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UNDERSTANDING THE PROPERTIES OF ISOSPECTRAL POINTS AND PAIRS IN GRAPHS: THE CONCEPT OF ORTHOGONAL RELATION

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Abstract

The mathematical property "orthogonal relationship" is used in proving the fact that isospectrality, isocodality and isocoefficiency of vertices within a graph are all equivalent. The same is true for isospectrality, "strict isocodality" and "strict isocoefficiency" of pairs (including edges) within a graph, whereas the "weak" versions of the latter properties are necessary but not sufficient for isospectrality of pairs. Similarly, necessary and sufficient conditions for isospectrality of vertices and pairs in different graphs are derived. In all these proofs, the concept of "orthogonal relation" plays a major role in that it allows the use of tools of elementary linear algebra.

1. Introduction

Much work has been devoted to the study of isospectral and endospectral graphs and to the discussion of the properties of the special vertices encountered in such graphs, termed isospectral and endospectral vertices or points. For leading references, see the book by Trinajstić [1] and the recent reviews by Randić [2,3].

Chemists, of course, are interested not only in atoms, but in bonds or, more generally, in relations between atoms, called pairs. Quite naturally, therefore, in the present context isospectral/endospectral edges [4] and pairs [5,6] were at least cursorily examined. In these studies, interesting properties of such vertices and pairs were detected: isospectral graphs may be produced whenever one or the other of two special sites (vertices, edges, pairs) is "perturbed" in some arbitrary manner (whence the term isospectral for such sites), the eigenvector coefficients associated with such sites may exhibit some regularities ("isocoefficiency") [7], and the numbers of possible walks in a graph may be equal for two such sites throughout all different lengths ("isocodality") [8].

Typically, however, such properties were discussed on a phenomenological basis, without describing the mathematical relations between them in general. There

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is one noticeable exception: Herndon and Ellzey [7] rigorously proved the equivalence of isospectrality and isocoefficiency of vertices within a graph. Apart from this, the development of the mathematics underlying these phenomena leaves much to be desired. In the case of isospectral edges and pairs, not even consistent definitions were given and, partly for this reason, necessary and sufficient conditions for isospectrality of these are not known.

From a mathematical point of view, isospectrality of graphs formally resembles isomorphism of graphs, in that both are equivalence relations, the former less demanding than the latter. Similarly, isospectrality of vertices is a less demanding equivalence relation than symmetry of vertices, the former giving a coarser partition of vertices than the latter. Our aim in the present study was to use these analogies in order to derive simple and elegant mathematical proofs of the equivalence of the properties mentioned above, or to point out wherever they are not equivalent, which may happen in the case of vertices in different graphs or in the case of pairs including edges even within a single graph.

To achieve this goal, we found it useful to introduce another property, the "orthogonal relationship". After demonstrating in section 2 the orthogonal relationship of isospectral graphs, we use this property in treating isospectral vertices within a single graph in section 3, isopectral pairs within a single graph in section 4, and isospectral vertices and pairs in different graphs in section 5.

2. Isospectral graphs

All graphs in this paper are undirected and may contain loops or multiple edges.

DEFINITION

Two graphs G and H with adjacency matrices A and B are called *isospectral*, if A and B have the same spectrum (the same eigenvalues) or, equivalently, the same characteristic polynomial $p_G(x) = \det(A + xI)$ [9,10].

By the well-known spectral theorem of linear algebra (see, e.g. [11]) for a symmetric linear map, there exists an orthogonal basis consisting of eigenvectors of this map. Moreover, matrices A and B have the same eigenvalues if and only if they are similar, that is, there exists a regular transformation S such that

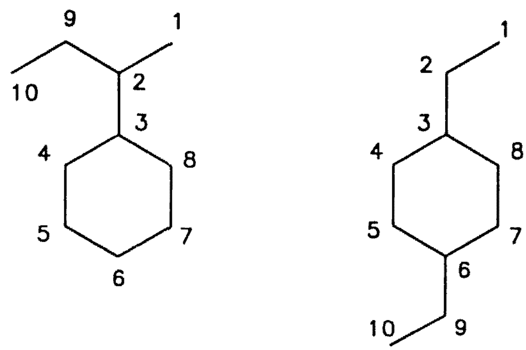
$$SA = BS \tag{1}$$

holds. By the spectral theorem for symmetric matrices, S can be chosen as an orthogonal matrix (that is, a regular matrix S with $S^{-1} = S^{\mathrm{T}}$, where S^{T} is the transposed matrix).

Examples

(i) If G and H are isomorphic graphs, then there exists a permutation matrix S (which is a special kind of orthogonal matrix) which transforms one form of the adjacency matrix, say A, into the other, B, so fulfilling eq. (1). Therefore, isomorphic graphs are isospectral.

(ii) A famous example of two isospectral but not isomorphic graphs [2, 12] is that of the carbon frames of 2-phenylbutadiene (**1**) and 1,4-divinylbenzene (**2**), shown in fig. 1.



1 **2**

Fig. 1. Two non-isomorphic isospectral graphs.

The reader can easily check that matrix T_1 given below is orthogonal and converts the adjacency matrix A of **1** into that of **2**, B, in the sense of eq. (1):

$$T_1 = \begin{pmatrix} 0.5 & 0 & -0.5 & 0 & 0.5 & 0 & 0.5 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ -0.5 & 0 & 0.5 & 0 & 0.5 & 0 & 0.5 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0.5 & 0 & 0.5 & 0 & 0.5 & 0 & -0.5 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0.5 & 0 & 0.5 & 0 & -0.5 & 0 & 0.5 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

T_1 can be derived by methods outlined in the next section. Of course, by the non-isomorphy of the two graphs, we cannot expect a permutation matrix to act as an orthogonal transformation here.

3. Isospectral vertices within a graph (endospectral vertices)

DEFINITION

Two vertices i and j ($1 \leq i \leq j \leq n$) in a graph are referred to as *isospectral vertices* [7] or *endospectral vertices* [3] or points, if every perturbation at i or j, respectively, yields two isospectral graphs.

The expression "every perturbation" includes attachment of any arbitrary fragment and more, as is shown below.

The following formula was given by Hosoya [13,14]: If a graph is composed of two subgraphs G and H with adjacency matrices A and B, which are joint in exactly one common vertex i (as in fig. 2), then the characteristic polynomial p_{AiB} of the graph is given by the formula

$$p_{AiB}(x) = p_A(x)p_{B-i}(x) + p_{A-i}(x)p_B(x) - xp_{A-i}(x)p_{B-i}(x), \tag{2}$$

where p_A and p_B are the characteristic polynomials of A and B, p_{A-i} and p_{B-i} those of the same graphs reduced by vertex i.

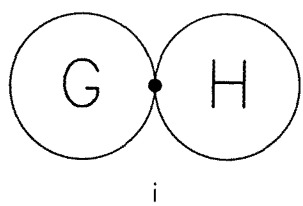


Fig. 2. A graph composed of two subgraphs joined in vertex i (schematic).

Equation (2) is a generalization of Heilbronner's formula [15] for the characteristic polynomial of a graph formed from two simpler graphs by joining them over an additional edge as in fig. 3.

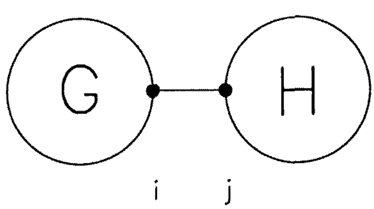


Fig. 3. A graph composed of two subgraphs joined by an edge i, j (schematic).

Now we are able to prove a simple criterion for endospectrality of two points in a graph.

LEMMA 3.1

To check whether two particular vertices i and j in a graph are endospectral, it is sufficient to verify isospectrality of the two graphs obtained by one of the following perturbations:

(i) Removal of i or j in turn.

(ii) "Marking" of i or j in turn by a loop (entering "1" in diagonal elements a_{ii} (a_{jj}) of the adjacency matrix).

(iii) Addition of a new vertex at site i or j in turn.

Proof

Use the following characteristic polynomials:

p for the original graph G,

p_{-i} for G with vertex i removed,

p_i for G with vertex i marked,

p_{i+} for G with a new vertex added at i,

p_{i+H} for G with an arbitrary fragment H (that is, another graph) attached at i (in the sense of fig. 2),

q for this fragment H,

q_- for H reduced by the vertex which serves for joining it to G (in the sense of fig. 2).

By elementary manipulations of the corresponding determinants, it can be proven that

$$p_i(x) = p(x) + p_{-i}(x). \tag{3}$$

By (2), it is seen that

$$p_{i+H}(x) = p(x)q_-(x) + p_{-i}(x)q(x) - xp_{-i}(x)q_-(x) \tag{4}$$

holds. Perturbation (iii) is obviously a special case of attaching a fragment at i, where

$$q(x) = x^2 - 1$$

and

$$q_-(x) = x$$

hold, so that (4) reduces to

$$p_{i+}(x) = xp(x) - p_{-i}(x). \tag{5}$$

Of course, corresponding formulas hold for vertex j. Now let perturbation (i) result in two isospectral graphs, that is

$$p_{-i}(x) = p_{-j}(x). \tag{6}$$

From (6) and (3), we at once obtain

$$p_i(x) = p_j(x) \tag{6'}$$

(corresponding to perturbation (ii)), and from (6) and (5) similarly

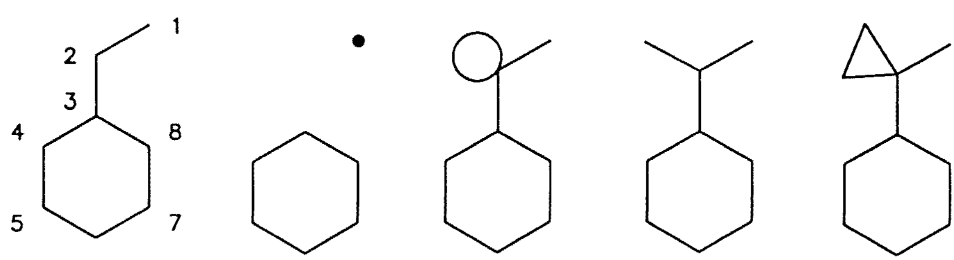
$$p_{i+}(x) = p_{j+}(x) \tag{6''}$$

(corresponding to perturbation (iii)). Obviously, eqs. (6), (6′), and (6″) are equivalent. Using (4) and (6), we see that they are even equivalent to

$$p_{i+H}(x) = p_{j+H}(x),$$

which means that i and j meet the definition of endospectral points. In other words, equality of the characteristic polynomials obtained by one sort of perturbation ((i), (ii), or (iii)) is sufficient for equality obtained by any other perturbation. □

Some perturbations are drawn in fig. 4. Note that the expression "attachment of any arbitrary fragment" is not limited to attachment via a single edge (fig. 3), but that attachment via many edges is allowed (fig. 2) by the very general nature of formulas (2) and (4), as exemplified by graph **7** (fig. 4).



3 **4** **5** **6** **7**

Fig. 4. A graph (**3**) containing endospectral vertices (2 and 6) and endospectral pairs ((2, 4) and (4, 6)), and the results of some perturbations at its vertex 2 (**4**–**7**). **4**: vertex removed, corresponding to perturbation (i); **5**: a loop added, corresponding to perturbation (ii); **6**: a new vertex added, corresponding to perturbation (iii); **7**: a two-vertex fragment added via two edges.

Examples

(i) Equivalence by symmetry is a special case of endospectrality of vertices. Two vertices i and j in a graph with adjacency matrix A are equivalent by symmetry if and only if there exists a permutation matrix S with

$$SA = AS \tag{7}$$

and

$$Se_i = e_j, \tag{8}$$

where e_i and e_j are the ith and jth unit vectors. This means S is the matrix of an automorphism of the graph, which transforms vertex i into vertex j.

(ii) A non-trivial example is provided by graph **3** given in fig. 4. Here, vertices 2 and 6, not equivalent by symmetry, will turn out to be endospectral. Note that the isospectral molecular graphs of fig. 1 are derivatives of **3**: a two-vertex group (vertices 9 and 10) has been attached to vertex 2 (leading to **1**) or vertex 6 (leading to **2**).

Isospectral *graphs*, on the one hand, are always related by an orthogonal transformation, since they correspond to similar matrices. For the special case of isomorphic graphs, a permutation transforms one representation of the graph into another. On the other hand, *vertices* equivalent by symmetry, which are a special kind of endospectral vertices, are related by a permutation, which is a special kind of orthogonal transformation. It is therefore quite natural to ask whether endospectral vertices in general are in some sense "orthogonally related". This turns out to be the case. In order to examine this in detail, we first give a definition.

DEFINITION

Two vertices i and j in a graph with adjacency matrix A are said to be *orthogonally related* if there exists an orthogonal matrix S with properties (7)

$$SA = AS$$

and (8)

$$Se_i = e_j.$$

S is called an *orthogonal relation* between i and j.

Obviously, this is a generalization of the relation which holds between vertices which are equivalent by symmetry. Instead of a permutation, we here admit an orthogonal transformation in general.

Example

Vertices 2 and 6 in **3** are in fact orthogonally related. An orthogonal relation is given by the matrix

$$T_2 = \begin{pmatrix} 0.5 & 0 & -0.5 & 0 & 0.5 & 0 & 0.5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ -0.5 & 0 & 0.5 & 0 & 0.5 & 0 & 0.5 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0.5 & 0 & 0.5 & 0 & 0.5 & 0 & -0.5 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0.5 & 0 & 0.5 & 0 & -0.5 & 0 & 0.5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix},$$

where T_2 is the restriction of T_1 (given above) to the first eight rows and columns, corresponding to the fact that graph **3** is **1** (or **2**) without vertices 9 and 10. Later in this section we shall derive this matrix.

Before clarifying the association between endospectrality and orthogonal relationship, we give two further definitions of properties which are frequently discussed [2,7,8].

DEFINITION

Let A^ν be the νth power of the adjacency matrix A of a graph of n vertices. Let the elements of A^ν be denoted as $a_{ij}^{(\nu)}$ $(i, j = 1, \ldots, n)$. Then the vertices i and j are called *isocodal* if the corresponding diagonal elements are equal for i and j in all powers of A:

$$a_{ii}^{(\nu)} = a_{jj}^{(\nu)} \qquad (\nu = 0, 1, 2, \ldots). \tag{9}$$

By the Cayley–Hamilton theorem [11], it is sufficient for isocodality to show the validity of (9) for $\nu = 1, \ldots, n-1$ [8].

DEFINITION

Two vertices i and j are called *isocoefficient* if for each eigenspace V of A and each orthonormal basis $\{x_1, \ldots, x_m\}$ of V the sum over the squared ith coefficients is equal to the sum over the squared jth coefficients:

$$\sum_{r=1}^{m} x_{ri}^2 = \sum_{r=1}^{m} x_{rj}^2, \tag{10}$$

where $x_r = (x_{r1}, \ldots, x_{rn})^{\mathrm{T}}$ for $r = 1, \ldots, m$.

For each eigenvector $x = (x_1, \ldots, x_n)^T$ belonging to a non-degenerate eigenvalue of A (that is, $m = 1$), (10) reduces to

$$x_i^2 = x_j^2, \tag{11}$$

which means that the coefficients for i and for j have the same absolute value. We can achieve validity of (11) even for degenerate eigenspaces as follows.

LEMMA 3.2

Let i and j be isocoefficient vertices in a graph with adjacency matrix A. Then an orthonormal basis $\{x_1, \ldots, x_m\}$ of each eigenspace V of dimension m of A can be chosen so that

$$x_{ri}^2 = x_{rj}^2 \tag{12}$$

holds for all $r = 1, \ldots, m$.

Proof

Let $\{y_1, \ldots, y_m\}$ be an arbitrary orthonormal basis of V. Together with an orthonormal basis of the orthogonal complement $V^\perp$, this provides a basis for $\mathbb{R}^n$. We intend to transform the basis of V in an appropriate way while leaving that of $V^\perp$ invariant. That is, the matrix

$$Y = \begin{pmatrix} y_{11} & \cdots & y_{m1} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ y_{1n} & \cdots & y_{mn} \end{pmatrix}$$

should be transformed into a matrix

$$X = \begin{pmatrix} x_{11} & \cdots & x_{m1} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ x_{1n} & \cdots & x_{mn} \end{pmatrix}$$

under the following conditions:

$$\sum_{r=1}^{m} x_{rk} x_{rl} = \sum_{r=1}^{m} y_{rk}\, y_{rl} \qquad (k, l = 1, \ldots, n) \tag{13}$$

and (12)

$$x_{ri}^2 = x_{rj}^2 \qquad (r = 1, \ldots, m).$$

Equations (13) are required by orthonormality of both the given and the desired basis of $\mathbb{R}^n$ (there are constant scalar products of the rows, both over $\mathbb{R}^n$ and $V^\perp$, leading to invariance of the sums in (13)). The rows $y_{.k}$ $(k = 1, \ldots, n)$ of Y generate a subspace W of dimension m. The presumed isocoefficiency may be written as

$$\| y_{.i} \| = \| y_{.j} \|,$$

where $\| \cdot \|$ is the Euclidean norm. Therefore, we can choose an orthogonal map $T : W \to W$ with all eigenvalues real (take a reflection by an appropriate hyperplane of $\mathbb{R}^n$) and

$$Ty_{.i} = y_{.j}$$

being satisfied. After transforming T into diagonal form by

$$T = U^{-1}DU$$

with a diagonal matrix D, containing the eigenvalues of T (which all are $+1$ or -1), and an orthogonal basis transformation matrix U, we have

$$Uy_{.j} = DUy_{.i}.$$

That is, the coefficients of $Uy_{.j}$ and $Uy_{.i}$ differ at most in their signs. Therefore, defining the kth row of X as

$$x_{.k} = Uy_{.k}$$

solves the problem raised above. □

(The statement of this lemma is given in [4] without proof.)

Example

Vertices 2 and 6 in **3** are both isocodal and isocoefficient, as the reader may check by inspection of tables 1 and 2, where the first powers of A and an orthonormal base of eigenvectors for A are listed.

In the remainder of this section, the equivalence of all four properties defined above will be proven.

Table 1

The first eight powers of the adjacency matrix A of **3**.

$$A = \begin{pmatrix} 0&1&0&0&0&0&0&0\\ 1&0&1&0&0&0&0&0\\ 0&1&0&1&0&0&0&1\\ 0&0&1&0&1&0&0&0\\ 0&0&0&1&0&1&0&0\\ 0&0&0&0&1&0&1&0\\ 0&0&0&0&0&1&0&1\\ 0&0&1&0&0&0&1&0 \end{pmatrix} \qquad A^2 = \begin{pmatrix} 1&0&1&0&0&0&0&0\\ 0&2&0&1&0&0&0&1\\ 1&0&3&0&1&0&1&0\\ 0&1&0&2&0&1&0&1\\ 0&0&1&0&2&0&1&0\\ 0&0&0&1&0&2&0&1\\ 0&0&1&0&1&0&2&0\\ 0&1&0&1&0&1&0&2 \end{pmatrix}$$

$$A^3 = \begin{pmatrix} 0&2&0&1&0&0&0&1\\ 2&0&4&0&1&0&1&0\\ 0&4&0&4&0&2&0&4\\ 1&0&4&0&3&0&2&0\\ 0&1&0&3&0&3&0&2\\ 0&0&2&0&3&0&3&0\\ 0&1&0&2&0&3&0&3\\ 1&0&4&0&2&0&3&0 \end{pmatrix} \qquad A^4 = \begin{pmatrix} 2&0&4&0&1&0&1&0\\ 0&6&0&5&0&2&0&5\\ 4&0&12&0&6&0&6&0\\ 0&5&0&7&0&5&0&6\\ 1&0&6&0&6&0&5&0\\ 0&2&0&5&0&6&0&5\\ 1&0&6&0&5&0&6&0\\ 0&5&0&6&0&5&0&7 \end{pmatrix}$$

$$A^5 = \begin{pmatrix} 0&6&0&5&0&2&0&5\\ 6&0&16&0&7&0&7&0\\ 0&16&0&18&0&12&0&18\\ 5&0&18&0&12&0&11&0\\ 0&7&0&12&0&11&0&11\\ 2&0&12&0&11&0&11&0\\ 0&7&0&11&0&11&0&12\\ 5&0&18&0&11&0&12&0 \end{pmatrix} \qquad A^6 = \begin{pmatrix} 6&0&16&0&7&0&7&0\\ 0&22&0&23&0&14&0&23\\ 16&0&52&0&30&0&30&0\\ 0&23&0&30&0&23&0&29\\ 7&0&30&0&23&0&22&0\\ 0&14&0&23&0&22&0&23\\ 7&0&30&0&22&0&23&0\\ 0&23&0&29&0&23&0&30 \end{pmatrix}$$

$$A^7 = \begin{pmatrix} 0&22&0&23&0&14&0&23\\ 22&0&68&0&37&0&37&0\\ 0&68&0&82&0&60&0&82\\ 23&0&82&0&53&0&52&0\\ 0&37&0&53&0&45&0&52\\ 14&0&60&0&45&0&45&0\\ 0&37&0&52&0&45&0&53\\ 23&0&82&0&52&0&53&0 \end{pmatrix} \qquad A^8 = \begin{pmatrix} 22&0&68&0&37&0&37&0\\ 0&90&0&105&0&74&0&105\\ 68&0&232&0&142&0&142&0\\ 0&105&0&135&0&105&0&134\\ 37&0&142&0&98&0&97&0\\ 0&74&0&105&0&90&0&105\\ 37&0&142&0&97&0&98&0\\ 0&105&0&134&0&105&0&135 \end{pmatrix}$$

Table 2

The eigenvalues and an orthonormal basis of eigenvectors of **3**.

Eigenvalues							
– 2.13578	– 1.41421	– 1.00000	– 0.66215	0.66215	1.00000	1.41421	2.13578
Eigenvectors							
– 0.14407	0.35355	0.00000	0.59518	– 0.59518	0.00000	0.35355	– 0.14407
0.30771	– 0.50000	0.00000	– 0.39410	– 0.39410	0.00000	0.50000	– 0.30771
– 0.51312	0.35355	0.00000	– 0.33423	0.33423	0.00000	0.35355	– 0.51312
0.39410	0.00000	– 0.50000	0.30771	0.30771	0.50000	0.00000	– 0.39410
– 0.32860	– 0.35355	0.50000	0.13048	– 0.13048	0.50000	– 0.35355	– 0.32860
0.30771	0.50000	0.00000	– 0.39410	– 0.39410	0.00000	– 0.50000	– 0.30771
– 0.32860	– 0.35355	– 0.50000	0.13048	– 0.13048	– 0.50000	– 0.35355	– 0.32860
0.39410	0.00000	0.50000	0.30771	0.30771	– 0.50000	0.00000	– 0.39410

THEOREM 3.3

For two vertices i and j of a graph G with adjacency matrix A, the following statements are equivalent:

(i) i and j are endospectral,

(ii) i and j are isocoefficient,

(iii) i and j are orthogonally related,

(iv) i and j are isocodal.

Proof

(i) $\Leftrightarrow$ (ii)

The equivalence of endospectrality and isocoefficiency has been shown by Herndon and Ellzey [7]. Their proof can be simplified using lemma 3.1: Instead of considering substitution of an arbitrary fragment at site i or j, it is sufficient to simply add a vertex at i or j in turn. We will give more details of the proof in the next section, where it is modified for endospectral pairs (see proof of theorem 4.2).

(ii) $\Rightarrow$ (iii)

We assume vertices i and j to be isocoefficient and choose a particular orthonormal basis of $\mathbb{R}^n$, consisting of eigenvectors of A, so that condition (12) is satisfied for all these eigenvectors. This is possible by lemma 3.2. Now we are able to transform this basis into another orthonormal basis of $\mathbb{R}^n$, likewise consisting of eigenvectors of A, so that the jth coefficients of the latter basis are exactly equal to the ith coefficients of the former: we have just to multiply each vector of the first basis by $+1$ or -1 according to equality ot inequality of the signs of its ith and jth coefficient. So, by matching of corresponding eigenvectors, an orthogonal basis transformation $S : \mathbb{R}^n \to \mathbb{R}^n$ is constructed with properties (7) and (8) being valid, that is, vertices i and j are orthogonally related. (By this construction, it becomes clear that S has the same eigenvectors as A, but with all eigenvalues having an absolute value of 1.)

(iii) $\Rightarrow$ (i)

Vertices i and j are assumed to be orthogonally related. By lemma 3.1, it is sufficient to prove isospectrality of the graphs G_i and G_j which emerge from G by marking i or j by a loop. Their adjacency matrices have the form

$$A_i = A + E_i,$$

$$A_j = A + E_j,$$

where E_i (E_j) is the matrix with entry 1 in the ith (jth) diagonal element and 0 elsewhere.

By assumption, we have an orthogonal relation S with (7)

$$SA = AS,$$

which can be written as

$$SA_i - SE_i = A_jS - E_jS.$$

On the other hand, assumption (8)

$$Se_i = e_j$$

proves to be equivalent to

$$SE_i = E_jS.$$

So, we obtain

$$SA_i = A_jS,$$

which is by (1) the isospectrality of graphs G_i and G_j.

(iii) $\Rightarrow$ (iv)

Again we presume the existence of an orthogonal relation S between i and j. If we write $\langle x, y\rangle$ for the usual scalar product of vectors x and y, we can conclude by conditions (8), (7), and the orthogonality of S that

$$a_{ii}^{(\nu)} = \langle e_i, A^\nu e_i\rangle = \langle S^{-1}e_j, A^\nu e_i\rangle = \langle e_j, SA^\nu e_i\rangle$$
$$= \langle e_j, A^\nu S e_i\rangle = \langle e_j, A^\nu e_j\rangle = a_{jj}^{(\nu)}$$

holds for $\nu = 0, 1, 2, \ldots$, showing the isocodality of i and j.

(iv) $\Rightarrow$ (iii)

Now we assume i and j to be isocodal and define V as the smallest A-invariant subspace of $\mathbb{R}^n$ which contains e_i. Let m be the dimension of V. Then, e_i, Ae_i, $A^2e_i, \ldots, A^{m-1}e_i$ serve as a basis for V. Now define a map $S : V \to W = S(V)$ by letting

$$SA^\nu e_i = A^\nu e_j \qquad (\nu = 0, \ldots, m-1).$$

Then S is an orthogonal transformation. This is established by the presumption of isocodality: For basis vectors $A^\nu e_i$, $A^\mu e_i$ $(0 \le \nu, \mu \le m-1)$ of V, we have

$$\langle SA^\nu e_i, SA^\mu e_i\rangle = \langle A^\nu e_j, A^\mu e_j\rangle = \langle e_j, A^{\mu+\nu} e_j\rangle = a_{jj}^{(\mu+\nu)}$$
$$= a_{ii}^{(\mu+\nu)} = \langle e_i, A^{\mu+\nu} e_i\rangle = \langle A^\nu e_i, A^\mu e_i\rangle.$$

Therefore W, as an orthogonal image of V, is also an A-invariant m-dimensional subspace of $\mathbb{R}^n$. Moreover, on V, condition (7)

$$SA = AS$$

holds by definition: For $\nu \in \mathbb{N}$, we have

$$SA^\nu e_i = A^\nu e_j = A^\nu S e_i.$$

Our aim is to extend S to the whole $\mathbb{R}^n$. To do this, we regard $\mathbb{R}^n$ as a direct sum of orthogonal subspaces as follows:

$$\mathbb{R}^n = V \cap W \;\oplus\; V \cap W^\perp \;\oplus\; V^\perp \cap W \;\oplus\; V^\perp \cap W^\perp.$$

Some of these spaces may have dimension 0. All spaces are A-invariant, as already known for V and W. This is true by orthogonal complements of A-invariant subspaces being A-invariant themselves, and by the same holding for intersections of spaces with this property each.

The next step is to prove the existence of an orthonormal basis of $\mathbb{R}^n$ which consists of eigenvectors of A and is representable as the union of bases of the four subspaces. This follows from the fact that A, restricted on each subspace, as a symmetrical map has an orthonormal basis of eigenvectors. We have already defined $S : V \to W$. Now $S : V^\perp \to W^\perp$ has to be constructed appropriately. Let $x \in V$ be an element of the above basis, that is, an eigenvector associated with an eigenvalue λ of A. Then

$$ASx = SAx = S\lambda x = \lambda Sx,$$

that is, with $x \in V$, its image $Sx \in W$ also has to be an eigenvector of A associated with the same eigenvalue. Therefore, V and W contain eigenvectors which belong to the same set of eigenvalues of A. Consequently, the remaining eigenvalues are associated with both $V^{\perp}$ and $W^{\perp}$, and it is possible to define S on $V^{\perp}$ such that for each basis eigenvector $y \in V^{\perp}$, its image $Sy \in W^{\perp}$ belongs to the same eigenvalue μ. Then

$$SAy = S\mu y = \mu Sy = ASy$$

holds, and therefore for all $y \in \mathbb{R}^n$ condition (7)

$$SA = AS$$

is fulfilled. Now $S : \mathbb{R}^n \to \mathbb{R}^n$ is a map meeting all requirements for an orthogonal relation between vertices i and j. □

Let us make a few remarks about alternatives to the proof given here. First, there exists a way to prove the equivalence of endospectrality (i) and isocodality (iv) directly [8, 16]. This proof uses the identity of the spectral moments (which are defined to be the traces of A, A^2, A^3 and so on) of isopectral graphs, which is easily established. This is applied, for example, to the two graphs obtained by marking vertex i or j in turn. By complete induction, it can be shown that the identity of spectral moments is equivalent to isocodality of i and j. To prove this, we need the fact that spectral moments and eigenvalues contain equivalent information, which is known but not obvious. (According to Gantmacher [17], the method for determining the coefficients of the characteristic polynomial using the spectral moments goes back to Le Verrier and applies Newton's formulas.) This proof (which to our knowledge has not been described in detail) seems to be rather lengthy, while our proof (via the concept of orthogonal relation) uses elementary linear algebra exclusively. This is particularly true for (iii) $\Rightarrow$ (iv) and (iii) $\Rightarrow$ (i), performed above, and also for a direct proof of (iii) $\Rightarrow$ (ii), given here as an extra proof (presumption and notation are as above, while eq. (10) has to be proven):

$$\sum_{r=1}^{m} x_{ri}^2 = \sum_{r=1}^{m} \langle e_i, x_r \rangle^2 = \sum_{r=1}^{m} \langle S e_i, S x_r \rangle^2 = \sum_{r=1}^{m} \langle e_j, S x_r \rangle^2 = \sum_{r=1}^{m} (S x_r)_j^2 = \sum_{r=1}^{m} x_{rj}^2,$$

where $(Sx_r)_j$ denotes the jth coefficient of Sx_r and the last equality holds since the sum of squares over each row does not change under an orthogonal transformation.

Graph **3** may serve as an example for the construction of an orthogonal relation between two isocodal vertices.

We show how the orthogonal map which is represented by matrix T_2 given above can be constructed using the isocodality of vertices 2 and 6. We use the method outlined in part (iv) $\Rightarrow$ (iii) of the proof.

The matrices B and C given below contain the columns

$$e_2, Ae_2, \ldots, A^5 e_2 \quad (B),$$

$$e_6, Ae_6, \ldots, A^5 e_6 \quad (C),$$

where e_2 and e_6 are the second and sixth unit vector and A is the adjacency matrix of **3**, given in table 1. So,

$$B = \begin{pmatrix} 0 & 1 & 0 & 2 & 0 & 6 \\ 1 & 0 & 2 & 0 & 6 & 0 \\ 0 & 1 & 0 & 4 & 0 & 16 \\ 0 & 0 & 1 & 0 & 5 & 0 \\ 0 & 0 & 0 & 1 & 0 & 7 \\ 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 1 & 0 & 7 \\ 0 & 0 & 1 & 0 & 5 & 0 \end{pmatrix}, \quad C = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 2 \\ 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 2 & 0 & 12 \\ 0 & 0 & 1 & 0 & 5 & 0 \\ 0 & 1 & 0 & 3 & 0 & 11 \\ 1 & 0 & 2 & 0 & 6 & 0 \\ 0 & 1 & 0 & 3 & 0 & 11 \\ 0 & 0 & 1 & 0 & 5 & 0 \end{pmatrix}.$$

The rank of both B and C is $m = 6$, and by the equality of rows 4 and 8 and of rows 5 and 7, this is the maximal number of linearly independent iterations of A on e_2 and e_6. We have to find a matrix S with

$$SB = C.$$

Using the pseudo-inverse [17] B^+ of B, defined as

$$B^+ = (B^{\mathrm{T}}B)^{-1}B^{\mathrm{T}}$$

($B^{\mathrm{T}}B$ being regular, since B has maximal rank), we obtain

$$S = CB^+ = C(B^{\mathrm{T}}B)^{-1}B^{\mathrm{T}}.$$

S, restricted on the space V generated by the columns of matrix B, is an orthogonal map with

$$Se_2 = e_6,$$

but not orthogonal on $\mathbb{R}^8$. Hereby,

$$V = W = \{(x_1, \ldots, x_8)^{\mathrm{T}} : x_5 = x_7, x_4 = x_8\}$$

and therefore the orthogonal complement $V^{\perp} = W^{\perp}$ is generated by

$$y_1 = \tfrac{1}{2}(0,0,0,1,1,0,-1,-1)$$

and

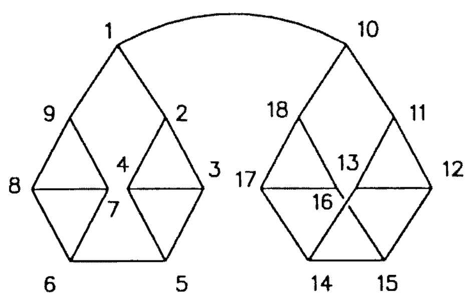
$$y_2 = \tfrac{1}{2}(0,0,0,1,-1,0,1,-1),$$

where y_1 and y_2 are orthonormal eigenvectors of A associated with eigenvalues 1 and -1. So we define T_2 by

$$T_2 x = \begin{cases} Sx, & x \in V, \\ y_1, & x = y_1, \\ y_2, & x = y_2. \end{cases}$$

T_2 is orthogonal on the whole $\mathbb{R}^8$. This matrix was given above. It can be interpreted as a somewhat frustrated reflection by the axis connecting vertices 4 and 8, which are invariant, while vertex 2 is mapped onto 6 and vice versa. The same matrix can be constructed by the "matching" method outlined in part (ii) $\Rightarrow$ (iii) of the proof, using the isocoefficiency of vertices 2 and 6 in the orthonormal system of eigenvectors given in table 2.

The latter method was used for another example, graph **8** (fig. 5). Here, vertices 1 and 10 are endospectral [6, 18]. In this case, the orthogonal relation is



8

Fig. 5. A graph containing endospectral vertices (1 and 10).

not unique, due to the occurrence of degenerate eigenvalues. One solution, probably the simplest one, is given by matrix T_3 below. T_3 represents an "unsuccessful attempt" to force the two halves of **8** to coincide.

$$
T_3 = (1/4)\begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & -2 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 2 \\
0 & 0 & 3 & -1 & 0 & 0 & -1 & -1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 \\
0 & 0 & -1 & 3 & 0 & 0 & -1 & -1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 \\
0 & 0 & 0 & 0 & 2 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 2 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -2 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 2 & 0 & 0 & 0 \\
0 & 0 & -1 & -1 & 0 & 0 & 3 & -1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 \\
0 & 0 & -1 & -1 & 0 & 0 & -1 & 3 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 \\
0 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 2 \\
4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & -2 \\
0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 3 & -1 & 0 & 0 & -1 & -1 & 0 \\
0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & -1 & 3 & 0 & 0 & -1 & -1 & 0 \\
0 & 0 & 0 & 0 & 2 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & -2 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 2 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -2 & 2 & 0 & 0 & 0 \\
0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & -1 & -1 & 0 & 0 & 3 & -1 & 0 \\
0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & -1 & -1 & 0 & 0 & -1 & 3 & 0 \\
0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 2
\end{bmatrix}
$$

4. Isospectral pairs within a graph (endospectral pairs)

DEFINITION

Two unordered pairs of vertices (i, j) and (k, l) $(i < j;\ k < l;\ 1 \le i, j, k, l \le n)$ in a graph are called *isospectral pairs* or *endospectral pairs* (of vertices) if every perturbation at pair (i, j) or (k, l) in turn results in two isospectral graphs.

The expression "every perturbation" needs a precise interpretation. One kind of perturbation is attachment of an arbitrary fragment at (i, j) or (k, l). Examples of such fragments are: an additional edge between i and j (k and l); more generally, a new "bridge" (chain) of arbitrary length between i and j; loops at i and j. Also, erasing pair (i, j) or (k, l) should be allowed. Moreover, even an asymmetrical perturbation (treating i differently from j) is allowed, provided that either vertex in (k, l) is treated identically to its "corresponding" vertex in (i, j). What is the exact meaning of "correspondence" between vertices? Let us assume that i and k are "corresponding" vertices, as are j and l. Then we postulate that perturbing i or k in turn, while leaving j and l unchanged, leads to isospectral graphs. This is exactly the requirement that the *vertices* i and k are endospectral, and also (by the same reasoning) the vertices j and l. We conclude that correspondence between vertices has to be interpreted as endospectrality. Hence, we obtain pairwise endospectrality of the vertices as a necessary condition for endospectrality of the pairs. We note that this requirement has a perfect analogue in a condition for pairs which are equivalent by symmetry: for these, it is necessary (but not sufficient) that the vertices forming the pairs are in pairwise identical cells of the automorphism partition. Moreover, such pairs provide a first (trivial) example of endospectral pairs.

Unfortunately, there is no analogue for pairs to the Hosoya formula for vertices, eq. (2). Therefore, we lack a theorem like the above (lemma 3.1) which could facilitate the direct verification of endospectrality of pairs. The more desirable is a characterization of endospectral pairs by related properties which would enable us to verify endospectrality of pairs without attaching legions of fragments. In fact, it will become apparent that the concept of orthogonal relation is a valuable tool to reach this goal.

First, the definitions of orthogonal relationship, isocodality and isocoefficiency of pairs will be given, followed by examples. Then we will prove the main theorem (4.2) about endospectral pairs, which is fully analogous to that about endospectral vertices (3.3).

DEFINITION

Two pairs (i, j) and (k, l) in a graph with adjacency matrix A are called *orthogonally related* if there exists an orthogonal matrix S with (7)

$$SA = AS$$

and

$$(Se_i = e_k \quad \text{and} \quad Se_j = e_l)$$

or (14)

$$(Se_i = e_l \quad \text{and} \quad Se_j = e_k).$$

If S can be chosen even as a permutation matrix, then S corresponds to an automorphism of the graph which maps pair (i, j) onto pair (k, l), so rendering them equivalent by symmetry.

DEFINITION

Using the notation introduced in section 2, we call two pairs (i, j) and (k, l) (*weakly*) *isocodal* if the corresponding matrix elements are equal for (i, j) and (k, l) in all powers of A:

$$a_{ij}^{(\nu)} = a_{kl}^{(\nu)} \qquad (\nu = 0, 1, 2, \ldots). \tag{15}$$

The pairs are called *strictly isocodal* if additionally

$$(a_{ii}^{(\nu)} = a_{kk}^{(\nu)} \text{ and } a_{jj}^{(\nu)} = a_{ll}^{(\nu)} \text{ for } \nu = 0, 1, 2, \ldots)$$

or (16)

$$(a_{ii}^{(\nu)} = a_{ll}^{(\nu)} \text{ and } a_{jj}^{(\nu)} = a_{kk}^{(\nu)} \text{ for } \nu = 0, 1, 2, \ldots)$$

holds.

Expression (16) means that the vertices are pairwise isocodal and therefore, which is equivalent, pairwise endospectral.

DEFINITION

Two pairs (i, j) and (k, l) are called *(weakly) isocoefficient* if for each eigenspace V of A and each orthonormal basis $\{x_1, \ldots, x_m\}$ of V the sum over the products of the ith and jth coefficient is equal to the sum over the products of the kth and lth coefficient:

$$\sum_{r=1}^{m} x_{ri} x_{rj} = \sum_{r=1}^{m} x_{rk} x_{rl}, \tag{17}$$

where $x_r = (x_{r1}, \ldots, x_{rn})^{\mathrm{T}}$ for $r = 1, \ldots, m$. The pairs are called *strictly isocoefficient* if in addition

$$\left(\sum_{r=1}^{m} x_{ri}^2 = \sum_{r=1}^{m} x_{rk}^2 \text{ and } \sum_{r=1}^{m} x_{rj}^2 = \sum_{r=1}^{m} x_{rl}^2 \text{ for each eigenspace}\right)$$

or (18)

$$\left(\sum_{r=1}^{m} x_{ri}^2 = \sum_{r=1}^{m} x_{rl}^2 \text{ and } \sum_{r=1}^{m} x_{rj}^2 = \sum_{r=1}^{m} x_{rk}^2 \text{ for each eigenspace}\right)$$

holds.

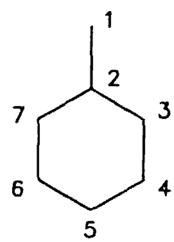
Expression (18) means that the vertices are pairwise isocoefficient and therefore, which is equivalent, pairwise endospectral.

Examples

(i) Pairs which are equivalent by symmetry meet all the requirements given and therefore are orthogonally related, strictly isocodal, and strictly isocoefficient.

(ii) Pairs (2, 4) and (4, 6) in **3** are both strictly isocodal and strictly isocoefficient, as is seen by inspection of tables 1 and 2. In fact, the vertices are pairwise endospectral: 2 and 6 served as an example for endospectral points in section 2, and 4 is endospectral to itself.

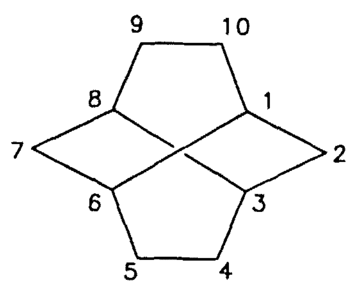
(iii) Lowe and Davis [4] give an example for two pairs (edges (1, 2) and (4, 5) in **9**, fig. 6) which are both isocodal and isocoefficient, but neither strictly isocodal nor strictly isocoefficient. Graph **8** provides examples of (weakly) isocodal and isocoefficient pairs (both edges and non-edges), as listed in [6].



9

Fig. 6. A graph containing two (weakly) isocodal and (weakly) isocoefficient edges (1, 2) and (4, 5).

(iv) In the graph of twistane (**10**, fig. 7), pairs (1, 5) and (1, 9) are both strictly isocodal and strictly isocoefficient [6]. Obviously, the vertices are pairwise equivalent by symmetry and thus endospectral. The following theorem (4.2) shows that (1, 5) and (1, 9) are endospectral pairs.



10

Fig. 7. The graph of twistane containing two endospectral pairs (1, 5) and (1, 9).

(v) A rather complex example, going back to Balaban [19], is provided by graph **14** in ref. [6]. There we gave an (incomplete) list of endospectral points and pairs in this graph, and further simple examples of endospectral points and pairs may be found there.

LEMMA 4.1

Let (i, j) and (k, l) be strictly isocoefficient pairs of vertices in a graph with adjacency matrix A. For each eigenspace V of dimension m of A, the orthonormal basis $\{x_1, \ldots, x_m\}$ can be chosen such that even

$$x_{ri}x_{rj} = x_{rk}x_{rl} \tag{19}$$

and

$$\left(x_{ri}^2 = x_{rk}^2 \text{ and } x_{rj}^2 = x_{rl}^2\right)$$

or (20)

$$\left(x_{ri}^2 = x_{rl}^2 \text{ and } x_{rj}^2 = x_{rk}^2\right)$$

holds for $r = 1, \ldots, m$.

The proof, not given here, is a slight modification of the proof of lemma 3.3.

Now it will be shown that the properties strict isocodality, strict isocoefficiency, and orthogonal relationship are adequately defined such that each of them is necessary and sufficient for endospectrality of pairs.

THEOREM 4.2

For two pairs (i, j) and (k, l) in a graph, the following statements are equivalent:

(i) The pairs are endospectral.

(ii) The pairs are strictly isocoefficient.

(iii) The pairs are orthogonally related.

(iv) The pairs are strictly isocodal.

Proof

We use methods very similar to those of the proof of theorem 3.4. Therefore, we will often refer the reader to the former proof in order to avoid repetitions.

(i) $\Rightarrow$ (ii)

Two pairs (i, j) and (k, l) are assumed to be endospectral. We imitate the proof of Herndon and Ellzey [7]. By the presumption of endospectrality, attachment of one new vertex in i and j results in a graph H_1 which is isospectral to H_2 resulting from attaching the new vertex in k and l. If (without restriction) $i = 1$ and $j = 2$, the adjacency matrix of H_1 is given by

$$A_1 = \begin{pmatrix} a_{11} & a_{12} & & \cdots & a_{1n} & 1 \\ a_{21} & a_{22} & & \cdots & a_{2n} & 1 \\ \vdots & \vdots & & \cdots & \vdots & 0 \\ a_{n1} & a_{n2} & & \cdots & a_{nn} & \vdots \\ 1 & 1 & 0 & \cdots & & 0 \end{pmatrix}.$$

A_1 is transformed into a matrix D_1 of dimension $n + 1$:

$$D_1 = \begin{pmatrix} \lambda_1 & & & & x_{1i} + x_{1j} \\ & \lambda_2 & & & x_{2i} + x_{2j} \\ & & \ddots & & \vdots \\ & & & \lambda_n & x_{ni} + x_{nj} \\ x_{1i} + x_{1j} & x_{2i} + x_{2j} & \cdots & x_{ni} + x_{nj} & 0 \end{pmatrix}.$$

Here, the upper left part is an $n \times n$ diagonal matrix which contains the eigenvalues $\lambda_1, \ldots, \lambda_n$ of A. The $(n + 1)$st column and row contain the sums of the ith and jth coefficient of each eigenvector (associated with $\lambda_1, \ldots, \lambda_n$), where the eigenvectors form an orthogonal basis of $\mathbb{R}^n$. This transformation of A_1 into D_1 corresponds to a basis transformation from the canonical basis into a new one, which consists of the above orthogonal system of eigenvectors (each vector completed by an $(n + 1)$st component 0) and the $(n + 1)$st unit vector. Likewise, the matrix A_2, which describes the graph with a new vertex adjacent to k and l, is transformed into a matrix D_2 equal to D_1 with the exception that the indices i and j are replaced by k and l, while the eigenvalues $\lambda_1, \ldots, \lambda_n$ are the same as in D_1 by the isospectrality of H_1 and H_2. Now D_1 and D_2, being derived from A_1 and A_2 by a basis transformation, also have identical eigenvalues. It can be shown that this is equivalent to

$$\sum_{r=1}^{m} (x_{ri} + x_{rj})^2 = \sum_{r=1}^{m} (x_{rk} + x_{rl})^2,$$

where the summation is done over all components belonging to the same eigenvalue. With the pairwise isocoefficiency of the vertices (18), which follows from their pairwise endospectrality, we also know that

$$\sum_{r=1}^{m} \left(x_{ri}^2 + x_{rj}^2\right) = \sum_{r=1}^{m} \left(x_{rk}^2 + x_{rl}^2\right),$$

and so we obtain (17)

$$\sum_{r=1}^{m} x_{ri} x_{rj} = \sum_{r=1}^{m} x_{rk} x_{rl},$$

which completes the proof of the strict isocoefficiency of the pairs (i, j) and (k, l).

(ii) $\Rightarrow$ (iii)

We assume pairs (i, j) and (k, l) to be strictly isocoefficient. As in the corresponding part of the former proof, we can choose an orthonormal basis consisting of eigenvectors $x_1, \dots, x_n$ of A, which fulfill conditions (19) and (20). If in some vector x_r the kth coefficient (which may correspond to the ith) still differs from the ith in its sign, we define y_r by $y_r = -x_r$. Then we have

$$y_{rk} = -x_{rk} = x_{ri}$$

and by (19) also

$$y_{rl} = -x_{rl} = x_{rj}.$$

If x_{rk} already equals x_{ri}, we set $y_r = x_r$. Then all the kth (lth) coefficients of the basis $\{y_1, \dots, y_n\}$ agree exactly with the ith (jth) coefficients of the basis $\{x_1, \dots, x_n\}$, and the basis transformation $S : \mathbb{R}^n \to \mathbb{R}^n$, defined by

$$Sx_r = y_r \qquad (r = 1, \dots, n),$$

has the desired properties (7) and (14). Hence, S serves as an orthogonal relation of (i, j) and (k, l).

(iii) $\Rightarrow$ (i)

We assume (i, j) and (k, l) to be orthogonally related by a transformation S with (7)

$$SA = AS$$

and (14), say

$$Se_i = e_k \quad \text{and} \quad Se_j = e_l.$$

We have to show that each perturbation at (i, j) or (k, l) in turn provides two isospectral graphs.

Let the adjacency matrix of the graph perturbed in pair (i, j) be denoted as A_{ij}, the other (perturbed in (k, l)) as A_{kl}. Both matrices have identical dimension, which is not necessarily n. Now we have to find an orthogonal matrix T of the same dimension, for which it holds that

$$TA_{ij} = A_{kl}T. \tag{21}$$

It will be shown that T exists and can be chosen as follows. For each $r \in \{1, \dots, n\}$, corresponding to a vertex r of the given graph, let

$$Te_r = Se_r \qquad (r \le n),$$

particularly by (14)

$$Te_i = e_k \quad \text{and} \quad Te_j = e_l. \tag{22}$$

(The components i and j may be missing if the perturbation is erasure of at least one of these vertices.) For each additional component r belonging to an attached fragment let

$$Te_r = e_r \qquad (r > n).$$

That is, vertices which are not part of the original graph are invariant under T. We have to show that by this choice of T eq. (21) is satisfied, independently of the kind of perturbation used. There are several types of perturbations which have to be differentiated:

- eliminating one or both vertices of a pair,
- eliminating the edge connecting the vertices of a pair (if any),
- attaching a loop ("marking") at one or both vertices of a pair,
- joining the vertices of a pair by a new edge,
- attaching an arbitrary fragment at the pair.

We give the proof in detail for the last case only, since it is in some sense the most general case; the others are similar, as well as easier to treat.

Let A be the adjacency matrix of the given graph (of dimension n) and B that of the fragment (of dimension m) which is attached. Without restriction, we can assume that $i = 1$, $j = 2$, $k = n - 1$, $l = n$. Then the connection between A and B is described by a $2 \times m$ matrix.

$$C = \begin{pmatrix} c_{11} & \cdots & \cdots & c_{1m} \\ c_{21} & \cdots & \cdots & c_{2m} \end{pmatrix}$$

and we have

$$A_{ij} = \begin{pmatrix} a_{11} & \cdots & & \cdots & a_{1n} & c_{11} & \cdots & c_{1m} \\ \cdot & & & & \cdot & c_{21} & \cdots & c_{2m} \\ \cdot & & & & \cdot & 0 & \cdots & 0 \\ \cdot & & & & \cdot & \vdots & & \vdots \\ \cdot & & & & \cdot & \vdots & & \vdots \\ a_{n1} & \cdots & & \cdots & a_{nn} & 0 & \cdots & 0 \\ c_{11} & c_{21} & 0 & \cdots & 0 & b_{11} & \cdots & b_{1m} \\ \vdots & \vdots & \vdots & & \vdots & \vdots & & \vdots \\ c_{1m} & c_{2m} & 0 & \cdots & 0 & b_{m1} & \cdots & b_{mm} \end{pmatrix},$$

$$A_{kl} = \begin{pmatrix} a_{11} & \dots & & \dots & a_{1n} & 0 & \dots & 0 \\ \cdot & & & & \cdot & \vdots & & \vdots \\ \cdot & & & & \cdot & 0 & \dots & 0 \\ \cdot & & & & \cdot & c_{11} & \dots & c_{1m} \\ a_{n1} & \dots & & \dots & a_{nn} & c_{21} & \dots & c_{2m} \\ 0 & \dots & 0 & c_{11} & c_{21} & b_{11} & \dots & b_{1m} \\ \vdots & & \vdots & \vdots & \vdots & \vdots & & \vdots \\ 0 & \dots & 0 & c_{1m} & c_{2m} & b_{m1} & \dots & b_{mm} \end{pmatrix}.$$

T, defined as above, by (22) has the form

$$T = \begin{pmatrix} S & O \\ O & I \end{pmatrix} = \begin{pmatrix} 0 & 0 & s_{13} & \dots & s_{1n} & & & \\ \vdots & \vdots & \vdots & & \vdots & & & \\ 0 & 0 & s_{n-2,3} & \dots & s_{n-2,n} & & & \\ 1 & 0 & 0 & \dots & 0 & & & \\ 0 & 1 & 0 & \dots & 0 & & & \\ & & & & & 1 & & \\ & & & & & & \ddots & \\ & & & & & & & 1 \end{pmatrix},$$

where I is the unit matrix and O the null matrix. The validity of (21), agreement of both matrix products, is easily checked using eq. (7).

(iii) $\Rightarrow$ (iv)

The presumptions are as in the preceding part of the proof. We have to prove strict isocodality of pairs (i, j) and (k, l). Thereby, (16) is a direct consequence of the fact that the *vertices* are pairwise orthogonally related and therefore isocodal. So we have to prove only (15). This is done by

$$\begin{aligned} a_{ij}^{(\nu)} &= \langle e_i, A^\nu e_j \rangle = \langle S^{-1} e_k, A^\nu e_j \rangle = \langle e_k, SA^\nu e_j \rangle \\ &= \langle e_k, A^\nu S e_j \rangle = \langle e_k, A^\nu e_l \rangle = a_{kl}^{(\nu)} \end{aligned}$$

for $\nu = 0, 1, 2, \dots$.

(iv) $\Rightarrow$ (iii)

Here, the point is to conclude from the strict isocodality of pairs (i, j) and (k, l) not only that the vertices are pairwise related by two orthogonal mappings (which follows from theorem 3.3), but to show that there exists a single transformation

S which effects both. The method is very similar to that of the corresponding part of the former proof. If (16), say,

$$a_{ii}^{(\nu)} = a_{kk}^{(\nu)} \text{ and } a_{jj}^{(\nu)} = a_{ll}^{(\nu)}$$

holds for all $\nu = 0, 1, 2, \ldots$, we define V as the smallest A-invariant subspace of $\mathbb{R}^n$ containing e_i and e_j. Let m be the dimension of V. We define $S : V \rightarrow W = S(V)$ by

$$SA^\nu e_i = A^\nu e_k, \quad SA^\nu e_j = A^\nu e_l \qquad (\nu = 0, \ldots, m-1).$$

S is an orthogonal transformation. This is shown, without restriction, for "mixed" scalar products of base vectors $A^\nu e_i$, $A^\mu e_j$ using (15):

$$\langle A^\nu e_i, A^\mu e_j \rangle = \langle e_i, A^{\mu+\nu} e_j \rangle = a_{ij}^{(\mu+\nu)} = a_{kl}^{(\mu+\nu)}$$

$$= \langle e_k, A^{\mu+\nu} e_l \rangle = \langle A^\nu e_k, A^\mu e_l \rangle = \langle SA^\nu e_i, SA^\mu e_j \rangle.$$

(This can be interpreted as the invariance of "angles" under S.) The remainder of the proof (extension of S to $\mathbb{R}^n$) is exactly the same as for theorem 3.3. □

By this theorem it is seen that the pairs of example (ii) are endospectral, again with T_2 as orthogonal relation (already known from the preceding section about endospectral vertices). The pairs of examples (iv) and (v) are endospectral, whereas those of example (iii) are not.

5. Isospectral vertices and pairs in different graphs

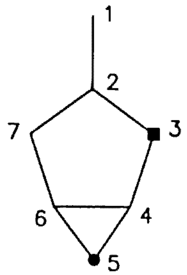
Randić pointed out that there are vertices in different graphs which are related by similar properties (e.g. isocodality) as the endospectral vertices treated in section 3 [2]. We shall characterize these points as isospectral by deducing the situation to that of endospectral points [20].

DEFINITION

Vertices i in a graph G and j in a graph H are called *isospectral* if every perturbation at i (producing graph G_i) and at j (producing graph H_j) leads to isospectral graphs G_i and H_j. Similarly, pairs (i, j) and (k, l) in different graphs are called *isospectral* if every perturbation in (i, j) and (k, l) results in two isospectral graphs.

Examples

(i) Randić [2,8] has given two examples, one of which (discussed earlier by Schwenk [21]) is shown in fig. 8. He noted that vertex 5 in graph **11** is isospectral



11

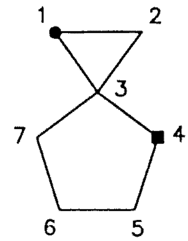


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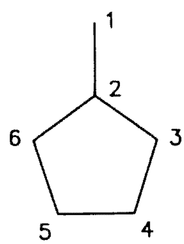
Fig. 8. Two graphs containing isospectral vertices and pairs.



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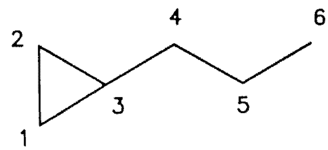

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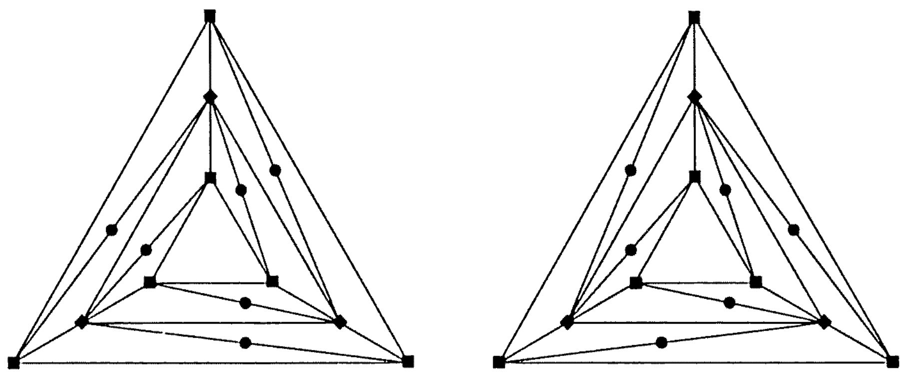
Fig. 9. Graphs resulting from erasure of an isospectral vertex from **11** or **12**.

to vertex 1 in **12**. If the special vertices are erased, a single graph (**13**, fig. 9) is obtained.

The same example was found independently by Lowe and Soto [5], who noted that the isospectral graphs **11** and **12** are also obtained by bridging pair (1, 5) or pair (3, 6) in graph **14** (fig. 9) by a one-vertex bridge. In fact, it can be shown that vertices 3 of **11** and 4 of **12** are also isospectral vertices. Moreover, we find that the pairs (3, 5) in **11** and (1, 4) in **12** (as well as pairs (3, 7) in **11** and (4, 7) in **12**) are isospectral pairs.

(ii) A rather complex example of isospectral graphs with several isospectral points and pairs is given by the two well-known graphs of Fisher [22] or their simplification given by Randić [2], which is shown in fig. 10. By proposition 5.1 (see below), it is shown that each point in **15** marked by a symbol is isospectral to a point in **16** marked by the same symbol. Moreover, we found a list of several isospectral pairs in these graphs. Note that in contrast to the situation in Randić's



15 **16**

Fig. 10. The simplified Fisher graphs containing isospectral vertices and pairs.

examples erasing a point in **15** and its isopectral counterpart in **16** results in two isospectral but not isomorphic graphs.

The reader may have noticed that graphs containing isospectral points or pairs are themselves isospectral graphs. Now we give a characterization of isospectral points and pairs which shows that this is necessary.

PROPOSITION 5.1

Vertices i in G and j in H (or pairs (i, j) in G and (k, l) in H) are isospectral if and only if the graphs G and H are isospectral and the vertices (pairs) are endospectral vertices (pairs) in the disjoint union of G and H.

Proof

Isospectrality of graphs G and H is necessary for that of the vertices (pairs), since the "void" perturbation ("do nothing") also should result in isospectral graphs. The remainder of the proof is done by inspection of the disjoint union of G and H and application of the definitions of endospectral and isospectral vertices (pairs).

□

Example

In fig. 11, two graphs are shown (**17**, **18**) which are not isospectral. Although the vertices marked by a dot are endospectral in the disjoint union of **17** and **18** (this follows from their isocodality which was pointed out by Randić [23,24]), they cannot be isospectral vertices in the sense of the above definition.

17 **18**

Fig. 11. Two graphs containing isocodal vertices.

Note that endospectrality of vertices (pairs) in the disjoint union implies isocodality and isocoefficiency as well. Therefore, these properties are *not* sufficient for isospectrality of vertices or pairs in different graphs.

Our last proposition characterizes isospectral vertices and pairs (in different graphs) by the concept of orthogonal relation.

PROPOSITION 5.2

Vertices i in a graph G (adjacency matrix A) and j in a graph H (adjacency matrix B) are isospectral if and only if there exists an orthogonal relation between them, that is, an orthogonal transformation S with (1)

$$SA = BS$$

and (8)

$$Se_i = e_j.$$

Pairs (i, j) in G and (k, l) in H are isospectral if and only if there exists an orthogonal transformation S for which instead of (8) condition (14) holds (known from section 4).

Proof

The proof is drawn here for vertices only; for pairs it is done in an analogous manner.

First, let i and j be isospectral vertices. Then, by proposition 5.1, G and H are isospectral graphs and i and j are endospectral vertices in the disjoint union $G \cup H$ of G and H and therefore isocoefficient. By a similar method as was used in part (ii) $\Rightarrow$ (iii) of the proof of theorem 3.3, an orthogonal map S can be defined which maps the eigenvectors of A onto those of B which belong to the same eigenvalues, in such a way that S has properties (1) and (8).

For the backward direction of the proof, we presume the existence of an orthogonal transformation S with properties (1) and (8). By (1), the isospectrality of graphs G and H is seen. It remains to be shown that i and j are endospectral vertices in the disjoint union $G \cup H$. In fact, by (1) and (8) it can be shown that

$$U = \begin{pmatrix} O & S^{-1} \\ S & O \end{pmatrix}$$

serves as an orthogonal relation between i and j in $G \cup H$. □

Example

This proposition is illustrated by orthogonal matrix T_4 which transforms graph **11** into **12**, at the same time mapping the vertices and the pairs as listed above.

$$T_4 = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0.5 & -0.5 & 0 & 0.5 & 0 & 0.5 & 0 \\ -0.5 & 0.5 & 0 & 0.5 & 0 & 0.5 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0.5 & 0.5 & 0 & 0.5 & 0 & -0.5 & 0 \\ 0.5 & 0.5 & 0 & -0.5 & 0 & 0.5 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

6. Conclusion

In the orthogonal relationship we found a simple means to demonstrate the equivalence of all the properties dealt with here. Moreover, this property is a generalization of the equivalence by symmetry. Of all the four properties discussed here, we would like to rate it the most valuable, since from it the others can be derived by straightforward lines of reasoning, the opposite directions, as a rule, being more difficult.

In other words, we would have welcomed it if this property had been selected to characterize vertices and pairs that are "somewhat less than equivalent by symmetry", the more so since it is mathematically completely analogous to the isospectrality of graphs, which characterizes graphs which are "somewhat less than isomorphic".

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