Notes on Isocodal Graphs

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A simple explanation is given for the existence of the Randić–Kleiner endospectral tree. It is also shown that joining two copies of the Schwenk tree at both endospectral points in the two possible ways delivers a pair of isocodal graphs (the smallest known by now).

Isocodal graphs are nonisomorphic graphs with a 1-1 correspondence for the vertices such that corresponding vertices have equal counts of self-returning walks for all lengths.[1] These graphs have also identical ordered structural codes or walk codes.[2,3] The concept of isocodal graphs was introduced in connection with isospectral[4,5] (cospectral[6]) graphs. Nonisomorphic graphs with identical characteristic polynomials and consequently with identical graph-theoretical spectra are named isospectral (cospectral) graphs.[7] Many isocodal graphs may be constructed from endospectral graphs. An endospectral graph is a graph with a pair (or several sets) of topologically distinct vertices (called endospectral vertices)[8,9] having identical self-returning walks. The term endospectral graph was suggested by Randić.[10] Ten years ago we produced all endospectral trees with up to 16 vertices[11] using our tree-generating computer program based on the N-tuple code.[12–14] (A tree is a connected acyclic graph).[15]

Randić[16] introduced in 1980 the concept of isocodal vertices as nonequivalent vertices (in the same or different graphs) having identical self-returning walk counts for all lengths. A recent discussion about the isocodal and isospectral points in different context may be found in a report by Rücker and Rücker.[17] Our computer algorithm for routinely generating all trees up to a given size[12] allowed us to systematically search for examples among the trees with isocodal vertices with up to 16 vertices. This search revealed that there are isospectral trees without isocodal vertices, that there are nonisospectral trees with isocodal vertices and that there are trees containing several isocodal vertices. Table 2 of the resulting article[18] shows as the smallest nonzero entry a rooted tree of size 5 that has the same number of self-returning walks of length up to 32 as a rooted tree of size 7. These two trees with a suitable numbering of their vertices (1 for roots, denoted by black dots, in both trees) are shown in Figure 1.

The adjacency matrices corresponding to trees in Figure 1 are given as follows

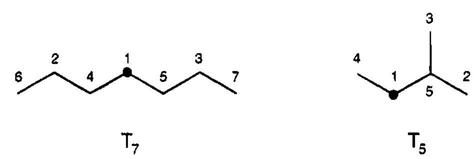

Figure 1. Two smallest rooted trees possessing the same number of self-returning walks. Roots are denoted by black dots.

$$\mathbf{A}(T_7) = \left[\begin{array}{ccc|cccc} 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ \hline 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \end{array}\right]$$

$$\mathbf{A}(T_5) = \left[\begin{array}{ccc|cc} 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 \\ \hline 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \end{array}\right]$$

or the adjacency matrices squared (one should note that in adjacency matrices for trees, only even powers have nonzero diagonal elements):

$$\mathbf{B}(T_7) = \left[\begin{array}{ccc|cccc} 2 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 2 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 2 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 2 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 2 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 \end{array}\right]$$

$$\mathbf{B}(T_5) = \left[\begin{array}{ccc|cc} 2 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 3 \end{array}\right]$$

Due to the zero off-diagonal blocks, powers of $\mathbf{B}(T_7)$ and $\mathbf{B}(T_5)$ contain as their upper left 3×3 submatrix just the

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same powers of the matrices:

$$\mathbf{C}(\mathrm{T}_7) = \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 0 \\ 1 & 0 & 2 \end{bmatrix}$$

$$\mathbf{C}(\mathrm{T}_5) = \begin{bmatrix} 2 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}$$

Now there is a matrix

$$\mathbf{X} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1/2 & 1/2 \\ 0 & 1/2 & 1/2 \end{bmatrix}$$

with

$$\mathbf{X}^k = \begin{bmatrix} 1 & 0 & 0 \\ 0 & ? & ? \\ 0 & ? & ? \end{bmatrix}$$

and

$$\mathbf{C}(\mathrm{T}_7) \times \mathbf{X} = \mathbf{X} \times \mathbf{C}(\mathrm{T}_7) = \mathbf{C}(\mathrm{T}_5)$$

so that

$$[\mathbf{C}(\mathrm{T}_5)]^k = [\mathbf{C}(\mathrm{T}_7) \times \mathbf{X}]^k = \mathbf{C}(\mathrm{T}_7)^k \times \mathbf{X}^k$$

which implies that for all even powers (this true for all powers because odd powers are necessarily zero for self-returning walks) the first diagonal elements of the matrices are equal, that is, the vertices labeled by 1 in both, T_7 and T_5, trees are indeed isocodal. If we combine T_7 and T_5 trees with a graph with two equivalent vertices by identifying the two roots with the two equivalent vertices, then these identified vertices are isocodal (or endospectral vertices as they are now in the same graph). For example, with K_2 graph, one obtains a tree with 12 vertices (see Figure 2).

This tree was also among cases summarized in Table 2 of ref 18. But, this is just the tree, denoted by E_6 in Figure 3 from a paper by Randić and Kleiner[8] which they described as "found in this work" without giving any hints on how they found it, although one could surmise that the endospectral trees they reported are a result of systematic examination of all trees with 12 vertices. The properties of this tree listed in their article all become obvious by the explanation given above. Randić and Kleiner apparently considered only alternative schemes to that of Jiang to construct endospectral trees. They did not consider why trees that are not derived by their construction are endospectral.[19] This question is considered in our report.

Endospectral tree E_6 is named 12.435 in another paper on endospectral trees.[11] This was the first tree found in which endospectral vertices are adjacent. The only other trees with adjacent endospectral vertices are 14.1423, 14.2932, 16.110 94, and 16.175 17. These trees are depicted in Figure 3.

Having adjacent endospectral vertices means that one can insert between such vertices other fragments. In this way one can obtain, for example, from 12.435 the following endospectral trees: 13.1136, 14.2632, and 14.2932. Trees 13.1136 and 14.2632 are depicted in Figure 4, while tree 14.2932 is already given in Figure 3. Note that sym-

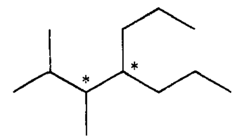
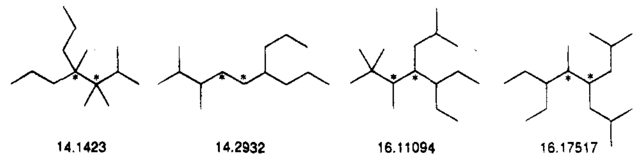
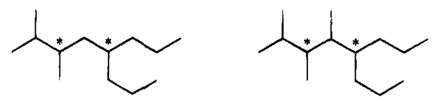


Figure 2. An endospectral tree with two endospectral vertices denoted by stars.



14.1423 14.2932 16.11094 16.17517

Figure 3. Endospectral trees labeled in the text as 14.1423, 14.2932, 16.110 94, and 16.175 17.



13.1136 14.2632

Figure 4. Endospectral trees labeled in the text as 13.1136 and 14.2632.

metrically introduced equivalent vertices, such as the two central vertices in tree 14.2932, are necessarily endospectral.

The endospectral trees depicted in Figures 3 and 4 can be considered as "reducible", that is, they can be derived from smaller trees. Of more interest are trees that cannot be reduced. For example, the irreducible trees 16.110 94 and 16.175 17 have distinct origin for the coincidence of self-returning walks of endospectral vertices.

Sometimes one can find that some building blocks, such as T_5 and T_7 which make up the endospectral tree 12.435, are subspectral. In the case mentioned, T_5 is subspectral to T_7, that is, the spectrum of T_5 is contained in the spectrum of T_7:

12.435

$$\mathrm{T}_5\text{: } \pm 1.8478, \pm 0.7654, 0$$

$$\mathrm{T}_7\text{: } \pm 1.8478, \pm 1.4142, \pm 0.7654, 0$$

Two trees T* and T are subspectral if tree T* is subspectral to tree T, that is, if all eigenvalues (spectrum) of T* are contained in the spectrum of T.[20] Tree T, being larger than T*, has additional eigenvalues and is referred to as superspectral to T*.[21] This property extends to all trees with adjacent endospectral points. Thus, endospectral tree 14.2932 has two fragments T_6 and T_8 obtained by cutting the bond between the adjacent vertices in 14.2932. T_6 is subspectral T_8, that is

14.2932

$$\mathrm{T}_6\text{: } \pm 2.0000, \pm 1.0000\ 0, 0$$

$$\mathrm{T}_8\text{: } \pm 2.0000, \pm 1.4142, \pm 1.0000, 0, 0$$

The observed subspectrality is an interesting property.[22] However, it appears that one cannot always obtain subspectral components. This is illustrated for endospectral tree 16.175 17 which breaks up by cutting the bond between the adjacent vertices into the seven (T_7) and nine (T_9) vertices components. T_7 is not subspectral to T_9:

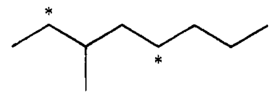


Figure 5. The endospectral tree of Schwenk. The endospectral vertices are denoted by stars.

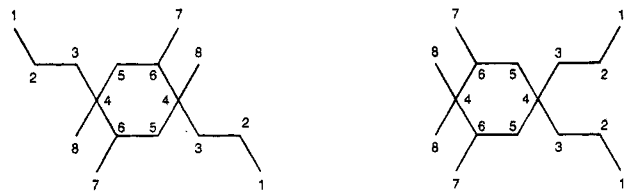


Figure 6. The pair of the smallest isocodal graphs obtained by combining two copies of the Schwenk tree at both endospectral vertices. Note that identical self-returning walk counts are denoted by equally labeled vertices.

16.175 17

$$T_7: \pm 2.0000, \pm 1.0000, \pm 1.0000, 0$$

$$T_9: \pm 2.0000, \pm 1.7321, \pm 1.0000, 0, 0, 0$$

Although the same eigenvalues appear in T_7 as in T_9, the multiplicity of ± 1 is different.

Ivanciuc and Balaban[1] use the above trees 12.435, 16.110 94, and 16.175 17 under the labels T_8, T_{25}, and T_{28} to construct isocodal graphs (given in Schemes 5, 10, and 11 of ref 1). However, their construction of isocodal graphs appears complicated. Given any nonisomorphic pair of rooted trees with isocodal roots (nonisomorphic only as rooted trees, that is, two endospectral vertices of the same tree are allowed as roots) and a graph with two equivalent vertices, then joining two copies of each member of the pair with the latter graph by identifying each of the equivalent vertices with two of the roots is possible in two noisomorphic ways (equal members to the same vs not to the same vertex) with identical self-returning walk count configurations for both. But there is a simpler way to construct even smaller isocodal graphs. Given two copies of an endospectral graph, i.e., a graph with two nonequivalent, but isocodal vertices, there are two ways to join them by identifying those special vertices of the first copy to those of the second copy, namely joining the equivalent vs joining the nonequivalent pairs. The resulting graphs are obviously nonisomorphic, but all four joining points are isocodal, as are every four copies of the same other vertex in the original endospectral graph. The smallest example for this construct and the smallest pair of isocodal graphs known so far uses two copies of the Schwenk endospectral tree.[23] The Schwenk tree is depicted in Figure 5.

In Figure 6 we give two graphs obtained by joining two copies of the Schwenk tree at both endospectral vertices. These are the two smallest isocodal graphs having only 16 vertices with identical self-returning walk counts for equally labeled vertices.

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