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Note on Acyclic Structures and their Self-Returning Walks*

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All rooted trees up to 16 vertices are generated and the self--returning walks for the roots are calculated. The systematic search for isocodal vertices in the same tree or in different trees revealed that there are isospectral trees without isocodal points, that there non-isospectral trees with isocodal points, and that there are single trees containing several isocodal vertices.

Recently one of us[1] proposed a systematic search for acyclic structures in which non-equivalent vertices may have the same walk-based atomic codes, i. e. the same numbers of self-returning walks for each length of walk. The name given to such vertices was *isocodal* vertices.[2]

Since we are in position to generate all trees for a given number of vertices,[7,8] we decided to carry out the above proposal. Firstly we developed a computer program to generate the adjacency matrix A of a tree from the N-tuple representation[7] of the tree. Then we generated all rooted trees up to 16 vertices. Computing the powers of the adjacency matrices up to 32, we obtained the numbers of self-returning walks for the root as the sequence of the first elements of the diagonal of the powers of A. Then we sorted the rooted trees by lexicographic order[7,9] of the walk-based atomic codes, so it was easy to enumerate the rooted trees having the same walk-based atomic codes up to length 32.

In Table I we show in how many cases the walk-based atomic codes were unique (up to length 32), appeared twice, three times, etc.

In Table II it is shown in how many cases a root of a tree with n vertices has the same walk-based atomic codes as a root of a tree with m vertices.

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TABLE I

Number of Walk-based Atomic Codes Occuring n Times Among the Trees up to 16 Vertices (up to Length 32)

n	number
1	342419
2	14699
3	1283
4	151
5	36
6	1
7	1

TABLE II

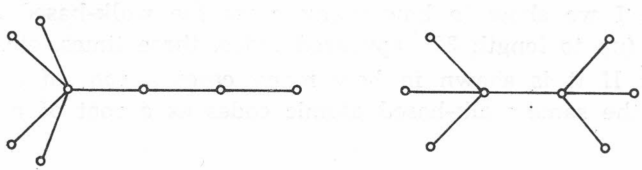
Cross-table of the Occurence of Isocodal Vertices

n \ m	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
6	0	0	0	0	0	0	0	2	0	1	0	0	0	0	0	0
7	0	0	0	0	0	0	0	0	6	1	4	0	1	0	0	0
8	0	0	0	0	0	0	0	0	0	15	3	8	2	4	0	1
9	0	0	0	0	0	0	0	0	1	0	46	6	24	4	13	2
10	0	0	0	0	0	0	0	0	0	3	2	105	17	62	18	23
11	0	0	0	0	0	0	0	0	0	0	13	6	317	44	155	42
12	0	0	0	0	0	0	0	0	0	0	0	44	20	795	123	433
13	0	0	0	0	0	0	0	0	0	0	0	0	133	54	2338	358
14	0	0	0	0	0	0	0	0	0	0	0	0	0	364	162	6180
15	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1107	462
16	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	3012

One may see that up to order 6 (i. e., the number of vertices), the walk-based atomic codes are unique. At order 7 three exists a tree which has the same walk-based atomic codes as a tree of order 5 (up to lenght 32). With respect to equal number of vertices, the walk-based atomic codes are unique up to order 8 (see the diagonal elements of the array shown in Table 2). At the order 9 there exists a tree with two isocodal vertices.

After this analysis we examined the characteristic polynomials of the generated trees. We found several interesting results worth reporting. These are as follows:

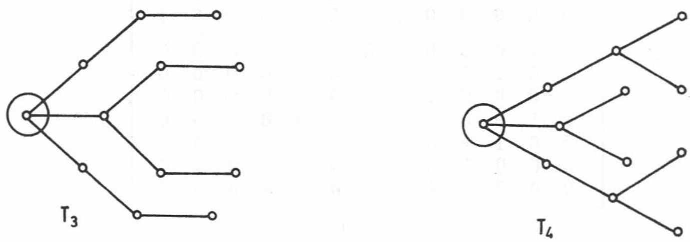
(i) Examples of isocpectral trees with no isocodal vertices, such as a pair shown below.



T_1 T_2

Characteristic polynomial: $P(T_1; x) = P(T_2; x) = x^8 - 7x^6 + 9x^4$

(ii) Examples of trees with isocodal vertices which are not isospectral, such as a pair of trees shown below.

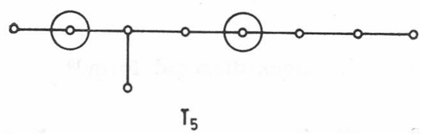


Characteristic polynomial: $P(T_3; x) = x^{12} - 11x^{10} + 43x^8 - 75x^6 + 58x^4 - 16x^2$

Characteristic polynomial: $P(T_4; x) = x^{12} - 11x^{10} + 41x^8 - 59x^6 + 24x^4$

The proof that the walk-based atomic codes of the root-vertices (denoted by circles) in T_3 and T_4 are equal for each lenght of walk is given in the *Appendix*.

(iii) Example of a single tree with several isocodal vertices, such as a tree given below.

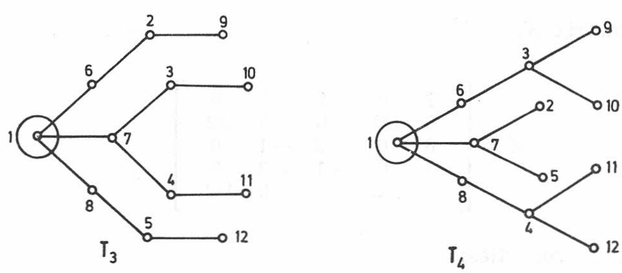


APPENDIX

Proof that two non-isospectral trees have isocodal vertices

The rooted trees T_3 and T_4 have different characteristic polynomials, $P(T_3; x) \neq P(T_4; x)$, and are evidently non-isospectral. We will show that the walk-based atomic codes of the root-vertices in T_3 and T_4, i. e. the first entry of the even powers of the adjacency matrix, are equal for each length of walk.

Since trees are necessarily bichromatic structures, after a convenient labelling of the vertices of T_3 and T_4 we obtain the corresponding adjacency matrices $A(T_3)$ and $A(T_4)$,



$$A(T_3) = \left[\begin{array}{ccccc:ccccccc}
0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\
\hdashline
1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{array}\right]$$

$$A(T_4) = \left[\begin{array}{ccccc:ccccccc}
0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
\hdashline
1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{array}\right]$$

These matrices are given in the block-diagonal form,[10]

$$A(T_3) = \begin{bmatrix} 0 & B_1 \\ B_1^{\mathrm{T}} & 0 \end{bmatrix} \qquad A(T_4) = \begin{bmatrix} 0 & B_2 \\ B_2^{\mathrm{T}} & 0 \end{bmatrix}$$

It is clear that for higher powers of $A(T_3) \cdot A(T_3)$ (or $A(T_4) \cdot A(T_4)$), the first entries (i. e., the first entry of the first row and column) are only dependent on $B_1 B_1^{\mathrm{T}}$ (or $B_2 B_2^{\mathrm{T}}$). Therefore, we need to consider only these submatrices in the further discussion. These submatrices are in our case given as,

$$C_2 = B_2 B_2^{\mathrm{T}} = \begin{bmatrix} 3 & 1 & 1 & 1 & 1 \\ 1 & 2 & 0 & 0 & 0 \\ 1 & 0 & 2 & 1 & 0 \\ 1 & 0 & 1 & 2 & 0 \\ 1 & 0 & 0 & 0 & 2 \end{bmatrix} \quad \text{and} \quad C_1 = B_1 B_1^{\mathrm{T}} = \begin{bmatrix} 3 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 3 & 0 & 0 \\ 1 & 0 & 0 & 3 & 0 \\ 1 & 1 & 0 & 0 & 1 \end{bmatrix}.$$

There exists a matrix X,

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

with the following properties:

(i)

$$X = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & & & & \\ 0 & & Y & & \\ 0 & & & & \\ 0 & & & & \end{bmatrix}$$

(ii)

$$X^n = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & & & & \\ 0 & & Y^n & & \\ 0 & & & & \\ 0 & & & & \end{bmatrix} \text{for all } n \in N$$

(iii)

$$C_1 X = X C_1 = C_2.$$

From (iii) follows

$$C_2^n = (C_1 X)^n = C_1^n X_1^n.$$

The consequence of properties (ii) and (iv) is that the first entries of C_1^n and C_2^n are equal for all n $\in$ N. This ends the proof.

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SAŽETAK

Bilješka o acikličkim strukturama i njihovim samovraćajućim šetnjama

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Generirana su sva stabla s korijenovima do 16 čvorova i za korijene su izračunane samovraćajuće šetnje. Sustavno traganje za čvorovima istog koda unutar zadanog stabla ili pak među različitim stablima je pokazalo da postoje izospektralna stabla bez točaka istog koda, zatim neizospektralna stabla sa točkama istog koda, te posebna stabla sa više točaka istog koda.