that  $u_1$  and  $u_2$  are clearly linearly dependent over  $\mathbb{F}_p$ . Since  $u_1^{\mathrm{T}}e = u_2^{\mathrm{T}}e = p$ , we must have  $u_1 \neq -u_2$  and hence  $u_1 \neq \pm u_2$  as  $u_1$  and  $u_2$  are distinct. Noting that  $u_1^{\mathrm{T}}u_1 = u_2^{\mathrm{T}}u_2 = p^2$  and using Lemma 20 we have  $u_1^{\mathrm{T}}u_2 = 0$ . This proves (i).

By the assumptions on v,  $c_1$  and  $c_2$ , we see that  $c_1v \not\equiv c_2v \pmod{p}$ . Noting that  $w_1 \equiv c_1v$  and  $w_2 \equiv c_2v$ , we have  $w_1 \not\equiv w_2$  and hence  $w_1 \not\equiv w_2$ . Now, (ii) holds by a similar argument as in (i).

**Theorem 29.** Let v be an m-dimensional integral vector with each entry nonzero modulo p. For each  $k \in \{1, 2, ..., p-1\}$ , let  $\mathcal{R}_k$  denote the collection of all perfect p-representatives of kv. Then v can generate a primitive matrix if and only if  $\sum_{k=1}^{p-1} |\mathcal{R}_k| = m$ .

Proof. Suppose Q is a primitive matrix generated from v. Since every entry of v is nonzero (mod p), we see from Remark 22 that Q contains no integral entries. Let z be any column of pQ. Then each entry of z is nonzero modulo p and of course  $z \not\equiv 0 \pmod{p}$ . Thus  $z \equiv kv \pmod{p}$  for some  $k \in \{1, 2, \ldots, p-1\}$ . Consequently, by the regularity and orthogonality of Q, we find that z is a perfect p-representative of kv, i.e.,  $z \in \mathcal{R}_k$ . Thus, we have  $\sum_{k=1}^{p-1} |\mathcal{R}_k| \ge m$ . By Proposition 28, all these p-1 sets  $\mathcal{R}_k$ 's are disjoint and any two vectors in  $\bigcup_{k=1}^{p-1} \mathcal{R}_k$  are orthogonal in  $\mathbb{R}^m$ . Thus the strict inequality  $\sum_{k=1}^{p-1} |\mathcal{R}_k| > m$  can never hold and hence  $\sum_{k=1}^{p-1} |\mathcal{R}_k| = m$ .

Suppose  $\sum_{k=1}^{p-1} |\mathcal{R}_k| = m$ . We construct an integral matrix  $\hat{Q}$  using all the *m* vectors in  $\bigcup_{k=1}^{p-1} \mathcal{R}_k$ . Using Definition 27 and Proposition 28, we can check that  $\frac{1}{p}\hat{Q}$  is a primitive matrix and  $\frac{1}{p}\hat{Q}$  is generated by *v*.

#### 3.2 Constructing all perfect *p*-representatives

**Definition 30.** For two integral vectors v and w, we call w the shortest *p*-representative of v if  $w \equiv v \pmod{p}$  and  $|w_i| \leq \frac{p-1}{2}$  for each entry  $w_i$  of w.

Remark 31. For a given integral vector v, there may be no, unique or many perfect p-representatives of v. Nevertheless, the shortest p-representative of v always exists and is unique. Also note that the shortest p-representative of v has the shortest Euclidian length among all vectors that are congruent to v modulo p.

### **Example 32.** Let n = 6, p = 3,

$$v = \begin{pmatrix} 2\\2\\2\\1\\1\\1 \end{pmatrix} \quad \text{and} \quad \hat{Q} = \begin{pmatrix} 2 & -1 & -1 & 1 & 1 & 1\\-1 & 2 & -1 & 1 & 1 & 1\\-1 & -1 & 2 & 1 & 1 & 1\\1 & 1 & 1 & 2 & -1 & -1\\1 & 1 & 1 & -1 & 2 & -1\\1 & 1 & 1 & -1 & -1 & 2 \end{pmatrix}$$

Then the shortest 3-representative of v is  $(-1, -1, -1, 1, 1, 1)^{T}$ . All the first 3 columns of  $\hat{Q}$  are perfect 3-representatives of v, while the remaining three columns are perfect 3-representatives of 2v.

The next lemma indicates that all perfect p-representatives of a vector v are very close to its shortest p-representative in the sense of Hamming distance. Recall that the Hamming distance of two vectors is the number of positions in which they differ.

**Lemma 33.** For an integral vector v with each entry nonzero modulo p, let w be a perfect p-representative and u be the shortest p-representative of v. Then the Hamming distance of w and u is at most 3. Moreover, for any index i such that  $w_i \neq u_i$ , either (i)  $w_i = u_i + p$  and  $u_i < 0$ , or (ii)  $w_i = u_i - p$  and  $u_i > 0$ .

*Proof.* Let *i* be an index such that  $w_i \neq u_i$ . As  $w_i \equiv u_i \pmod{p}$  and  $|u_i| \leq \frac{p-1}{2}$ , it is not difficult to see that  $|w_i| \geq \frac{p+1}{2}$  and consequently,  $w_i^2 > \frac{p^2}{4}$ . Therefore, there are at most 3 different such indices as  $w^T w = p^2$ . This proves the first part of this lemma. Note that  $w_i = u_i + kp$  for some integer *k*. It is easy to verify the remaining part using the obvious restriction that  $|w_i| < p$ .

The following proposition is immediate from Lemma 33.

**Proposition 34.** For an integral vector v with each entry nonzero modulo p, let u be the shortest p-representative of v. If v has at least one perfect p-representative, then  $|u^{\mathrm{T}}e - p| \leq 3p$  and  $u^{\mathrm{T}}u \leq p^2$ .

Using the entry sum of the shortest *p*-representative of a vector v, we can know more about its perfect *p*-representatives. Let  $e_i$  denote the *i*-th standard unit vector in  $\mathbb{R}^n$ .

**Lemma 35.** For an integral vector v with each entry nonzero modulo p, let u be the shortest p-representative of v. Suppose that  $u^{\mathrm{T}}e - p = sp$  for some  $s \in \{-3, -2, \ldots, 3\}$  and  $u^{\mathrm{T}}u \leq p^2$ . Then any perfect p-representative w of v can be written as

$$w = u + \sum_{i \in I} pe_i - \sum_{j \in D} pe_j, \tag{11}$$

where I and D are disjoint (possibly empty) subsets of  $\{1, 2, ..., n\}$  satisfying the following conditions:

(i)  $|I| + |D| \leq 3;$ (ii) |D| - |I| = s;(iii)  $u_i < 0$  for each  $i \in I$  and  $u_j > 0$  for  $j \in D;$  and (iv)  $\sum_{k \in I \cup D} |u_k| = \frac{1}{2p} u^{\mathrm{T}} u + \frac{p}{2} (|I| + |D| - 1).$ 

*Proof.* By Lemma 33, we know that w can be expressed as in (11) where I and D are disjoint subsets of  $\{1, 2, \ldots, n\}$  satisfying (i) and (iii). By (11), we have

$$w^{\mathrm{T}}e = u^{\mathrm{T}}e + p(|I| - |D|) = p + sp + p(|I| - |D|).$$

Thus,  $w^{\mathrm{T}}e = p$  is equivalent to (ii). It remains to check (iv). Due to (iii), we can rewrite (11) as

$$w = u - p \sum_{k \in I \cup D} \operatorname{sgn}(u_k) e_k.$$
(12)

Since  $e_k$ 's are standard unit vectors, we have

$$w^{\mathrm{T}}w = u^{\mathrm{T}}u + p^{2}\sum_{k\in I\cup D}e_{k}^{\mathrm{T}}e_{k} - 2p\sum_{k\in I\cup D}\mathrm{sgn}(u_{k})u^{\mathrm{T}}e_{k} = u^{\mathrm{T}}u + p^{2}(|I| + |D|) - 2p\sum_{k\in I\cup D}|u_{k}|.$$
(13)

Now it is straightforward to see that  $w^{\mathrm{T}}w = p^2$  if and only if (iv) holds.

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The following table gives a more visual description of Lemma 35. We may call the desired set I (resp. D) an *increasing* subset (resp. *decreasing* subset). For any  $s \in \{-3, -2, \ldots, 3\}$ , all possible pairs (|I|, |D|) for the sizes of I and D are rather restricted due to (i) and (ii). For example, when s = -3, we must have (|I|, |D|) = (3, 0); when s = -1, we have (|I|, |D|) = (1, 0), or (2, 1). In Table 1, we use

$$\underbrace{\uparrow \cdots \uparrow}_{a} \underbrace{\downarrow \cdots \downarrow}_{b} \left( \frac{1}{2p} u^{\mathrm{T}} u + \frac{p}{2} (a+b-1) \right)$$

to denote an adjustment strategy corresponding to the case (|I|, |D|) = (a, b), that is, a negative entries of u are increased by p while b positive entries of u are decreased by p, with the requirement that the sum of the absolute values of all these a + b entries is  $\frac{1}{2p}u^{\mathrm{T}}u + \frac{p}{2}(a+b-1)$ . For example, ' $\uparrow\uparrow\uparrow\uparrow(\frac{1}{2p}u^{\mathrm{T}}u+p)$ ' corresponds to the case (|I|, |D|) =(3,0) with the restriction that  $\sum_{k\in I} |u_k| = \frac{1}{2p}u^{\mathrm{T}}u + p$ . The symbol '--' at the middle of Table 1 means  $I = D = \emptyset$ . This only happens when the length of the shortest prepresentative is exactly p.

$\frac{1}{p}(u^{\mathrm{T}}e - p)$	adjustment strategy
-3	$\uparrow \uparrow \uparrow (\frac{1}{2p}u^{\mathrm{T}}u + p)$
-2	$\uparrow \uparrow (\frac{1}{2p} u^{\mathrm{T}} u + \frac{p}{2})$
-1	$\uparrow(\frac{1}{2p}u^{\mathrm{T}}u)$ or $\uparrow\uparrow\downarrow(\frac{1}{2p}u^{\mathrm{T}}u+p)$
0	$(\frac{1}{2p}u^{\mathrm{T}}u-\frac{p}{2}=0)$ or $\uparrow\downarrow(\frac{1}{2p}u^{\mathrm{T}}u+\frac{p}{2})$
1	$\downarrow (\frac{1}{2p}u^{\mathrm{T}}u)$ or $\uparrow \downarrow \downarrow (\frac{1}{2p}u^{\mathrm{T}}u+p)$
2	$\downarrow \downarrow (\frac{1}{2p}u^{\mathrm{T}}u + \frac{p}{2})$
3	$\downarrow \downarrow \downarrow (\frac{1}{2p}u^{\mathrm{T}}u + p)$

Table 1: Generating all possible perfect *p*-representatives from the shortest one

#### 3.3 The algorithm

Now we can summarize the above discussions in Algorithm 1. We give two examples for illustrations.

Algorithm 1 Finding generalized cospectral mate

**Input:** a graph  $G \in \mathcal{F}_n^p$ . **Output:** DGS or the unique generalized cospectral mate of G. 1: Compute any nontrivial solution v to  $W^{\mathrm{T}}z \equiv 0 \pmod{p}$ . 2: if  $v^{\mathrm{T}}v \equiv 0 \pmod{p}$  then Set  $S := \{i: v_i \equiv 0 \pmod{p}\}.$ 3: Remove zero entries  $v_i, i \in S$  from v to obtain a vector  $v^*$ . 4: Set  $\mathcal{R} := \emptyset$ . 5:for k from 1 to p-1 do 6: 7: Compute the shortest *p*-representative u of  $kv^*$ . if  $\left|\frac{1}{n}(u^{\mathrm{T}}e-p)\right| \leq 3$  and  $u^{\mathrm{T}}u \leq p^{2}$  then 8: Find all possible perfect p-representatives from u by Table 1. 9: 10: Update  $\mathcal{R}$  by appending all perfect *p*-representatives of  $kv^*$ . if  $|\mathcal{R}| = n - |S|$  then 11: Construct a primitive matrix Q using  $\mathcal{R}$  and unit vectors  $e_i$ 's,  $i \in S$ . 12:return graph H with adjacency matrix  $Q^{\mathrm{T}}A(G)Q$ . 13:14: return DGS.

**Example 36.** Let n=16 and G be the graph with adjacency matrix

Using Mathematica, we can find that  $G \in \mathcal{F}_n^p$  for p = 5. Indeed, the last invariant factor of W is

 $d_n = 2 \times 5^2 \times 11 \times 41 \times 28573 \times 260723 \times 71447889577.$ 

A nontrivial solution to  $W^{\mathrm{T}}z \equiv 0 \pmod{5}$  is  $v = (4, 0, 0, 0, 0, 0, 2, 1, 2, 1, 0, 0, 2, 2, 0, 1)^{\mathrm{T}}$ . Clearly,  $v^{\mathrm{T}}v \equiv 0 \pmod{5}$ . Now  $S = \{2, 3, 4, 5, 6, 11, 12, 15\}$ , the indices for the zero entries of v. Removing these zero entries we obtain  $v^* = (4, 2, 1, 2, 1, 2, 2, 1)^{\mathrm{T}}$ . Table 2 illustrates the iterations of the *for* loop.

When k = 1, we have  $u = (-1, 2, 1, -3, 1, 2, 2, 1)^{\mathrm{T}}$  and hence  $s = \frac{1}{5}(u^{\mathrm{T}}e - 5) = 1$ . According to Table 1 and noting that  $\frac{1}{2p}u^{\mathrm{T}}u = 2$  and  $\frac{1}{2p}u^{\mathrm{T}}u + p = 7$ , all potential perfect *p*-representatives of *u* must be obtained from *u* either by the strategy ' $\downarrow$  (2)', or ' $\uparrow \downarrow \downarrow$  (7)'. As there are exactly four entries equal to 2, we can obtain four perfect *p*-representatives by

k	shortest 5-representative $u$	$\frac{1}{5}(u^{\mathrm{T}}e-5)$	$u^{\mathrm{T}}u$	perfect 5-representatives
1	$(-1, 2, 1, 2, 1, 2, 2, 1)^{\mathrm{T}}$	1	20	$\begin{array}{c} (-1,-3,1,2,1,2,2,1)^{\mathrm{T}} \\ (-1,2,1,-3,1,2,2,1)^{\mathrm{T}} \\ (-1,2,1,2,1,-3,2,1)^{\mathrm{T}} \\ (-1,2,1,2,1,2,-3,1)^{\mathrm{T}} \end{array}$
2	$(-2, -1, 2, -1, 2, -1, -1, 2)^{\mathrm{T}}$	-1	20	$(3, -1, 2, -1, 2, -1, -1, 2)^{\mathrm{T}}$
3	$(2, 1, -2, 1, -2, 1, 1, -2)^{\mathrm{T}}$	-1	20	$\begin{aligned} &(2,1,3,1,-2,1,1,-2)^{\mathrm{T}}\\ &(2,1,-2,1,3,1,1,-2)^{\mathrm{T}}\\ &(2,1,-2,1,-2,1,1,3)^{\mathrm{T}} \end{aligned}$

 Table 2:
 Sufficient perfect 5-representatives

the strategy ' $\downarrow$  (2)'. No perfect *p*-representatives can be obtained by the strategy ' $\uparrow \downarrow \downarrow$  (7)' since otherwise *u* would contain one negative entry  $u_{j_1}$  together with two positive entries  $u_{j_2}$  and  $u_{j_3}$  satisfying  $\sum_{t=1}^{3} |u_{j_t}| = 7$ , which is clearly impossible. Thus,  $|\mathcal{R}| = 4$  after the first iteration of the *for* loop.

In the third iteration,  $|\mathcal{R}|$  reaches 8, which is the dimension of  $v^*$ . Now, using  $\mathcal{R}$  and S, we can construct

	1	$^{-1}$	-1	$^{-1}$	-1	3	2	2	2	0	0	0	0	0	0	0	0 \	\
	1	0	0	0	0	0	0	0	0	<b>5</b>	0	0	0	0	0	0	0	
		0	0	0	0	0	0	0	0	0	<b>5</b>	0	0	0	0	0	0	
		0	0	0	0	0	0	0	0	0	0	5	0	0	0	0	0	
		0	0	0	0	0	0	0	0	0	0	0	5	0	0	0	0	
		0	0	0	0	0	0	0	0	0	0	0	0	5	0	0	0	
1		-3	2	2	2	$^{-1}$	1	1	1	0	0	0	0	0	0	0	0	
$O^{-1}$		1	1	1	1	2	3	-2	-2	0	0	0	0	0	0	0	0	
$Q = \frac{1}{5}$		2	-3	2	2	$^{-1}$	1	1	1	0	0	0	0	0	0	0	0	·
0		1	1	1	1	2	-2	3	-2	0	0	0	0	0	0	0	0	
		0	0	0	0	0	0	0	0	0	0	0	0	0	5	0	0	
		0	0	0	0	0	0	0	0	0	0	0	0	0	0	5	0	
		2	2	-3	2	$^{-1}$	1	1	1	0	0	0	0	0	0	0	0	
		2	2	2	-3	$^{-1}$	1	1	1	0	0	0	0	0	0	0	0	
		0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	5	
		1	1	1	1	2	-2	-2	3	0	0	0	0	0	0	0	0,	/

Now  $Q^{\mathrm{T}}AQ$  gives the adjacency matrix for the generalized cospectral mate of G. Indeed,

direct computation shows that

**Example 37.** Let n=16 and G be the graph with adjacency matrix

This graph is in  $\mathcal{F}_n$ , according to the standard prime decomposition  $d_n = 2 \times 5^2 \times 7 \times 63689 \times 3118319 \times 2740960403$ . Now  $v = (2,3,0,1,1,4,0,4,3,1,1,0,0,0,4,1)^{\mathrm{T}}$  is a nontrivial solution to  $W^{\mathrm{T}}z \equiv 0 \pmod{5}$ . Removing all zero entries, we obtain  $v^* = (2,3,1,1,4,4,3,1,1,4,1)^{\mathrm{T}}$ . Table 3 summarizes the execution of Algorithm 1. As the

k	shortest 5-representative $u$	$\frac{1}{5}(u^{\mathrm{T}}e-5)$	$u^{\mathrm{T}}u$	perfect 5-representatives
1	$(2, -2, 1, 1, -1, -1, -2, 1, 1, -1, 1)^{\mathrm{T}}$	-1	20	$(2,3,1,1,-1,-1,-2,1,1,-1,1)^{\mathrm{T}}$ $(2,-2,1,1,-1,-1,3,1,1,-1,1)^{\mathrm{T}}$
2	$(-1, 1, 2, 2, -2, -2, 1, 2, 2, -2, 2)^{\mathrm{T}}$	0	35	
3	$(1, -1, -2, -2, 2, 2, -1, -2, -2, 2, -2)^{\mathrm{T}}$	-2	35	
4	$(-2, 2, -1, -1, 1, 1, 2, -1, -1, 1, -1)^{\mathrm{T}}$	-1	20	$(3, 2, -1, -1, 1, 1, 2, -1, -1, 1, -1)^{\mathrm{T}}$

Table 3: Insufficient perfect 5-representatives

total number of perfect p-representatives is less than the number of nonzero entries in v, the graph is DGS.

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Table 4 gives some experimental results on the DGS-property of graphs with at most 20 vertices. Using Mathematica, for each  $n \in \{10, 11, \ldots, 20\}$ , we randomly generate 10,000 graphs. The second column records the number of graphs that are in  $\mathcal{F}_n$ , while the last column records further the number of graphs which are not DGS, using Algorithm 1. It seems that the density of  $\mathcal{F}_n$  is nearly stable (about 3%), while the density of non-DGS graphs in  $\mathcal{F}_n$  decreases dramatically as n increases.

Haemers [1, 4] conjectured that almost all graphs are determined by their spectra. A weaker version of Haemers' conjecture is that almost all graphs are DGS. We note that the observed phenomenon of the decreasing density of non-DGS graphs is consistent with the prediction of the weaker version of Haemers' conjecture, and therefore provides some evidence for it.

n	$\# \ \mathcal{F}_n$	# Non-DGS
10	278	52
11	280	41
12	296	30
13	323	22
14	323	23
15	330	7
16	344	3
17	353	4
18	347	2
19	300	0
20	335	2

Table 4:  $\mathcal{F}_n$  and Non-DGS graphs in  $\mathcal{F}_n$ 

# 4 A conjecture

In this paper, we have presented an algorithm to check whether a graph  $G \in \mathcal{F}_n$  is DGS or not. The key ingredient of the algorithm is to decide whether a vector can generate a primitive matrix. Although this can be done algorithmically, it is still very desirable to give some more 'evident' conditions either for guaranteeing a vector to generate a primitive matrix, or for ruling out such a possibility. Inspired by some numerical experiments using Algorithm 1, we propose the following conjecture for further study. **Conjecture 38.** Let v be an n-dimensional integral vector with each entry nonzero modulo p. Suppose that  $v^{\mathrm{T}}e \equiv 0 \pmod{p}$  and  $v^{\mathrm{T}}v \equiv 0 \pmod{p}$ . Then (i) If  $n \leq 8$  then v can always generate some primitive matrix. (ii) If  $n \geq 2p + 1$  then v cannot generate any primitive matrix.

We remark that if Conjecture 38 is true, then the final results of Examples 36 and 37 can be easily predicted once the nontrivial solutions of  $W^T z \equiv 0 \pmod{p}$  were found. Indeed, in Example 36, the nontrivial solution v of  $W^T z \equiv 0 \pmod{p}$  has exactly 8 nonzero entries, which constitutes a vector  $v^*$ . Noting that  $(v^*)^T e \equiv 0 \pmod{p}$  and  $(v^*)^T v^* \equiv 0 \pmod{p}$ , Conjecture 38 (i) implies that  $v^*$  and hence v can generate a primitive matrix. Nevertheless, in Example 37, the nontrivial solution v has exactly 11 nonzero entries, which reaches 2p+1 (noting p = 5). Thus, we may 'predict' that v cannot generate any primitive matrix assuming Conjecture 38 (ii).

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