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Strongly cospectral vertices

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Abstract

Two vertices a and b in a graph X are cospectral if the vertex-deleted subgraphs $X \setminus a$ and $X \setminus b$ have the same characteristic polynomial. In this paper we investigate a strengthening of this relation on vertices, that arises in investigations of continuous quantum walks. Suppose the vectors e_a for a in $V(X)$ are the standard basis for $\mathbb{R}^{V(X)}$. We say that a and b are strongly cospectral if for each eigenspace U of $A(X)$, the orthogonal projections of e_a and e_b are either equal or differ only in sign. We develop the basic theory of this concept and provide constructions of graphs with pairs of strongly cospectral vertices. Given a continuous quantum walk on a graph, each vertex determines a curve in complex projective space. We derive results that show that the closer these curves are, the more "similar" the corresponding vertices are.

1 Introduction

Let $E_1, \ldots, E_d$ be the distinct orthogonal projections onto the eigenspaces of a graph X. If $a \in V(X)$, we use e_a to denote the characteristic vector of a, viewed as a 1-element subset of $V(X)$. Vertices a and b are *cospectral* if the projections $E_r e_a$ and $E_r e_b$ have the same length; they are *strongly cospectral* if $E_r e_a = \pm E_r e_b$.

The idea of cospectral vertices goes back to Schwenk [12], where he used it to show that the proportion of trees on n vertices that are determined by the characteristic polynomial goes to zero as $n \to \infty$. Strongly cospectral vertices appear first in [6], where Fan and the author used them to study properties of continuous quantum walks. The goal of this paper is to develop the basic theory of strongly cospectral vertices.

To start our work, we set up some machinery for working with quantum states. We will represent a quantum state in $\mathbb{C}^n$ by a *density matrix*, a positive semidefinite $n \times n$ matrix with trace one. A density matrix D represents a *pure state* if $\mathrm{rk}(D) = 1$, in which case $D = zz^*$ for some unit vector z. We will only be concerned with pure states in this paper and generally they will be associated to vertices of a graph X—if $a \in V(X)$, then e_a denotes the standard basis vector in $\mathbb{C}^{V(X)}$ indexed by a and

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our focus will be on pure states of the form $D_a = e_a e_a^T$. If D is a pure state then $D^2 = D$ and D represents orthogonal projection onto the column space of D; thus D corresponds to a point in complex projective space.

If X is a graph with adjacency matrix A, the *continuous quantum walk* on X is determined by the family of unitary matrices

$$U(t) = \exp(itA), \qquad t \geq 0.$$

The understanding is that if, initially, our system is in the state associated with the density matrix D, then at time t its state is given by

$$U(t)DU(-t).$$

It is easy to check that this is a density matrix, which we denote by $D(t)$, and that $D(t)$ is pure if and only if D is. It follows that, if our initial state D is pure, a quantum walk determines a curve in projective space, namely the set of points $D(t)$. (If our initial state were not pure, we would have a curve on a Grassmannian, but we will not go there.)

Given distinct vertices a and b in X, one question of interest to physicists is whether there is a time t such that D_b lies on the curve containing D_a; equivalently if there is a time t such that $U(t)D_aU(-t) = D_b$. If there is such a time, we say that we have *perfect state transfer* from a to b at time t. If we do have perfect state transfer at time t, then

$$\|D_a(t) - D_b\| = 0.$$

Since, as it happens, perfect state transfer is rare, we might decide to settle for less: we could ask whether, given $\epsilon > 0$, there is a time t such that

$$\|D_a(t) - D_b\| < \epsilon.$$

If this is possible (for all positive ϵ) we have *pretty good state transfer* from a to b. Pretty good state transfer occurs more often than perfect state transfer. For example we get perfect state transfer between the end-vertices of the path P_n if and only if $n = 2$ or $n = 3$, but we have pretty good state transfer between the end-vertices of P_n if and only if $n + 1$ is a power of two, a prime, or twice a prime. For details see Banchi et al. [1]; more recent work on this topic appears in [4, 14].)

Let $\theta_1, \ldots, \theta_m$ be the distinct eigenvalues of the adjacency matrix A of the graph X. For each eigenvalue θ_r there is an idempotent matrix E_r representing orthogonal projection onto the eigenspace with eigenvalue θ_r. If f is a function defined on the eigenvalues of A, then

$$f(A) = \sum_r f(\theta_r) E_r$$

and, in particular

$$U(t) = \sum_r e^{it\theta_r} E_r.$$

Hence

$$D(t) = \sum_{r,s} e^{it(\theta_r - \theta_s)} E_r D E_s$$

and so $D_a(t) = D_b$ if and only if

$$\sum_{r,s} e^{it(\theta_r - \theta_s)} E_r D_a E_s = D_b = \sum_{r,s} E_r D_b E_s$$

and this holds if and only if

$$e^{it(\theta_r - \theta_s)} E_r D_a E_s = E_r D_b E_s$$

for all r, s. Now all six matrices in this equality are real, whence we deduce that if perfect state transfer occurs,

$$e^{it(\theta_r - \theta_s)} = \pm 1$$

and, for each r,

$$E_r D_a E_r = E_r D_b E_r.$$

(The diagonal entries in both sides are necessarily non-negative since density matrices are positive semidefinite and E_r is symmetric, whence both sides are positive semidefinite.) This leads us to the conclusion that, if perfect state transfer from a to b occurs, then for each r.

$$E_r e_a = \pm E_r e_b$$

Our ruminations have lead to the conclusion that, if there is perfect state transfer between vertices a and b, then these two vertices are strongly cospectral. This is the basic reason we find this property to be interesting.

We discuss our main results. We show that if vertices a and b in X are strongly cospectral, then any automorphism of X that fixes a must fix the vertex b. (So the concept has combinatorial implications.) We provide a number of characterizations, for example: vertices a and b are strongly cospectral if and only if they are cospectral and all poles of the rational function $\phi(X \setminus \{a, b\}, t)/\phi(X, t)$ are simple. We use this to provide constructions of graphs with pairs of strongly cospectral vertices. We show that cospectral vertices and strongly cospectral vertices are connected by mappings that can viewed as relaxations of automorphisms. Thus we prove that a and b are strongly cospectral if and only if there is an orthogonal matrix Q, a rational polynomial in A, such that $Q^2 = I$ and $Qe_a = e_b$.

In the final three sections of the paper, we consider the geometry of the orbits of the pure states of the form D_a. As we noted above, there is perfect state transfer from a to b if and only if D_b lies in the orbit of D_a; equivalently if and only if the orbits of D_a and D_b coincide. Further we have pretty good state transfer if and only if D_b lies in the closure of the orbit of D_a, that is, if and only if the closures of the two orbits are equal. However the geometry of the orbits provides information about purely graph-theoretic properties: we prove that if the orbits of D_a and D_b are sufficiently close, then a and b must be cospectral and, if they are even closer, then a and b must be strongly cospectral.

2 Cospectral Vertices

We view the relation of being strongly cospectral as a combination of two relations. The first of these two is an older concept: two vertices a and b in a graph X are *cospectral* if the characteristic polynomials of the vertex-deleted subgraphs $X \setminus a$ and $X \setminus b$ are equal, that is,

$$\phi(X \setminus a, t) = \phi(X \setminus b, t).$$

It is immediate that if there is an automorphism of X that maps a to b, then a and b are cospectral. Cospectral vertices were first introduced in Schwenk's fundamental paper [12]; here Schwenk noted that the vertices u and v in the tree in Figure 1 are cospectral, but lie in different orbits of the automorphism group of the tree. Using this he was able to show that the proportion of trees on n vertices that are determined by their characteristic polynomial goes to zero as $n \to \infty$.

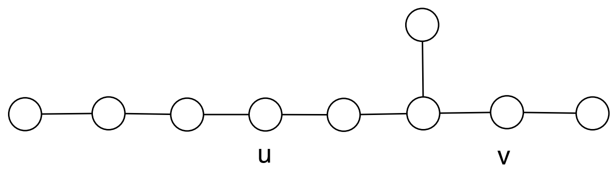

Figure 1: A pair of cospectral vertices

There are a surprising number of characterizations of cospectral vertices. We will list them in the next section, but we need first to introduce more terminology.

Suppose S is a subset of the vertices a graph X with characteristic vector z and $n = |V(X)|$. We define the *walk matrix* M_S relative to S to be the $n \times n$ matrix with the vectors

$$z,\ Az, \dots, A^{n-1}z$$

as its columns. The case of interest to us will be when S is a single vertex a and, in this case, we will refer to the *walk matrix relative to a*. We will use e_S to denote the characteristic vector of S. The column space of M_S is A-invariant, and so it is a module over the ring $\mathbb{R}[A]$ of real polynomials in A. It is in fact a cyclic module, generated by the first column z of M_S. We call it the *walk module* relative to S.

We see that the ij-entry of $M_S^T M_S$ is $z^T A^{i+j-2} z$, and so it is equal to the number of walks on X with length $i + j - 2$ that start and end on a vertex in S. Hence if $S = \{a\}$, then this entry is the number of closed walks in X that start at a and have length $i + j - 2$. We define $W_S(X, t)$ to be the generating function

$$\sum_{k \geq 0} z^T A^k z t^k = z^T (I - tA)^{-1} z.$$

Lemma 2.1. *Let a and b be vertices in X. Then $W_a(X, t) = W_b(X, t)$ if and only if $M_a^T M_a = M_b^T M_b$.*

Proof. It should be clear that, if the walk-generating functions are equal, the matrix products are equal. For the converse, let $\theta_1, \dots, \theta_m$ denote the distinct eigenvalues of A and let $E_1, \dots, E_m$ denote the corresponding orthogonal projections onto the distinct eigenspaces of A. Then for any vector z,

$$z^T(I - tA)^{-1}z = \sum_r \frac{z^T E_r z}{1 - t\theta_r}.$$

Since $m \le n$, it follows that the generating function $z^T(I - tA)^{-1}z$ is determined by its first m coefficients. $\square$

3 Characterizing Cospectral Vertices

We give a comprehensive list of characterizations of cospectral vertices. The first four appear already in [8]

Theorem 3.1. *Let a and b be vertices in the graph X with corresponding walk matrices M_a and M_b. The following statements are equivalent:*

(a) a and b are cospectral.

(b) $\phi(X \setminus a, t) = \phi(X \setminus b, t)$.

(c) $W_a(X, t) = W_b(X, t)$.

(d) For each spectral idempotent E_r we have $(E_r)_{a,a} = (E_r)_{b,b}$.

(e) For any non-negative integer k we have $(A^k)_{a,a} = (A^k)_{b,b}$.

(f) $M_a^T M_a = M_b^T M_b$.

(g) The $\mathbb{R}[A]$-modules generated by $e_a - e_b$ and $e_a + e_b$ are orthogonal subspaces of $\mathbb{R}^{V(X)}$.

Proof. Claims (a) and (b) are equivalent, because (b) is the definition of cospectral. From the proof of Lemma 2.1 we have

$$t^{-1} W_v(X, t^{-1}) = \frac{\phi(X \setminus v, t)}{\phi(X, t)}$$

and, from [7, p. 30],

$$\frac{\phi(X \setminus v, t)}{\phi(X, t)} = \sum_r \frac{(E_r)_{v,v}}{t - \theta_r}. \tag{3.1}$$

Hence (b), (c) and (d) are equivalent. Since any power of A is a linear combination of the spectral idempotents E_r, and since the spectral idempotents are polynomials in A, we see that (d) and (e) are equivalent. By the discussion in the previous section, (c) and (f) are equivalent.

We turn to (g). The given modules are orthogonal if and only if for all non-negative i and j, we have

$$\langle A^i(e_a - e_b), A^j(e_a + e_b)\rangle = 0,$$

equivalently if and only if

$$(e_a - e_b)^T A^k(e_a + e_b) = 0$$

for all $k \geq 0$. This is equivalent in turn to

$$(e_a - e_b)^T E_r(e_a + e_b) = 0$$

for each spectral idempotent E_r. As

$$(e_a - e_b)^T E_r(e_a + e_b) = e_a^T E_r e_a - e_b^T E_r e_b - e_b^T E_r e_a + e_a^T E_r e_b$$

and

$$e_b^T E_r e_a = (E_r)_{b,a} = (E_r)_{a,b} = e_b^T E_r e_a$$

we find that $(e_a - e_b)^T E_t(e_a + e_b) = 0$ for all r if and only if $e_a^T E_r e_a = e_b^T E_r e_b$ for all r. □

We make some remarks. One consequence of part (g) of the theorem is that if two vertices of X are cospectral, then the characteristic polynomial of X factors non-trivially over $\mathbb{Q}$. More precisely, the characteristic polynomials of the respective restrictions of A to the modules generated by $e_a - e_b$ and $e_a + e_b$ are disjoint factors of $\phi(X, t)$.

A graph is said to be *walk regular* if for each non-negative integer k, the diagonal of A^k is constant or, equivalently if the diagonals of the spectral idempotents are constant. In a walk-regular graph, any two vertices are cospectral; in particular any two vertices of a strongly regular graph are cospectral.

Finally, since $E_r = E_r^T E_r$, we have

$$(E_r)_{v,v} = e_v^T E_r^T E_r e_v = \|E_r e_v\|^2,$$

whence vertices a and b are cospectral if and only if the eigenspace projections $E_r e_a$ and $E_r e_b$ have the same length for each r. It follows (as we would hope) that strongly cospectral vertices are cospectral.

4 Parallel Vertices: Characterizations

We have developed some of the theory of cospectral vertices and noted that strongly cospectral vertices are cospectral. To characterize strongly cospectral vertices, we need a second condition. Two vertices a and b in X are *parallel* if, for each r, one of the vectors $E_r e_a$ and $E_r e_b$ is a scalar multiple of the other. Equivalently a and b are parallel if and only if the vectors $E_r e_a$ and $E_r e_b$ are parallel for each r. As an immediate consequence of the definition of strongly cospectral vertices, we have:

Lemma 4.1. *Two vertices in a graph are strongly cospectral if and only if they are cospectral and parallel.* □

If the eigenvalues of X are all simple, it is easy to see that any two vertices in X are parallel. It follows in this case that two vertices are strongly cospectral if and only if they are cospectral. (The eigenvalues of Schwenk's tree in Figure 1 are simple, and the vertices u and v there are strongly cospectral.)

Lemma 4.2. *The eigenvalues of X are all simple if and only if any two vertices of X are parallel.*

Proof. Suppose any two vertices of X are parallel. If $a \in V(X)$ and $E_r e_a \neq 0$, then for each r we have that $E_r e_b$ is a scalar multiple of $E_r e_a$. Hence $E_r e_a$ spans the eigenspace belonging to θ_r and so θ_r has multiplicity one. □

We use $\langle e_u \rangle_A$ to denote the $\mathbb{R}[A]$-module generated by e_u, and we call it the *walk module* relative to u. (When A is clear from the context, we may be lazy and write simply $\langle e_u \rangle$.) The *eigenvalue support* of a subset S of $V(X)$ with characteristic vector z is the set of eigenvalues θ_r such that $E_r z \neq 0$. (We will also refer to the eigenvalue support of an arbitrary vector.) Two cospectral vertices necessarily have the same eigenvalue support.

Lemma 4.3. *The walk modules generated by vertices a and b in X are equal if and only if a and b are parallel and have the same eigenvalue support.*

Proof. If $u \in V(X)$, the non-zero vectors $E_r e_u$ form an orthogonal basis for $\langle e_u \rangle$. Therefore if a and b are parallel with the same eigenvalue support, their walk modules are equal.

For the converse, let W_a and W_b denote the respective walk modules. If $W_a = W_b$ then $E_r W_a = E_r W_b$, but $E_r W_a$ and $E_r W_b$ are spanned respectively by $E_r e_a$ and $E_r e_b$. Therefore a and b are parallel with the same eigenvalue support. □

Finally we note that, by [9, Lemma 13.1], if we have pretty good state transfer from vertex a to vertex b, then a are b are strongly cospectral. (This result is a private communication from Dave Witte Morris.) Since perfect state transfer can be viewed as a special case of pretty good state transfer, it follows that vertices involved in perfect state transfer are necessarily strongly cospectral. (As we already noted in the Introduction.)

An old and well-known result states that a vertex-transitive graph with only simple eigenvalues is K_1 or K_2. This has been generalized—a walk regular graph with only simple eigenvalues is K_1 or K_2 (see e.g., [8, Theorem 4.8]). The following result generalizes this in turn.

Lemma 4.4. *If all vertices in X are strongly cospectral, then $|V(X)| \leq 2$.*

Proof. If all vertices of X are strongly cospectral to u, then the θ_r-eigenspace of X is spanned by $E_r e_u$, and therefore all eigenvalues of X are simple. As all vertices of X are cospectral, X is walk regular and as noted just above, a walk regular graph with only simple eigenvalues has at most two vertices. □

The four vertices of degree two in the Cartesian product of P_3 with K_2 are pairwise strongly cospectral, so we can have more than a pair of strongly cospectral vertices. (They are cospectral because they form an orbit under the action of the automorphism group. To see that they are parallel, it is easiest to note that the characteristic polynomial has only simple zeros; you can verify this using your favourite computer algebra package.)

5 Average States

If $\theta_1, \dots, \theta_m$ are the distinct eigenvalues of the adjacency matrix A of X, we use E_r to denote the matrix representing orthogonal projection onto the θ_r-eigenspace of A. So A has spectral decomposition

$$A = \sum_r \theta_r E_r.$$

We make use of some theory developed in [3]. The *commutant* comm(A) of a matrix A is the set of all matrices that commute with A. If A is $n \times n$, then comm(A) is a subspace of the space of $n \times n$ real matrices. This latter space is an inner product space, with inner product

$$\langle M, N \rangle = \operatorname{tr}(M^T N).$$

The norm $\|M\|$ of a matrix M is $\langle M, M \rangle^{1/2}$. The operation of orthogonal projection onto comm(A) is well defined; we denote the orthogonal projection of a matrix M onto comm(A) by $\Phi(M)$.

From Section 2 of [3], we have:

Lemma 5.1. *If A is a symmetric matrix with spectral idempotents $E_1, \dots, E_m$, then*

$$\Phi(M) = \sum_r E_r M E_r. \qquad \square$$

As Φ is linear and self-adjoint,

$$\langle \Phi(M), M - \Phi(M) \rangle = \langle M, \Phi(M) - \Phi^2(M) \rangle = \langle M, 0 \rangle = 0$$

and therefore

$$\|M\|^2 = \|M - \Phi(M)\|^2 + \|\Phi(M)\|^2.$$

This implies that $\|\Phi(M)\| \leq \|M\|$ for any M. Hence the operator norm of Φ is at most 1.

Lemma 5.2. *For any density matrix D and for any time t, we have $\Phi(D(t)) = \Phi(D)$.*

Proof. One line:

$$\Phi(D(t)) = \sum_r E_r U(t) D U(-t) E_r = \sum_r e^{it\theta_r} E_r D E_r e^{-it\theta_r} = \Phi(D). \qquad \square$$

We use $M \circ N$ to denote the Schur product of matrices M and N. The *average mixing matrix* $\widehat{M}_X$ of the graph X is

$$\widehat{M}_X = \sum_r E_r \circ E_r.$$

Our next result is Theorem 3.1 in [3].

Theorem 5.3. *If $a, b \in V(X)$, then*

$$(\widehat{M}_X)_{a,b} = \langle \Phi(D_a), \Phi(D_b) \rangle. \qquad \square$$

If $a \in V(X)$, then

$$\Phi(D_a) = \sum_r E_r e_a e_a^T E_r.$$

We calculate that

$$\|E_r e_a e_a^T E_r\| = e_a^T E_r e_a = (E_r)_{a,a}$$

and define

$$F_r = \frac{1}{(E_r)_{a,a}} E_r e_a e_a^T E_r.$$

Thus F_r represents orthogonal projection onto the span of $E_r e_a$ and the scalars

$$(E_r)_{a,a}, \qquad r = 1, \dots, m$$

are the eigenvalues of $\Phi(D_a)$.

Lemma 5.4. *Assume a and b are vertices in the graph X. Then:*

(a) a and b are cospectral if and only the average states $\Phi(D_a)$ and $\Phi(D_b)$ are similar.

(b) a and b are strongly cospectral if and only if $\Phi(D_a) = \Phi(D_b)$.

Proof. From Equation (3.1), we see that a and b are cospectral if and only if $\Phi(D_a)$ and $\Phi(D_b)$ are. For the second claim we note that a and b are cospectral, they are parallel if and only if $E_r e_a e_a^T E_r = E_r e_b e_b^T E_r$ for all r, that is, if and only if the projections F_r are the same for a and b. $\square$

The sum $\sum_r F_r$ is the matrix representing orthogonal projection onto the walk module generated by e_a.

We introduce spectral densities of subsets of vertices of a graph. Assume $S \subseteq V(X)$ and let z be the normalized characteristic vector of S. (So z is zero off S, constant on S and $z^T z = 1$.) The quantities

$$z^T E_r z, \quad (r = 1, \dots, m)$$

are non-negative and sum to 1. Hence they determine a probability density on the eigenvalues of A; this is the *spectral density* of S. We will only work with the case where S is a single vertex, where the value of the spectral density of vertex a on θ_r is $(E_r)_{a,a}$. Hence the spectral density is determined by the eigenvalues of $\Phi(D_a)$. The generating function for closed walks on a is the moment generating function for the spectral density at a and, viewed as a generating function, $U(t)_{a,a}$ is the characteristic function of the spectral density.

More background on average mixing appears in [10, 3].

6 An Uncomplicated Algebra

We need information about the matrix algebra generated by A and $e_a e_a^T$ for a vertex a. It is no harder to work with an arbitrary non-zero vector z in place of a vector e_a, so we do.

We use $\langle S \rangle$ to denote the algebra generated by a set of matrices. The algebra of interest to us is $\langle A, zz^T \rangle$, where A is an adjacency matrix and $z \in \mathbb{R}^N$.

Lemma 6.1. *Assume $\mathcal{A} = \langle A, zz^T \rangle$ for an adjacency matrix A with spectral decomposition $A = \sum_r \theta_r E_r$. Let S be the set of eigenvalues θ_r such that $E_r z \neq 0$. If $r \in S$, define*

$$F_r = \frac{1}{z^T E_r z} E_r zz^T E_r, \quad E'_r = E_r - F_r;$$

if $r \notin S$ then define $E'_r = E_r$. Then the matrices

$$E_r zz^T E_s, \ (r, s \in S),$$

together with the non-zero matrices E'_r, form a trace-orthogonal basis for $\mathcal{A}$.

Proof. Easy calculations show that the matrices F_r are idempotents (F_r represents orthogonal projection onto the span of $E_r z$) and they commute with the spectral idempotents. Further $E_k F_r = 0$ if $k \neq r$ and $E_r F_r = F_r$ if $r \in S$. One consequence of this is that the matrices E'_r are pairwise orthogonal and are orthogonal to each matrix F_s.

It is also easy to check that distinct matrices of the form $E_r zz^T E_s$ are trace-orthogonal.

Thus it only remains to verify that the given matrices span $\mathcal{A}$. The key is that

$$\begin{aligned}(A^k zz^T A^\ell)(A^m zz^T A^n) &= A^k z\, z^T A^{\ell+m} z\, z^T A^n \\ &= (z^T A^{\ell+m} z) A^k zz^T A^n,\end{aligned}$$

from which it ensues that $\mathcal{A}$ is spanned by matrices of the form $A^k zz^T A^\ell$, along with the powers of A. The span of the first set of matrices is equal to the span of the matrices $E_r zz^T E_s$ and the spectral idempotents span the space of polynomials in A; therefore we have an orthogonal basis as claimed. □

Corollary 6.2. *If the vertices a and b in X are parallel with the same eigenvalue support, then $\langle A, e_a e_a^T \rangle = \langle A, e_b e_b^T \rangle$.*

Proof. Suppose a and b are parallel. If θ_r and θ_s lie in the eigenvalue support of a and b, then $E_r e_a e_a^T E_s$ and $E_r e_b e_b^T E_s$ are non-zero scalar multiples of each other. From the previous lemma it follows that our two algebras are equal. □

Corollary 6.3. *Let X be a graph on n vertices and let a and b be parallel vertices in X with the same eigenvalue support. If the matrix Q commutes with A and $Qe_a = e_a$, then $Qe_b = e_b$.* □

Corollary 6.4. *If a and b are strongly cospectral vertices in X, then any automorphism of X that fixes a also fixes b.*

Given this corollary, it is an easy exercise to show that no two vertices in the Petersen graph are strongly cospectral, but more is true.

The *characteristic matrix* of a partition π is the matrix whose columns are the characteristic vectors of the cells of π. If P is the characteristic matrix of π, then $P\mathbf{1} = \mathbf{1}$ and P^TP is diagonal with positive diagonal entries. If $D = (P^TP)^{1/2}$ then the columns of PD^{-1} are pairwise orthogonal unit vectors, and we call this matrix the *normalized characteristic matrix* of π. We recall that a partition π of $V(X)$ is equitable if the column space of P is A-invariant. Alternatively, π is equitable if and only if $PD^{-2}P^T$ commutes with A. (Note that $PD^{-1}P^T$ represents orthogonal projection onto $\operatorname{col}(P)$.)

If π is a partition of $V(X)$ and $v \in V(X)$, then $\{v\}$ is a cell of π if and only if $PD^{-1}P^Te_v = e_v$.

Corollary 6.5. *If a and b are strongly cospectral vertices in X and $\{a\}$ is a cell in the equitable partition π, then $\{b\}$ is also a cell in π.* □

If X is a graph and $a \in V(X)$, the cells of the distance partition relative to a are the sets of vertices at a given distance from a. It is easy to verify that if X is strongly regular, then the distance partition relative to any vertex is equitable. We conclude that if X is strongly regular and not complete multipartite, no two distinct vertices in X are strongly cospectral.

7 Eigenspaces and Parallel Vertices

Our next result provides one way of deciding whether two vertices are parallel.

Lemma 7.1. *The projections of e_a and e_b onto the θ_r-eigenspace are parallel if and only if $(E_r)_{a,a}(E_r)_{b,b} - (E_r)^2_{a,b} = 0$.*

Proof. Observe that

$$(E_r)_{a,b} = e_a^TE_r^TE_re_b = \langle E_re_a, E_re_b\rangle$$

and for any vertex c

$$(E_r)_{c,c} = \langle E_re_c, E_re_c\rangle,$$

whence Cauchy-Schwarz implies that

$$(E_r)^2_{a,b} \le (E_r)_{a,a}(E_r)_{b,b}$$

with equality if and only if the vectors E_re_a and E_re_b are parallel. □

We point out that $(E_r)_{a,a}(E_r)_{b,b} - (E_r)^2_{a,b}$ is the determinant of the 2×2 submatrix of E_r with rows and columns indexed by a and b.

If u and v are vertices in X, we say an element f in $\mathbb{R}^{V(X)}$ is *balanced* if $f(u) = f(v)$ and is *skew* if $f(u) = -f(v)$. A subspace is balanced or skew if each vector in it is balanced or, respectively, skew.

Lemma 7.2. *Two vertices u and v in X are strongly cospectral if and only if each eigenspace is balanced or skew relative to the vertices u and v.*

Proof. If u and v are strongly cospectral, then either $E_r(e_u - e_v) = 0$ or $E_r(e_u + e_v) = 0$. Since $\operatorname{col}(E_r)$ is the θ_r-eigenspace, it follows that either each eigenvector in the θ_r-eigenspace is balanced, or each eigenspace is skew. The converse follows easily. □

Lemma 7.3. *Let S be a subset of $V(X)$ such that any two vertices in S are parallel and have the same eigenvalue support, of size s. Then $|S| \leq s$.*

Proof. Suppose $a \in S$. Denote the non-zero vectors $E_r e_a$ by $x_1, \dots, x_s$. Then for each vertex b in S, we can write e_b as a linear combination of $x_1, \dots, x_s$. Since the vectors e_b for b in S are linearly independent, we must have $|S| \leq s$. □

8 Parallel Vertices and a Rational Function

We need an identity due to Jacobi. A proof is given in [7, Theorem 4.1.2].

Theorem 8.1. *Let X be a graph. If $T \subseteq V(X)$, then*

$$\det(((tI - A)^{-1})_{T,T}) = \frac{\phi(X \setminus T, t)}{\phi(X, t)}.$$ □

Corollary 8.2. *Let $\theta_1, \dots, \theta_m$ be the distinct eigenvalues of X, with corresponding spectral idempotents $E_1, \dots, E_m$. If $T \subseteq V(X)$, the multiplicity of θ_r as a pole of $\phi(X \setminus T, t)/\phi(X, t)$ is at most equal to $\operatorname{rk}((E_r)_{T,T})$. Moreover, if $\operatorname{rk}((E_r)_{T,T}) = |T|$, then the multiplicty of θ_r as a pole is equal to $|T|$.*

Proof. We have

$$((tI - A)^{-1})_{T,T} = \sum_r \frac{1}{t - \theta_r} (E_r)_{T,T}.$$

Assume $F_s := (t - \theta_s)^{-1}(E_s)_{T,T}$. Fix r and let P be an orthogonal matrix such that $D = P^T(E_r)_{T,T}$ is diagonal. Let $H = \sum_{s:s \neq r} F_s$. Then

$$\frac{\phi(X \setminus T, t)}{\phi(X, t} = \det\left(\frac{1}{t - \theta_r} + P^T H P\right).$$

From the Laplacian expansion, this determinant is the sum of the determinants of the matrices we get from $P^T H P$ by replacing each subset of its columns by the corresponding set from $(t - \theta_r)^{-1} D$. The non-zero diagonal entries of this matrix have poles at θ_r, but the entries of $P^T H P$ do not. Hence the multiplicity of θ_r as a pole of $\phi(X \setminus T, t)/\phi(X, t)$ cannot exceed $\operatorname{rk}((E_r)_{T,T})$.

If $\operatorname{rk}((E_r)_{T,T}) = |T|$, then D is the identity matrix and the term $(t - \theta_r)^{-|T|}$ appears with coefficient equal to 1 in the expansion of $\phi(X \setminus T, t)/\phi(X, t)$.

We note that $(E_r)_{D,D}$ is the Gram matrix of the vectors $E_r e_u$, for u in D.

Lemma 8.3. *Distinct vertices a and b of X are parallel if and only all poles of the rational function $\phi(X \setminus \{a,b\},t)/\phi(X,t)$ are simple.*

Proof. By Corollary 8.2, if $T = \{a,b\}$ then the multiplicity of the pole at θ_r in $\phi(X \setminus T,t)/\phi(X,t)$ is equal to $\mathrm{rk}((E_r)_{T,T})$. We have

$$|(E_r)_{a,b}|^2 = (e_a^T E_r e_b)^2 = \langle E_r e_a, E_r e_b\rangle^2 \leq \|E_r e_a\|^2\|E_r e_b\|^2 = (E_r)_{a,a}(E_r)_{b,b}$$

whence it follows that $\mathrm{rk}((E_r)_{T,T}) = 1$ if and only if a and b are parallel. □

Corollary 8.4. *Distinct vertices a and b of X are strongly cospectral if and only if they are cospectral and all poles of $\phi(X \setminus \{a,b\},t)/\phi(X,t)$ are simple.* □

One merit of this result is that it enables us to decide if two vertices are parallel using exact arithmetic.

9 Constructing Strongly Cospectral Pairs

We present two constructions of strongly cospectral vertices.

Theorem 9.1. *Let Z be the graph obtained from vertex-disjoint graphs X and Y by joining a vertex u in X to a vertex v in Y by a path P of length at least one. If u and v are cospectral in Z, they are strongly cospectral.*

Proof. Assume $A = A(Z)$ and let $\phi_{u,v}(Z,t)$ denote the determinant of the uv-minor of $tI - A$. From the spectral decomposition of A, we have

$$\frac{\phi_{u,v}(Z,t)}{\phi(Z,t)} = ((tI-a)^{-1})_{u,v} = \sum_r \frac{(E_r)_{u,v}}{t-\theta_r},$$

showing that the poles of $\phi_{u,v}(Z,t)/\phi(Z,t)$ are simple. From [7, Corollary 2.2], we have

$$\phi_{u,v}(Z,t) = \sum_P \phi(X \setminus P,t)$$

where the sum is over all paths in X that join u to v. By construction there is only one path in Z that joins u to v, and therefore

$$\phi_{u,v}(Z,t) = \phi(X \setminus u,t)\phi(Y \setminus v,t).$$

If Q is the path we get from P by deleting its end-vertices,

$$\frac{\phi(Z \setminus \{u,v\},t)}{\phi(Z,t)} = \phi(Q,t)\frac{\phi(X \setminus u,t)\phi(Y \setminus v,t)}{\phi(Z,t)} = \phi(Q,t)\frac{\phi_{u,v}(Z,t)}{\phi(Z,t)}.$$

We conclude that the poles of $\phi(Z \setminus \{u,v\},t)/\phi(Z,t)$ are all simple and so, by Lemma 8.3, it follows that u and v are strongly cospectral. □

Note that u and v will be cospectral in Z if X and Y are cospectral and also $X \setminus u$ and $Y \setminus v$ are cospectral. We get interesting examples by taking two vertex-disjoint copies of Schwenk's tree from Figure 1 and joining the vertex u in the first copy to vertex v in the second by a path of positive length. This gives pairs of strongly cospectral vertices that do not lie in an orbit of the automorphism group of the resulting graph.

Now we consider a "rabbit-ear" construction. We use $\mathrm{mult}(\theta, X)$ to denote the multiplicity of θ as a zero if $\phi(X, t)$.

Lemma 9.2. *Let a be a vertex in X and let Z be formed from X by joining two new vertices of valency one to a. If* $\mathrm{mult}(0, X \setminus a) \leq \mathrm{mult}(0, X)$*, then the two new vertices are strongly cospectral in Z.*

Proof. Assume the two new vertices are b and c. Since $Z \setminus b$ and $Z \setminus c$ are isomorphic, b and c are cospectral. We have

$$\phi(Z, t) = t^2 \phi(X, t) - 2t\phi(X \setminus a, t)$$

and so we are concerned with the multiplicities of the poles of

$$\frac{\phi(X, t)}{t(t\phi(X, t) - 2\phi(X \setminus a, t))} = \frac{1}{t\big(t - 2\frac{\phi(X \setminus a, t)}{\phi(X, t)}\big)}.$$

By interlacing, the zeros of

$$t - 2\frac{\phi(X \setminus a, t)}{\phi(X, t)}$$

are simple (see, e.g., [11, Thm. 8.13.3]) and hence Lemma 8.3 yields that b and c are parallel if and only if 0 is not a zero of this rational function. We see that 0 is a zero of the rational function if and only if the multiplicity of 0 as an eigenvalue of $X \setminus a$ is greater than its multiplicity as an eigenvalue of X. □

10 Symmetries

An *orthogonal symmetry* of a graph X is an orthogonal matrix that commutes with A. If the eigenvalue θ_r of X has multiplicity m_r and $O(m)$ denotes the group of $m \times m$ orthogonal real matrices, then the orthogonal symmetries of X form a group isomorphic to the direct product of the orthogonal groups $O(m_r)$. Thus this group is determined entirely by the multiplicities of the eigenvalues of X and, given this, does not promise to be very useful. Nonetheless it does have its applications. Note that the permutation matrices in it form a group isomorphic to $\mathrm{Aut}(X)$.

If the idempotents in the spectral decomposition of A are $E_1, \ldots, E_m$ and $\sigma_r^2 = 1$ for each r, then

$$S = \sum_r \sigma_r E_r$$

satisfies $S^2 = I$. Since $S = S^T$, we see that S is orthogonal. Since S must be a polynomial in A, it follows that the 2^m matrices S form a subgroup of the orthogonal symmetries of X; this subgroup is an elementary abelian 2-group. Any automorphism of X that lies in this group must lie in the centre of $\mathrm{Aut}(X)$.

If a and b are cospectral then $A(X\backslash a)$ and $A(X\backslash b)$ are similar. Since these matrices are symmetric, there is an orthogonal matrix L say, such that $L^T A(X\backslash a)L = A(X\backslash b)$.

Lemma 10.1. *The vertices a and b in X are cospectral if and only if there is an orthogonal symmetry Q of X such that $Q^2 = I$ and $Qe_a = e_b$.*

Proof. Let $U(+)$ and $U(-)$ respectively denote the A-modules generated by $e_a + e_b$ and $e_a - e_b$. By Theorem 3.1(g), these two modules are orthogonal subspaces of $\mathbb{R}^{V(X)}$. Let $U(0)$ be the orthogonal complement of $U(+) + U(-)$. There is a unique orthogonal matrix Q such that $Qx = -x$ if $x \in U(-)$ and $Qx = x$ if x lies in $U(+)$ or $U(0)$. (Note that, since the eigenvalues of Q are 1 and -1, we have $Q^2 = I$.)

Since $U(0)$, $U(+)$ and $U(-)$ are A-invariant, they are spanned by eigenvectors of A and (by construction) Q is diagonal relative to a basis of eigenvectors. Therefore it commutes with A.

Clearly $Q^2 = I$. We also have

$$2Qe_a = Q((e_a + e_b) + (e_a - e_b)) = e_a + e_b - e_a + e_b = 2e_b,$$

and so $Qe_a = e_b$. Since $Q^2 = I$, we also have $Qe_b = e_a$.

Thus we have shown that a symmetry exists as required when a and b are cospectral. The converse is straightforward. □

It is interesting to note that if $a, b \in V(X)$ and some automorphism γ maps a to b, it does not necessarily follow that γ maps b to a. The lemma above implies that if γ maps a to b, then some orthogonal matrix swaps a and b, but this matrix need not be related to any automorphism of X.

Theorem 10.2. *The vertices a and b in X are strongly cospectral if and only there is an orthogonal symmetry Q of X such that Q is a polynomial in A, is rational, $Q^2 = I$ and $Qe_a = e_b$.*

Proof. We use exactly the same construction as in the previous theorem and then observe that it a and b are strongly cospectral, the subspaces $U(+)$ and $U(-)$ are both direct sums of eigenspaces of A. This implies that Q is a signed sum of the idempotents E_r, and hence is a polynomial in A.

Let $\mathbb{E}$ be the extension of the rationals by the eigenvalues of X and let α be an automorphism of $\mathbb{E}$. Assume a and b are strongly cospectral. Then E_r^α is an idempotent in the spectral decomposition of A, associated to the eigenvalue θ_r^α. Therefore $((E_r)_{a,a})^\alpha > 0$ and consequently $((E_r)_{a,b})$ and $((E_r)_{a,a})^\alpha$ must have the same sign. It follows that Q is fixed by all field automorphisms of $\mathbb{E}$ and therefore it is a rational matrix.

The converse is straightforward. □

We derive some of the consequences of the theory we have just developed.

Suppose X is walk regular and a and b are strongly cospectral. Then $Q_{a,a} = 0$ but, since Q is a polynomial in A, its diagonal is constant. Therefore $\mathrm{tr}(Q) = 0$. Since

$Q^2 = I$ its eigenvalues are all ± 1; we conclude that 1 and -1 have equal multiplicity and therefore $|V(X)|$ must be even.

Recall that the *r-th distance graph* X_r of X is the graph with vertex set $V(X)$, where two vertices are adjacent in X_r if they are distance r in X. (Thus $X_1 = X$.) We use A_r to denote the adjacency matrix of X_r and we set $A_0 = I$. We have $\sum_r A_r = J$. We define X to be *distance regular* if, for each r, the matrix A_r is a polynomial of degree r in A_1. It follows from the definition that J is a polynomial in A_1 and consequently A_r and J commute for each r. Therefore the distance graphs X_r are regular.

If A is the adjacency matrix of a distance-regular graph, then A^k is a linear combination of the matrices $A_0, \ldots, A_d$ (for any non-negative integer k). Accordingly the diagonal of A^k is constant for all k, and therefore any two vertices in X are cospectral.

We present a short proof of a result of Coutinho et al. [2].

Theorem 10.3. *Suppose X is a distance-regular graph of diameter d, with distance matrices $A_0, \ldots, A_d$. If a and b are distinct strongly cospectral vertices in X, then A_d is a permutation matrix of order two and $A_d e_a = e_b$.*

Proof. Let Q be the matrix provided by Theorem 10.2. Then Q lies in the Bose-Mesner algebra of the association scheme $\mathcal{A} = \{A_0, \ldots, A_d\}$ which contains X. Since $Qe_a = e_b$, the a-column of Q has exactly one nonzero entry, $Q_{a,b}$. This implies that Q is equal to one of the matrices A_r, and that A_r is a permutation matrix. □

A distance-regular graph is *primitive* if its distance-graphs $X_1, \ldots, X_d$ are connected, otherwise it is *imprimitive*. It is a standard result that if a distance-regular graph of diameter d is imprimitive, either X_2 is not connected (and X is bipartite), or X_d is not connected (in which case X is said to be *antipodal*). The d-cube is distance-regular, and both bipartite and antipodal. The previous theorem implies that a distance-regular graph which contains a pair of strongly cospectral vertices is imprimitive.

More results of this flavour can be found in Coutinho [5].

11 Automorphisms, Equitable Partitions

We proved (as Corollary 6.4) that if vertices a and b were strongly cospectral, then any automorphism of X that fixed a must also fix b. We also derived (as Corollary 6.5) a related result involving equitable partitions. In this section we derive analogs of these results, where the algebraic conditions (cospectral, strongly cospectral) are replaced by constraints on the geometry of the orbits of D_a and D_b.

Suppose that we have an equitable partition π of X in which $\{a\}$ is a singleton cell, and let Q represent orthogonal projection onto the space of functions constant on the cells of π. Then $2Q - I$ is orthogonal and commutes with A and $(2Q - I)e_a = e_a$. Now if b lies in a cell of π with size k, then

$$\|(Q - I)e_b\|^2 = (k-1)\frac{1}{k^2} + \left(\frac{1}{k} - 1\right)^2 = 1 - \frac{1}{k}$$

and so if $Qe_b \neq e_b$, we have $\|2(Q-I)e_b\| \geq \sqrt{2}$. Therefore:

Lemma 11.1. *Suppose $a, b \in V(X)$. If $\|D_a(t) - D_b\| < 1/\sqrt{2}$, then any equitable partition in which $\{a\}$ is a singleton cell must also have $\{b\}$ as a singleton cell.* □

The orbits of any automorphism of a graph form an equitable partition, and if the automorphism fixes the vertex a, then $\{a\}$ is a singleton cell of the partition. This yields the following.

Corollary 11.2. *Let a and b be vertices of X. If there is a time t such that $\|D_a(t) - D_b\| < 1/\sqrt{2}$, then any automorphism of X that fixes a must also fix b.* □

12 Close Orbits, Cospectral

Assume a and b are vertices in X. We know that if the orbits of D_a and D_b coincide, then a and b must be cospectral. The main result of this section is that if these orbits are just sufficiently close, then a and b are cospectral. Hence the geometry of the orbits provides combinatorial information.

Suppose

$$A = \sum_r \theta_r E_r$$

is the spectral decomposition of A. Here $\theta_1, \ldots, \theta_m$ are the distinct eigenvalues of A and E_r is the matrix that represents orthogonal projection onto the eigenspace belonging to θ_r. Since the spectral idempotents E_r form a basis for the vector space of real polynomials in A, and since E_r is a polynomial in A, it follows that the vectors $E_r e_a$ span the column space of M_a, more precisely, the non-zero vectors $E_r e_a$ form an orthogonal basis for $\mathrm{col}(M_a)$. Recall from Section 4 set of eigenvalues θ_r such that $E_r e_a \neq 0$ is the *eigenvalue support* of the vertex a. (Hence $\mathrm{rk}(M_a)$ is equal to the size of the eigenvalue support of a.)

Lemma 12.1. *Assume a and b are distinct vertices in the graph X and set $n = |V(X)|$. Let $A = \sum_r \theta_r E_r$ be the spectral decomposition of X and let F be the $m \times n$ matrix with $F_{r\ell} = \theta_r^{\ell-1}$. If a and b are not cospectral, then*

$$\max_r \{|(E_r)_{a,a} - (E_r)_{b,b}|\} \geq \frac{1}{\mathrm{tr}(FF^T)}.$$

Proof. Let N_a and N_b respectively denote the $n \times m$ matrices with columns consisting of the vectors $E_r e_a$ and $E_r e_b$. If M_a and M_b are the walk matrices of a and b respectively, then

$$M_a = N_a F, \quad M_b = N_b F$$

and

$$M_a^T M_a - M_b^T M_b = F^T (N_a^T N_a - N_b^T N_b) F. \tag{12.1}$$

The matrices $N_a^T N_a$ and $N_b^T N_b$ are diagonal with

$$(N_a^T N_a)_{r,r} = (E_r)_{a,a}, \quad (N_b^T N_b)_{r,r} = (E_r)_{b,b}.$$

Hence
$$F^T(N_a^T N_a - N_b^T N_b)F = \sum_r ((E_r)_{a,a} - (E_r)_{b,b}) F^T e_r e_r^T F. \tag{12.2}$$
Let η denote the maximum value over r of $|(E_r)_{a,a} - (E_r)_{b,b}|$. Then by the triangle inequality
$$\Big\| \sum_r ((E_r)_{a,a} - (E_r)_{b,b}) F^T e_r e_r^T F \Big\| \le \eta \sum_r \|F^T e_r e_r^T F\|. \tag{12.3}$$
We have
$$\|F^T e_r e_r^T F\|^2 = \operatorname{tr}(F^T e_r e_r^T F\, F^T e_r e_r^T F) = (e_r^T F F^T e_r)^2,$$
whence $\|F^T e_r e_r^T F\| = (FF^T)_{r,r}$ and therefore the right side in (12.3) is equal to $\eta \operatorname{tr}(FF^T)$.

If a and b are not cospectral then $M_a^T M_a \ne M_b^T M_b$ and, since these matrices are integer matrices, the norm of $M_a^T M_a - M_b^T M_b$ is at least 1. So Equations (12.1), (12.2) and (12.3) imply that
$$\frac{1}{\operatorname{tr}(FF^T)} \le \eta. \qquad \square$$

Our next lemma provides an upper bound on $|U(t)_{a,b}|$.

Lemma 12.2. *If $a, b \in V(X)$ and $E_1, \ldots, E_m$ are the spectral idempotents of A, then*
$$|(E_r)_{a,a} - (E_r)_{b,b}| < \sqrt{8}\sqrt{1 - |U(t)_{a,b}|}.$$

Proof. We have
$$U(t)_{a,b} = \sum_r e^{it\theta_r} (E_r)_{a,b}.$$
By the triangle inequality we have
$$|U(t)_{a,b}| \le \sum_r |(E_r)_{a,b}|.$$
Now
$$(E_r)_{a,b} = e_a^T E_r e_b = \langle E_r e_a, E_r e_b \rangle$$
and by Cauchy-Schwarz
$$|\langle E_r e_a, E_r e_b \rangle| \le \|E_r e_a\| \|E_r e_b\| = \sqrt{(E_r)_{a,a}}\sqrt{(E_r)_{b,b}}.$$
We conclude that
$$|U(t)_{a,b}| \le \sum_r \sqrt{(E_r)_{a,a}}\sqrt{(E_r)_{b,b}}.$$
Here the upper bound is the fidelity between the spectral densities at a and b, which we denote by vectors x and y respectively. As
$$2 - 2|U(t)_{a,b}| \ge 2 - 2\langle x, y \rangle = \langle x - y, x - y \rangle,$$

we have that for any r,

$$\left|\sqrt{(E_r)_{a,a}} - \sqrt{(E_r)_{b,b}}\right| \leq \sqrt{2 - 2|U(t)_{a,b}|},$$

and since, $(E_r)_{a,a} \leq 1$ and $(E_r)_{b,b} \leq 1$, we finally have our upper bound:

$$|(E_r)_{a,a} - (E_r)_{b,b}| < \sqrt{8}\sqrt{1 - |U(t)_{a,b}|}. \qquad \square$$

We now show that if the orbits of D_a and D_b are close enough, then a and b are cospectral.

Theorem 12.3. *Let $n = V(X)$, let ρ be the largest eigenvalue of A, and let a and b be vertices of X. If there is a time t such that*

$$|U(t)_{a,b}| \geq 1 - \frac{1}{8n^4\rho^{2n}}.$$

then a and b are cospectral.

Proof. We need an estimate for $\operatorname{tr}(FF^T)$. As $\operatorname{tr}(FF^T)$ is equal to the sum of the entries of the Schur product $F \circ F$, and as the maximum entry of F is ρ^{n-1}, we see that $\operatorname{tr}(FF^T) \leq n^2\rho^n$. Now the result follows from the previous two lemmas. $\square$

There is a simple relation between $1 - |U(t)_{a,b}|$ and the distance between orbits:

$$\|D_b - D_a(t)\|^2 = 2 - 2\langle D_b, D_a(t)\rangle = 2 - 2|U(t)_{a,b}|^2.$$

13 Closer Orbits, Strongly Cospectral

We prove an analog of the result of the previous section, showing that if the orbits of D_a and D_b are close enough, then a and b are strongly cospectral.

Two preliminary results are needed; the first is Theorem 9.3 in [10], the second is Lemma 3.1 from the same source.

Lemma 13.1. *Two vertices of X are strongly cospectral if and only if the corresponding rows of $\widehat{M}_X$ are equal.* $\square$

Lemma 13.2. *Let D denote the discriminant of the minimal polynomial of the adjacency matrix of X. Then the entries of $D^2\widehat{M}_X$ are integers.* $\square$

Lemma 13.3. *Let a and b be vertices in the graph X. There is a constant η (depending on X) such that if for some t we have*

$$\|D_a(t) - D_b\| < \eta,$$

then a and b are strongly cospectral.

Proof. Suppose $\|D_a(t) - D_b\| < \zeta$. Then, as we noted following the proof of Lemma 5.1, the operator norm of Φ is at most 1 and we can apply Lemma 5.2 to deduce that

$$\|\Phi(D_a) - \Phi(D_b)\| = \|\Phi(D_a(t)) - \Phi(D_b)\| \leq \|D_a(t) - D_b\| < \zeta.$$

If $u \in V(X)$, then Cauchy-Schwarz yields

$$|\langle \Phi(D_a) - \Phi(D_b), \Phi(D_u)\rangle| \leq \|\Phi(D_a) - \Phi(D_b)\| \, \|\Phi(D_u)\|.$$

Since D_u is pure, $\|D_u\| = 1$ whence $\|\Phi(D_u)\| \leq 1$. and it follows that the right side of this inequality is bounded above by ζ.

We conclude that the absolute value of an entry of $(e_a - e_b)^T \widehat{M}_X$ is bounded above by ζ. On the other hand, if D is the discriminant of the minimal polynomial of A, then $D^2 \widehat{M}_X$ is an integer matrix and, accordingly, if a and b are not strongly cospectral, some entry of $(e_a - e_b)^T \widehat{M}_X$ is bounded below by D^{-2}. □

It would not be too difficult to derive an estimate for η, it would be substantially smaller than the distance required to show that the vertices are cospectral.

This lemma implies that if there is pretty good state transfer from a to b, then a and b are strongly cospectral.

14 Problems

Is there a tree that contains a set of three vertices, any two of which are strongly cospectral?

We have shown that the distance between orbits of D_a and D_b provides a measure of 'similarity' between the vertices a and b. Are there further interesting properties of vertices related to this distance? We admit that computing this distance, even for specific graphs, is a difficult task. Are there interesting graphs where this computation is feasible?

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