TOWARDS AN ALGEBRA OF SINGS

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The spectrum of a graph is the spectrum of its adjacency matrix. Cospectral (or isospectral) graphs are graphs having the same spectrum. We develop some algebraic tools for treating sets of isospectral non-isomorphic graphs (SINGs). SINGs with eigenvalues greater than \(-\frac{1 + \sqrt{5}}{2} = -1.6180\) are classified.

1. INTRODUCTION

The spectrum of a graph is the spectrum of its adjacency matrix. Cospectral (or isospectral) graphs are graphs having the same spectrum.

Cospectral graphs have been studied since very beginnings of the development of the theory of graph spectra. The subject, although present in the investigations all the time, has recently attracted special attention (see, e.g., [6], [7]).

In this paper we study the phenomenon of cospectrality in graphs by outlining (in Sections 2 and 3) an algebra of sets of isospectral non-isomorphic graphs (SINGs). SINGs with eigenvalues greater than \(-\frac{1 + \sqrt{5}}{2} = -1.6180\) are classified in Section 5. Some remarks on the use of graph angles in treating SINGs are given in Section 6.

2. BASIC NOTIONS AND RESULTS

Let \(G\) be a simple graph with \(n\) vertices. We write \(V(G)\) for the vertex set of \(G\), and \(E(G)\) for the edge set of \(G\).

The characteristic polynomial \(\det(xI - A)\) of the adjacency matrix \(A\) of \(G\) is called the characteristic polynomial of \(G\) and denoted by \(P_G(x)\). The eigenvalues of \(A\) (i.e. the zeros of \(\det(xI - A)\)) and the spectrum of \(A\) (which consists of the \(n\) eigenvalues) are also called the eigenvalues and the spectrum of \(G\), respectively. The spectrum of a graph \(G\) is denoted by \(S(G)\). The eigenvalues of \(G\) are usually denoted by \(\lambda_1, \lambda_2, \ldots, \lambda_n\); they are real because \(A\) is symmetric. We shall assume that \(\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n\) and use the notation \(\lambda_i = \lambda_i(G)\) for \(i = 1, 2, \ldots, n\). The least eigenvalue \(\lambda_n(G)\) is also denoted by \(\lambda(G)\).
An overview of results on graph spectra is given in [2].

Graphs with the same spectrum are called isospectral or cospectral graphs. The term “(unordered) pair of isospectral non–isomorphic graphs” will be denoted by PING. More generally, a “set of isospectral non–isomorphic graphs” is denoted by SING. A two element SING is a PING. A SING may be empty (of course, if it has no elements) or trivial (if it consists of just one graph). A graph $H$, cospectral but non–isomorphic to a graph $G$, is called a cospectral mate of $G$.

Since eigenvectors of an adjacency matrix are not graph invariants it is reasonable to extend eigenvalue based techniques by some invariants of the eigenspaces called graph angles.

Let $G$ be a graph on $n$ vertices with distinct eigenvalues $\mu_1, \mu_2, \ldots, \mu_m$ ($\mu_1 > \mu_2 > \cdots > \mu_m$) and let $S_1, S_2, \ldots, S_m$ be the corresponding eigenspaces. Let $\{e_1, e_2, \ldots, e_n\}$ be the standard (orthonormal) basis of $\mathbb{R}^n$. The numbers $\alpha_{pq} = \cos \beta_{pq}$ ($p = 1, 2, \ldots, m; q = 1, 2, \ldots, n$), where $\beta_{pq}$ is the angle between $S_p$ and $e_q$, are called graph angles. The sequence $\alpha_{pq}$ ($q = 1, 2, \ldots, n$) is called the eigenvalue angle sequence corresponding to the eigenvalue $\mu_p$ ($p = 1, 2, \ldots, m$).

Let $x_i = (x_{i1}, x_{i2}, \ldots, x_{in})$ ($i = 1, 2, \ldots, n$) be orthonormal eigenvectors of $G$. Define $M_p = \{j \mid Ax_j = \mu_p x_j\}$. We have

$$\alpha_{pq}^2 = \sum_{j \in M_p} x_{jq}^2$$

for squares of angles of $G$. This formula holds for any choice of orthonormal eigenvectors of $G$ (cf. [8], p. 76).

Cosines of the angles between all-1 vector $j$ and eigenspaces $S_i, i = 1, 2, \ldots, m$ are called main angles of the graph. An eigenvalue is called main if the corresponding main angle is different from 0. Obviously, an eigenvalue is main if and only if it has an eigenvector the sum of whose coordinates is different from 0.

An overview of results on graph angles is given in [8] including the characterizing properties of graph angles.

As usual, $K_n, C_n$ and $P_n$ denote respectively the complete graph, the cycle and the path on $n$ vertices. Further, $K_{m,n}$ denotes the complete bipartite graph on $m + n$ vertices. The double star $D_{m,n}$ is the graph formed by adding an edge between the central vertices of stars $K_{1,m}$ and $K_{1,n}$.

The union of (disjoint) graphs $G$ and $H$ is denoted by $G \cup H$, while $mG$ denotes the union of $m$ disjoint copies of $G$. The graph $k_1 G_1 + \cdots + k_n G_n, k_1, \ldots, k_n$ being integers, is called a linear combination of graphs $G_1, \ldots, G_n$. The set of all linear combinations of graphs $G_1, \ldots, G_n$ is denoted by $L(G_1, \ldots, G_n)$.

### 3. OPERATIONS ON SINGs

A part of efforts in the research in area of combinatorics is devoted to enumeration of combinatorial structures of small cardinality. Such catalogues (nowdays usually in an electronic form) of “small” combinatorial structures serve, among
other things, to produce conjectures which are then treated theoretically. An example of this type is a table of cospectral graphs with least eigenvalue at least \(-2\) \[5, 6\]. When preparing this table it appeared to be useful to introduce some notions related to SINGs. Here we extend these ideas.

A SING is called complete if no graph outside the SING is cospectral to graphs from the SING; otherwise the SING is called incomplete. Two SINGs are said to be cospectral if the graphs in both of them have the same spectrum. Of course, the union of cospectral SINGs is a SING.

A subset of a SING is also a SING. The union and intersection of SINGs are also SINGs.

If the set of graphs \(\{G_1, G_2, \ldots, G_k\}\) is a SING and if \(G\) is any connected graph, then the set \(\{G_1 \cup G, G_2 \cup G, \ldots, G_k \cup G\}\) is also a SING. Each graph in the later SING has a component isomorphic to a fixed graph (to the graph \(G\)).

A SING \(S\) is called reducible if each graph in \(S\) contains a component isomorphic to a fixed graph. Otherwise, \(S\) is called irreducible. A reducible non-trivial SING can be reduced to an irreducible one by extracting one or several components common for each graph in the SING.

More generally, for two SINGs \(S = \{G_1, G_2, \ldots, G_k\}\) and \(P = \{H_1, H_2, \ldots, H_q\}\)

we define the composition \(S \circ P\) by

\[S \circ P = \{G \cup H \mid G \in S, H \in P\}\]

A subset of \(S \circ P\) is called a partial composition of SINGs \(S\) and \(P\).

A partial graph of a graph \(G\) is the union of some components of \(G\).

A SING \(S\) is weakly reducible if there is a graph \(H\) such that any graph in \(S\) contains a partial graph cospectral to \(H\). If \(G\) is not weakly reducible it is called strongly irreducible.

**Proposition 1.** If a SING contains a connected graph, it is irreducible and strongly irreducible.

We shall say that a SING \(P\) is relevant to the SING \(S\), denoted by \(P \vdash S\), if a graph in \(P\) is cospectral to a partial graph of a graph in \(S\). Any such graph \(G\) is called the basis of \((P, S)\).

**Proposition 2.** If \(P \vdash S\) and \(S \vdash P\), then \(P\) and \(S\) are cospectral.

If \(P \vdash S\), then for any basis \(G\) of \((P, S)\) we can define an expansion \(E(S, P, G)\) of \(S\) by \(P\) through the basis \(G\). The SING \(S\) is extended by graphs obtained from any graph of \(S\) which contains a partial graph isomorphic to \(G\) by replacing it with any other graph from \(P\). Obviously, the set \(E(S, P, G)\) is a SING.

The SINGs whose members belong to a set \(X\) of graphs are called \(X\)-SINGs.

We shall illustrate the usefulness of these notions by presenting some details concerning the mentioned table of cospectral graphs.
Towards an Algebra of SINGs

The table of cospectral graphs from [5], [6] contains irreducible SINGs in which graphs have the least eigenvalue at least \(-2\) and the number of vertices \(n\) is at most 8. Let \(\mathcal{L}\) be the set of graphs which have the least eigenvalue at least \(-2\). Such graphs are also called \(\mathcal{L}\)-graphs. The table contains the 201 irreducible \(\mathcal{L}\)-SINGs with at most 8 vertices. This number includes 178 pairs, 20 triplets and 3 quadruples of cospectral graphs.

In the table the SINGs are classified by the number of vertices and by the number of edges. Within a group with fixed numbers of vertices and edges the SINGs are classified lexicographically by their eigenvalues.

Given two graphs \(G\) and \(H\), we shall say that \(G\) is smaller than \(H\) if \(|V(G)| < |V(H)|\) and in the case \(|V(G)||V(H)|\) if \(|E(G)| < |E(H)|\). Any set of graphs has one or several smallest graphs in the above order of graphs. Since graphs in any SING have the same number of vertices and the same number of edges, we can compare SINGs as well in the above sense.

The smallest PING without the limitations on the least eigenvalue, which consists of graphs \(K_{1,4}\) and \(C_4 \cup K_1\), is also the first graph in our table.

The next PING which appears in the table consists of disconnected graphs \(K_{1,3} \cup K_2, P_3 \cup K_1\) and this is the smallest irreducible PING with such a property.

Although reducible SINGs should not be included in tables like our since they can easily be generated from irreducible ones, reducible SINGs are not quite uninteresting. Namely, although the reducible PINGs, for example, \(\{K_{1,4} \cup K_1, C_4 \cup 2K_1\}, \{K_{1,3} \cup K_2 \cup K_1, P_3 \cup 2K_1\}\) have been deleted from the table, the reducible SING \(\{K_{1,4} \cup K_2, C_4 \cup K_1 \cup K_2\}\) appears to be incomplete and can be extended to the triplet of cospectral graphs \(\{K_{1,4} \cup K_2, C_4 \cup K_1 \cup K_2, S_6 \cup K_1\}\) which does appear in the table (as the SING No. 7.1, the SING identification numbers refering to the table of [5], [6])! (Here \(S_6\) is the tree on 6 vertices with largest eigenvalue equal to 2).

In this context interesting is also the (irreducible) SING No. 8.2. It is a quadruple consisting of two (cospectral) reducible PINGs (first and third graph can be reduced to PING No. 6.2 while the other two reduce to the PING No. 7.2).

The PING No. 6.3 of the table of [5], [6] is reproduced in Fig. 1.

Its least eigenvalue \(\rho\), approximately equal to \(-1.5616\), is the least solution of the equation \(\lambda^2 - \lambda - 4 = 0\). This PING will be used in Section 5.

4. AN ALGEBRA OF SINGs

The SINGs in which the largest eigenvalue does not exceed 2 have been characterized in [3]. This was achieved by considering formal integer linear combinations of graphs in question and of their spectra. A basis of this module has been found.

The idea from [3] will be elaborated here in a more general setting.
A mapping $\phi$ from a set $S$ to the integer set $\mathbb{Z}$ is called a family of $S$. For $x \in S$ the value $\phi(x)$ is the multiplicity of $x$ in the family $\phi$. This definition extends the usual notion of a family; normally we would allow only non-negative multiplicities of elements of the family while here multiplicities could be negative.

Let $X, Y$ be a families of elements of a set $S$. For $k \in \mathbb{Z}$ we define $kX$ to be the family obtained from $X$ by multiplying the multiplicities of its elements by $k$. The union $X + Y$ of families $X, Y$ is the family consisting of elements contained in any of the two families with multiplicities being the sums of multiplicities in the corresponding families.

The family $k_1X_1 + \cdots + k_nX_n$, $k_1, \ldots, k_n$ being integers, is called a linear combination of families $X_1, \ldots, X_n$. The set of all linear combinations of families $X_1, \ldots, X_n$ is denoted by $L(X_1, \ldots, X_n)$. The set $L = L(X_1, \ldots, X_n)$ is an Abelian group w.r.t. the union $+$ of families and also a $\mathbb{Z}$-module. The corresponding ”subtraction” operation - in $L$ is introduced in a standard manner and used in [3].

A minimal set of families of $L$ which generates the whole set $L$ is called a basis of $L$.

The spectrum of a graph $G$ will be denoted by $\mathcal{S}(G)$. Obviously, we have

$$S(kG) = kS(G) = k \mathcal{S}(G) = \mathcal{S}(kG), \quad S(G \cup H) = S(G) + S(H) = \mathcal{S}(G) + \mathcal{S}(H) = \mathcal{S}(G \cup H).$$

The spectrum of a linear combination of graphs is the same linear combination of their spectra.

The mapping $G \rightarrow \mathcal{S}(G)$ is a homomorphism from $L(G_1, \ldots, G_n)$ onto $L(G_1, \ldots, G_n)$.

**Proposition 3.** The homomorphism $G \rightarrow \mathcal{S}(G)$ is an isomorphism if $L(G_1, \ldots, G_n)$ contains no non-trivial SING.

**Proof.** If for two distinct graphs $G$ and $H$ we have $\mathcal{S}(G) = \mathcal{S}(H) = \mathcal{S}(G \cup H) = \mathcal{S}(H)$ then graphs $G$ and $H$ form a non-trivial SING.

The following two propositions are immediate.

**Proposition 4.** A set of families is independent if each family has a member which does not belong to other families.

**Proposition 5.** Families of reals are independent if they all have mutually different largest (least) members.

If $G_1, \ldots, G_n$ is a basis of $L(G_1, \ldots, G_n)$ then $G_1, \ldots, G_n$ is called an $s$-basis of $L(G_1, \ldots, G_n)$.

The main result of [3] can be formulated in the following way.

**Theorem 1.** The set of all paths extended by the cycle $C_4$ is an $s$-basis of the set of graphs whose largest eigenvalue does not exceed 2.

In the next section SINGs in which the least eigenvalue is greater than $-\frac{1 + \sqrt{5}}{2}$ are classified.
5. THE PING WITH LARGEST LEAST EIGENVALUE

All graphs with least eigenvalue at least $-\sqrt{3}$ have been identified in [10]. The set of connected graphs with least eigenvalue at least $\tau = -(1 + \sqrt{5})/2 = -1.6180$ is denoted by $S_\tau$. A relevant particular result reads:

**Theorem 2.** The set $S_\tau$ consists of connected induced subgraphs of the following graphs:

1. graph (a) of Fig. 2 (i.e. the wheel $W_5$),
2. graph (f) of Fig. 2,
3. graph (k) of Fig. 2,
4. the graph $Y_{n,0}$ of Fig. 3 for some $n = 1, 2, \ldots$.

We have that $Y_{k,l}$ is the line graph of $X_{k,l}$ (see Fig. 3). Note that the complete graph $K_n$ is just $Y_{0,n}$, while the graph $Y_{1,m} = Q_m$ is just the line graph of a double star $D_{m,1}$. All graphs $Y_{k,l}$ belong to $S_\tau$, since $Y_{k,l}$ is an induced subgraph of $Y_{k+t,0}$.

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**Fig. 2**

(a) (b) (c) (d) (e) (f)

(g) (h) (i) (j) (k)

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**Fig. 3**
We shall prove the following proposition.

**Proposition 6.** The only PING with largest least eigenvalue and a minimal number of vertices is the PING of Fig. 1.

**Proof.** The graphs $Y_{k,0}$ can be obtained by adding a pendant vertex to each vertex of $K_k$. On page 60 of [2] one can find a formula for the characteristic polynomial of a graph obtained in this way (alternatively, one can use a more general formula for the corona of two graphs in the next section): 

$$P(Y_{k,0}; \lambda) = \lambda^k P(K_k; \lambda - \frac{1}{\lambda}) = (\lambda^2 - (k - 1)\lambda - 1)(\lambda^2 + \lambda - 1)^{k-1}.$$ 

Thus, the eigenvalues of $Y_{k,0}$ are simple eigenvalues $(k - 1 \pm \sqrt{(k - 1)^2 + 4})/2$, and eigenvalues $(\sqrt{5} - 1)/2$ and $-(1 + \sqrt{5})/2$, each with multiplicity $k - 1$.

The characteristic polynomial of graphs $Q_m$ can be calculated by Theorem 2.1 of [2], p. 60: 

$$(\lambda + 1)^{m-2}(\lambda^3 - (m - 2)\lambda^2 - m\lambda + m - 2).$$ 

The least eigenvalue of $Q_m$ is strictly decreasing with $m$ and tends to the smallest root of the equation $\lambda^2 + \lambda - 1$, i.e. to $\tau = -(1 + \sqrt{5})/2 = -1.6180$.

Since $Q_7$ and $Q_8$ have least eigenvalues $-1.5572$ and $-1.5645$, connected graphs are ordered by decreasing least eigenvalues as follows: 

$K_1, K_n (n \geq 2), Q_s (2 \leq s \leq 7)$ graphs (d) and (j) of Fig. 2 both with least eigenvalue $\rho = -1.56166, Q_t (t = 8, 9, ...)$.

Hence, graphs of the PING with largest least eigenvalue should contain graphs (d) and (j) of Fig. 2 as components and we readily get the PING of Fig. 1.

This completes the proof.

We can go on to describe all SINGs with eigenvalues greater than $\tau$.

By Theorem 2, except for the series $Q_t (t = 8, 9, ...)$, the only connected graph with least eigenvalue in the interval $(\tau, \rho)$ is the graph (k) of Fig. 2. However, no graph $Q_n$ has the least eigenvalue equal to the least eigenvalue of (k). Namely, we have $\lambda(Q_{26}) = -1.60111, \lambda(Q_{28}) = -1.6023$ while $\lambda(Q_{27}) = -1.6017$ coincides with least eigenvalue of (k) within four decimal places. More precise calculation shows that $\lambda(Q_{27}) = -1.60171$ and $\lambda(k) = -1.60168$.

This shows that any non-trivial irreducible SING with least eigenvalue greater than $\tau$ has least eigenvalue equal to $\rho$.

Let us denote by $D, J$ the graphs (d),(j) of Fig. 2. The spectrum of $D$ is $1 - \rho, 0, -1, \rho$ while the spectrum of $J$ reads $1 - \rho, 1, -1, -1, \rho$. The symmetric difference of these spectra contains the numbers $1, 0, -1$. The only graph with this spectrum is $K_2 \cup K_1$. This gives rise to PING of Fig. 1. Moreover, any irreducible PING with least eigenvalue $\rho$ contains the graphs of the form $kD \cup \ell J \cup sK_1 \cup tK_2$ for some integers $k, \ell, s, t$.

The following proposition can easily be proved.
Proposition 7. Let
\[ G_1 = kD \cup \ell J \cup sK_1 \cup tK_2, \quad G_2 = pD \cup qJ \cup uK_1 \cup vK_2 \]
where \( k, \ell, s, t, p, q, u, v \) are integers and \( q \geq \ell \). Put \( \Delta = q - \ell \). Then \( G_1 \) and \( G_2 \)
are cospectral if and only if \( k + \ell = p + q \), \( u = s + \Delta \), \( t = v + \Delta \).

Also the following statement holds.

Proposition 8. Any non-trivial irreducible SING with eigenvalues greater than \( \tau \) contains only graphs in which each components is isomorphic to one of graphs \( D, J, K_2, K_1 \).

In this way we arrive at the following theorem.

Theorem 3. The graph \( D \) together with graphs \( K_n \) (for \( n = 1, 2, \ldots \)) and \( Q_m \) (for \( m = 2, 3, \ldots \)) constitutes an \( s \)-basis of the set of graphs whose least eigenvalue is greater than \( \tau \).

Of course, the graph \( D \) can be replaced by the graph \( J \) in this theorem.

Next step would be to characterize SINGs with least eigenvalue \( \tau \). The only irreducible SING with this property that we know is the PING No. 7.12 of [5], [6].

6. USING GRAPH ANGLES

If, besides the spectrum, also the angles of a graph are known, we can say much more about the structure of the graph [8]. In many cases the graphs from a PING can be distinguished by their angles. However, there exist also cospectral graphs with the same angles.

Smallest such examples have been found by a computer search [4]. They have 10 vertices. In fact, there are 58 pairs of cospectral graphs on 10 vertices with the same angles (and with the same main angles). Among them there are just two (Nos. 1 and 2 in [4]) with least eigenvalue \(-2\). In both PINGs one graph is a line graph while the other is an exceptional one.

A case when the angles suffice to characterize graphs is noted in [1]. It is proved there that the graphs whose largest eigenvalue does not exceed 2 are characterized (up to isomorphism) by their eigenvalues and angles.

Angles can be very useful in treating SINGs which contain disconnected graphs. Connected graphs can be recognized by eigenvalues and angles. In this way irreducible SINGs containing at least one connected graph can be recognized. In many cases components or partial graphs of disconnected graphs can be reconstructed and eigenvalues and angles corresponding to particular components or partial graphs determined (cf. [8], Section 4.4). This means that, under some conditions, reducible SINGs can be recognized and the common components extracted, thus obtaining irreducible SINGs.
REFERENCES


