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On the spectral characterization of the p -sun and the (p, q) -double sun

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ABSTRACT

In 1973 Schwenk [7] proved that almost every tree has a cospectral mate. Inspired by Schwenk's result, in this paper we study the spectrum of two families of trees. The p -sun of order $2p + 1$ is a star $K_{1,p}$ with an edge attached to each pendant vertex, which we show to be determined by its spectrum among connected graphs. The (p, q) -double sun of order $2(p + q + 1)$ is the union of a p -sun and a q -sun by adding an edge between their central vertices. We determine when the (p, q) -double sun has a cospectral mate and when it is determined by its spectrum among connected graphs. Our method is based on the fact that these trees have few distinct eigenvalues and we are able to take advantage of their nullity to shorten the list of candidates.

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1. Introduction

The goal of this paper is to study the spectra of two families of graphs and to decide if they have a unique spectrum among connected graphs. The motivation for this type

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of study comes from complexity theory. The Graph Isomorphism Problem asks to decide whether two given graphs are isomorphic. From the viewpoint of computational complexity theory, it is a celebrated problem that it is not yet known whether it is solvable in polynomial time or not. Since checking whether two graphs are cospectral can be done in polynomial time, the isomorphism problem concentrates on checking isomorphism between cospectral graphs.

From the prospective of the spectral graph theory, this question is generally studied by analyzing the spectrum of matrices associated with graphs, identifying which graphs are uniquely determined by the spectrum (DS), up to isomorphism. If we know that a graph is DS, then we know its entire structure (vertices, edges, connectivity, subgraphs etc) just by looking at the eigenvalues of the associated matrix (a problem with order of n^3 time complexity). Hence one of the most important problems in the area is to decide which graphs are DS [9].

The question which graphs are DS arose in chemistry with Günthard and Primas [2] in 1956. All graphs were believed to be DS, until in 1957 Collatz and Sinogowitz [10] exhibit a pair of cospectral (non-isomorphic) trees.

A landmark result came in 1973, when Schwenk [7] proves that almost all trees are cospectral by showing that given a tree, it is possible to build a non-isomorphic pair with the same characteristic polynomial. Since then, many methods for constructing cospectral graphs have emerged, some of which can be found in [9], for instance. To this day, it is not known whether most graphs are DS or not, as there are results that reinforce both beliefs.

As van Dam and Haemers point out in the celebrated paper [9], it is not easy to show that a single graph has a unique spectrum among all graphs. In this paper, we are concerned with two families of graphs.

The p -sun (see Section 2 for definitions) has one vertex of degree $p > 2$, p vertices of degree 2 and p pendant vertices and, therefore, belongs to a wider class of trees known as starlikes (has exactly one of its vertices with degree greater than 2). In 2002, Lepovic and Gutman [5] show that no two non-isomorphic starlike trees are cospectral. In 2007, Omid and Tajbakhsh [6] show that if T is a starlike with maximum degree Δ , then the maximum degree of any cospectral graph with T must be less than Δ and it has at most two vertices of degree at least 5. In addition, they also show that all starlike trees are DS in relation to the Laplacian matrix.

More recently, in 2006, Wang and Xu [11] show that all starlike trees with a maximum degree 3 (T-shape trees) are determined by the spectrum, with only a few well-defined exceptions. We notice that the p -sun is also a T-shape tree and when $p = 3$ it is one of the exceptions. In this paper we will show that the p -sun is DS among connected graphs. On the other hand, we will see that this graph may have a cospectral mate, if we consider disconnected graphs.

The other family we study is the (p, q) -double sun, which is composed by a p -sun and a q -sun joined by an edge between their central vertices. We determine when the

(p, q) -double sun is DS among connected graphs. Moreover, when the (p, q) -double has a connected cospectral mate H , we determine precisely the graph H .

We point out that the p -sun and the (p, q) -double sun are important graphs as, for example, they are conjectured to be graphs with largest Randić energy [3]. We also emphasize that the technique used in our proofs is novel, as we use a localization algorithm and take advantage of relations between matching number and nullity.

The paper is organized as follows. In Section 2 we see some basic notions of (spectral) graph theory which are needed along the paper as well as some important preliminary results and a localization algorithm. Our first main result is presented in Section 3, where we show that the p -sun is DS among connected graphs. Section 4 is a guide for the proof of the results about (p, q) -double sun. Sections 5, 6, 7 and 8 contain the details of the analysis of trees having perfect matching and different values of the diameter. Finally, in Section 9, we discuss our results and suggest some research problems.

2. Preliminaries

In this section we set the notation, give basic definitions and state known results that will be used in this manuscript. We also set forward the main tool used to prove our main results.

We will deal with simple graphs $G = (V, E)$. A vertex with degree 0 is called *isolated* and a vertex with degree 1 is called *pendant*. Also a vertex with a pendant neighbor is called *quasi-pendant*.

An subset M of edges is called a *matching* of G if no two edges of M share a common vertex. A matching is called *maximum* in G if it has maximum cardinality among all matchings, and it is called *perfect* if every vertex of G is incident with (exactly) one edge in M . The cardinality of a maximum matching is called the *matching number* of G , denoted by $\mu(G)$. A tree with a perfect matching is denoted by *PM-tree* for short.

For a tree T on at least two vertices, a vertex $v \in T$ is called *mismatched* in T if there exists a maximum matching M of T that does not cover v ; otherwise, v is called *matched* in T . If a tree consists of only one vertex, then this vertex is considered mismatched.

The *distance* of two vertices u, v in G is the length (number of edges) of a shortest path between u and v in G . The greatest distance between any two vertices in G is the *diameter* of G , denoted $d(G)$. A vertex is *central* in G if its greatest distance from any other vertex is as small as possible.

With G we associate the *adjacency matrix* which is the 0-1 matrix A indexed by the vertices of G , where $A_{uv} = 1$ when u and v are adjacent in G and $A_{uv} = 0$ otherwise. The *spectrum* of G is the spectrum of its adjacency matrix. The *nullity* of the graph G , denoted by $\eta(G)$, is the multiplicity of the eigenvalue zero in the spectrum of G .

A graph is *determined by its spectrum* – DS for short – if there is no other non-isomorphic graph with the same spectrum. If there is such a non-isomorphic graph with the same spectrum, we say both are *cospectral mates*.

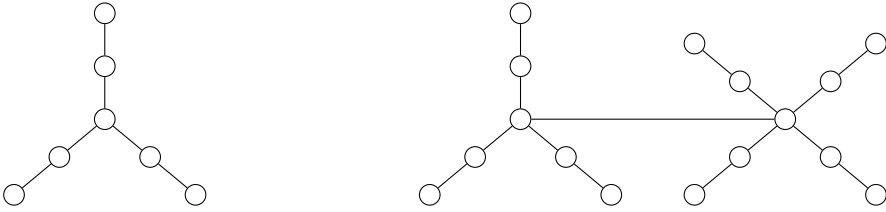


Fig. 1. The 3-sun with 7 vertices and the (3,4)-double sun with 16 vertices.

We understand that a sun graph has different forms in the literature. Here we follow the definition from Gutman et al. in [3]. Let $p \geq 1$. The tree of order $n = 2p + 1$ obtained from a star $K_{1,p}$ with an edge attached to each pendant vertex is called p -sun. For $p, q \geq 1$, the tree of order $n = 2(p + q + 1)$ obtained from the union of two suns, the p -sun and q -sun, by adding an edge between their central vertices is called (p, q) -double sun. Fig. 1 illustrates the graphs we are concerned in this note.

The following results may be found in van Dam and Haemers [9].

Proposition 2.1. *Let G be a connected graph with diameter d . Then G has at least $d + 1$ distinct eigenvalues.*

Lemma 2.2. *For the adjacency matrix of a graph G , the following can be deduced from the spectrum:*

- (i) *The number of vertices.*
- (ii) *The number of edges.*
- (iii) *Whether G is bipartite.*

From Jacobs et al. [4] we have the following algorithm which is used extensively in our results. The algorithm operates directly on a (rooted) tree and works bottom-up. The tree is rooted at an arbitrary vertex and the vertices are ordered v_1, \dots, v_n such that if v_i is a child of v_k , then $k > i$.

The algorithm *Diagonalize* finds a diagonal matrix D that is congruent to $A(T) + \alpha I$, for any real number α . Hence the next result follows [4]:

Theorem 2.3. *Let D be the matrix produced by *Diagonalize*($T, -\alpha$), for T a tree.*

- (i) *The number of positive entries in D is the number of eigenvalues of T greater than α .*
- (ii) *The number of negative entries in D is the number of eigenvalues of T less than α .*
- (iii) *If there are j zero entries in D , then α is an eigenvalue of T with multiplicity j .*

We would like to point out that Algorithm 1 may also be used to compute the characteristic polynomial $\det(\lambda I - A)$, where λ is an indeterminate. We may use *Diagonalize*($T, -\lambda$) to compute $\det(A - \lambda I)$. However we would be working over the

Algorithm 1: Diagonalize(T, α).

Input: tree T , scalar α
 Output: diagonal matrix D congruent to $A(T) + \alpha I$
 initialize $d(v) := \alpha$, for all vertices v
 order vertices bottom-up
for $k = 1$ to n **do**
 if v_k is a leaf **then**
 continue
 else if $d(c) \neq 0$ for all children c of v_k **then**
 $d(v_k) := d(v_k) - \sum \frac{1}{d(c)}$, summing over all children of v_k
 else
 select one child v_j of v_k for which $d(v_j) = 0$
 $d(v_k) := -\frac{1}{2}$
 $d(v_j) := 2$
 if v_k has a parent v_l , remove the edge $v_k v_l$
 end if
end for

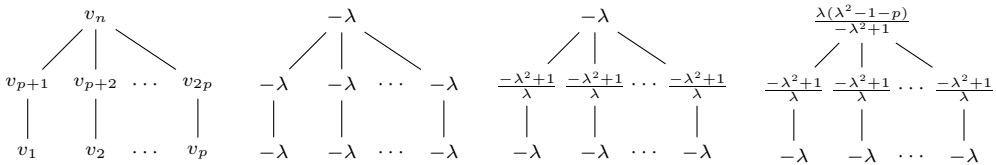


Fig. 2. Diagonalize algorithm step-by-step applied to the p -sun.

quotient field $\mathbb{R}(\lambda)$ of $\mathbb{R}[\lambda]$. The output of $\text{Diagonalize}(T, -\lambda)$ over $\mathbb{R}(\lambda)$ will be a diagonal matrix D whose product of the diagonal terms is $\det(A - \lambda I)$ and adjusting the sign by $(-1)^n$ we obtain $\det(\lambda I - A)$.

To emphasize the previous observation we will use the algorithm Diagonalize with $\alpha = -\lambda$ to obtain the characteristic polynomial $\phi_{p\text{-sun}}(\lambda)$ of the p -sun. We set the root to be the vertex of degree p and we begin by initializing each vertex with $d(v) := -\lambda$ and then we skip all the leaves and look at their quasi-pendant neighbors. According to the algorithm, for each one of these quasi-pendant vertices v_k , as they only have one child c with $d(c) = -\lambda$, we have $d(v_k) := d(v_k) - \sum \frac{1}{d(c)} = -\lambda - \frac{1}{-\lambda} = \frac{-\lambda^2+1}{\lambda}$.

Finally we look at the root v_n which has p children with $d(c) = \frac{-\lambda^2+1}{\lambda}$ each and so we find $d(v_n) := d(v_n) - \sum \frac{1}{d(c)} = -\lambda - \frac{p\lambda}{-\lambda^2+1} = \frac{\lambda(\lambda^2-1-p)}{-\lambda^2+1}$. We can see in Fig. 2 the algorithm being applied step-by-step to the tree. In the tree on the left we show the vertices named bottom-up and in the remaining trees the values $d(v)$ of each vertex are shown as they are calculated at each level up to the root.

To find $\det(A - \lambda I)$ we just multiply all the values $d(v)$ that the algorithm has computed. Then the characteristic polynomial of the p -sun is given by

$$\begin{aligned} \phi_{p\text{-sun}}(\lambda) &= (-1)^n \det(A - \lambda I) \\ \phi_{p\text{-sun}}(\lambda) &= (-1)^n (-\lambda)^p \left(\frac{-\lambda^2+1}{\lambda} \right)^p \left(\frac{\lambda(\lambda^2-1-p)}{-\lambda^2+1} \right) \end{aligned}$$

$$= \lambda(\lambda^2 - 1)^{p-1}(\lambda^2 - (p + 1)).$$

The following two results can be found in Gong *et al.* [1]. The first associates the matching number and the nullity of a tree, and the second ensures that every quasi-pendant vertex of a tree is matched.

Lemma 2.4. *Let T be a tree of order n , with nullity $\eta(T)$ and matching number $\mu(T)$. Then $\eta(T) = n - 2\mu(T)$.*

Lemma 2.5. *If v is a quasi-pendant vertex of a tree T , then v is matched in T .*

The following well known result about trees is stated here for easy reference.

Lemma 2.6. *A connected graph with n vertices is a tree if and only if it has $n - 1$ edges.*

We observe that any tree with nullity zero has a perfect matching, for Lemma 2.4 yields $\mu(T) = \frac{n}{2}$. Also every PM-tree has an even number of vertices since each edge has two vertices and no edge in a matching share a vertex with another. In particular, any tree T of order n (therefore $n - 1$ edges) and nullity $\eta(T) = 1$, has a matching number $\mu(T) = \frac{n-1}{2} \in \mathbb{Z}$, which means that half of its edges are matched by a maximum matching and thus all its vertices (but one) are covered, for T has an odd number of vertices.

2.1. Constructing a general tree with a given diameter

In order to determine the spectral characterization of the p -sun and the (p, q) -double sun, we will need to analyze trees with diameters up to 7. For this we need to understand the structure of such trees. As this may be of independent interest, we explain in this section how to construct general trees with a given diameter.

The following is well known, but we emphasize here for completeness.

Observation 2.7. Let T be a tree with diameter d . Then T has a path P with largest length d as a subgraph. If d is even, then P has an odd number of vertices and so it has one *central vertex* v . Similarly, if d is odd, then P has two central vertices with an edge e joining them. The vertex v and edge e are unique, independently of the largest path P . The edge e is called the *central edge* of the (odd diameter) tree T , while the vertex v is called the *central vertex* of the (even diameter) tree T .

The following is also well known.

Observation 2.8. If a tree has even diameter $2k$, then the distance from its central vertex v to any other vertex is at most k . If it has an odd diameter $2k + 1$, then the distance from any of its central vertices to any other vertex is at most $k + 1$ and a path which

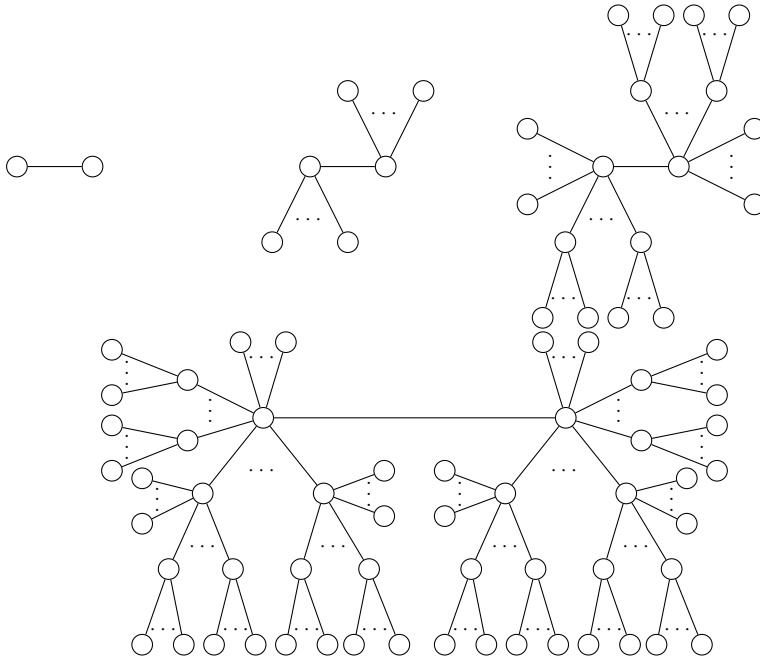


Fig. 3. General trees of diameters 1, 3, 5 (top) and 7 (bottom).

attains such maximum distance contains the central edge e . Moreover, there must be at least one path from each central vertex with length k that does not contain e .

Since we need a rooted tree to apply Algorithm 1, in what follows, we always choose the central vertex as the root; if the tree has an odd diameter, we choose either one of the central vertices.

Let d be a fixed diameter. We initialize the construction of the tree T according to the parity of d . If $d = 2k \geq 2$ is even, we initialize T with a vertex, and if $d = 2k + 1 \geq 3$, we initialize T with an edge. The rest of the procedure is the same, depending only on k , not the parity of d .

First we attach $p(v) \geq 2$ pendant vertices to each vertex v in T . We continue this procedure for a total of k steps, where at each step we attach $p(v) \geq 2$ pendant vertices to every vertex v present in T so far. The important thing is to attach an amount greater than 1 (but not necessarily equal) to every vertex at each step in order to yield a general tree.

We first exemplify this procedure by creating a general tree T with diameter 7. As $d = 2 \cdot 3 + 1$, we initialize T with an edge and then we have $k = 3$ steps to complete the process.

We observe that while constructing the general tree of diameter 7, we also construct general trees of diameter 1, 3 and 5 in the process. We refer to Fig. 3.

The only difference between constructing an odd and an even diameter tree is the first step, so in order to build T with diameter 6, we initialize it with a vertex, instead of an

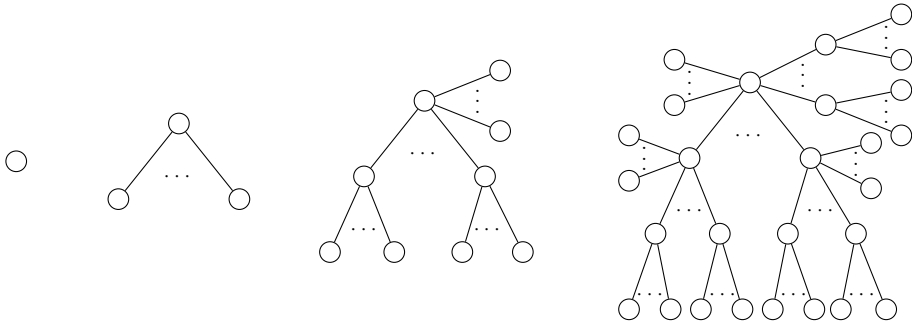


Fig. 4. Steps yielding to the general tree with $d = 6$.

edge. As $d = 2.3$, we only have $k = 3$ steps after the initial vertex. We also notice that a general tree with an odd diameter $2k + 1$ may be thought of as two general trees with an even diameter $2k$ connected by their central vertices. For instance, a general tree with diameter 7 can be seen as two general trees with diameter 6 connected by their central vertices. We refer to Fig. 4 for the construction of general trees of even diameter 0, 2, 4 and 6.

3. The p -sun is DS among connected graphs

In this section we prove that the p -sun is determined by its spectrum among connected graphs. Our method takes advantage of the fact that the sun has nullity one and only five distinct eigenvalues. Hence, by using Proposition 2.1, it suffices to determine all possible trees with diameter at most 4 whose eigenvalue 0 has multiplicity one. This discrimination turns out to be fairly simple and, by putting together the previous results, it allows us to show that the sun has no cospectral mates in the set of connected graphs.

Proposition 3.1. *The spectrum of the p -sun is*

$$\{0^{(1)}, -1^{(p-1)}, 1^{(p-1)}, -\sqrt{p+1}^{(1)}, \sqrt{p+1}^{(1)}\}$$

for $p \geq 1$.

Proof. The result follows by noticing that the characteristic polynomial of the p -sun computed in the previous section is $\lambda(\lambda^2 - 1)^{p-1}(\lambda^2 - (p + 1))$. \square

A tree with diameter 3 (see Fig. 3) (top) may be seen as two stars $K_{1,a}$ and $K_{1,b}$ with their centers connected by an edge. Hence we denote a diameter 3 tree of order n by $T(a, b)$, as in [8], where $n = a + b + 2$ with $a \geq b \geq 1$ leaves at each end of $T(a, b)$.

A tree with diameter 4 (see Fig. 4) may also be seen as a star $K_{1,\ell}$ with its center connected to the centers of k stars $K_{1,p_1}, \dots, K_{1,p_k}$. We denote it by $T(\ell, p_1, \dots, p_k)$, where $\ell \geq 0, k \geq 2$ and $p_i \geq 1$. We notice that the p -sun is the particular case $T(0, 1, \dots, 1)$ for $k = p$ and observe that $\ell \geq 0$ and $p_i \geq 1$ because this guarantees $d = 4$.

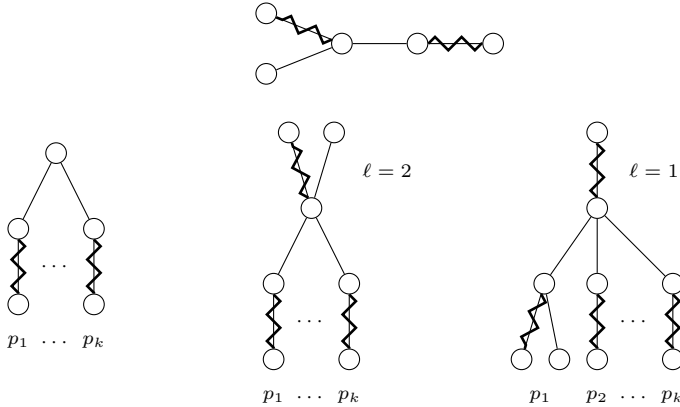


Fig. 5. The only trees with $d = 3$ (top) and $d = 4$ (bottom) and nullity one.

Lemma 3.2. Consider the set of trees.

- (i) The only tree with diameter 3 and nullity one is $T(2, 1)$.
- (ii) The only trees with diameter 4 and nullity one are the p -sun, $T(2, 1, \dots, 1)$ and $T(1, 2, 1, \dots, 1)$.

Proof. We recall that a tree with nullity one can have a single mismatched vertex. For item (i), we notice that if $a \geq b = 2$, then it is easy to see that $T(a, b)$ would have more than one mismatched vertex. By the same reasoning, in a diameter 4 tree, there can be at most one quasi-pendant vertex with two pendant vertices and hence item (ii) follows. We refer to Fig. 5 for an illustration. \square

We now state the main result of this section.

Theorem 3.3. Let $p \geq 1$ be an integer. Then the p -sun is determined by its spectrum among connected graphs.

Proof. We first notice that for $p = 1$ and $p = 2$, the p -sun trees are the paths P_3 and P_5 , respectively, which are DS. Hence we assume that $p \geq 3$. By Proposition 3.1 we know that the spectrum of the p -sun is $\{0^{(1)}, \pm 1^{(p-1)}, \pm \sqrt{p+1}^{(1)}\}$, where $n = 2p + 1 \geq 7$ is its order.

Suppose T is a connected graph non-isomorphic and cospectral with the p -sun. By Lemma 2.2 (ii), the number of edges of T is $n - 1$ and hence, by Lemma 2.6, we may assume T is a tree. By Proposition 2.1, as T has 5 distinct eigenvalues, its diameter is at most 4. As the only trees with diameter 1 and 2 are P_2 and $K_{1, n-1}$, respectively, and they both are determined by their spectra, they may be ruled out.

By Lemma 3.2 (i) the only tree with nullity one and diameter 3 is $T(2, 1)$, which has 5 vertices, so it cannot be cospectral with the p -sun.

Now only trees with diameter 4 remain to be considered and then, by Lemma 3.2 (ii), we shall verify whether T is isomorphic to either $T(2, 1, \dots, 1)$ or $T(1, 2, 1, \dots, 1)$. We first notice that the multiplicity of the eigenvalue 1 (or -1) of T equals $p - 1$, i.e., $\frac{n-3}{2}$.

If $T \simeq T(2, 1, \dots, 1)$, then it has order $n = 2k + 3$ and thus the eigenvalue 1 must have multiplicity k . After applying Algorithm 1 and using Theorem 2.3, we find out that its multiplicity is actually $k - 1$, so this tree cannot be cospectral with the p -sun.

In a similar manner, if $T \simeq T(1, 2, 1, \dots, 1)$, it has order $n = 2k + 3$ and so the eigenvalue 1 must also have multiplicity k , but using Theorem 2.3 we find out it actually has multiplicity $k - 2$.

Therefore the p -sun has no cospectral mates among connected graphs. \square

4. Spectral characterization of the (p, q) -double sun

This section is a guide for the spectral characterization of the (p, q) -double sun. The main result is the following.

Theorem 4.1. *Let $3 \leq p \leq q$ be integers and G the (p, q) -double sun with $n = 2(p + q + 1)$ vertices. Consider*

$$p' = \frac{1}{4}(n - 4 + 2\sqrt{(p - q)^2 + n - 5}).$$

- (a) G is DS among connected graphs if and only if p' is not a natural number.
- (b) G has a connected cospectral mate if and only if p' is a natural number.

We now explain how we achieve the proof of this result. Because we are considering only connected graphs, we may restrict the analysis to trees of diameter $d \leq 7$, because the (p, q) -double sun G has 8 distinct eigenvalues. As G has nullity 0, we restrict further to those trees with perfect matching.

In Section 5 we prove Proposition 5.4 showing that G has no cospectral mate among trees with diameter $d \leq 4$. In sections 6 and 7 we prove Propositions 6.2 and 7.3 showing, respectively, that G has no cospectral mates among trees of diameters 5 and 6.

In Section 8 we deal with PM-trees of diameter 7. There, we reduce the analysis to 4 prototype PM-trees. Proposition 8.2 shows that 3 of the 4 types are not cospectral with G . However, as Proposition 8.3 shows, one type may be cospectral with the (p, q) -double sun G , exactly when $p' = \frac{1}{4}(n - 4 + 2\sqrt{(p - q)^2 + n - 5})$ is a natural number.

Hence, collectively, Propositions 5.4, 6.2, 7.3, 8.2 and 8.3 prove Theorem 4.1.

The remaining of the paper is as follows. The rest of this section has some general results that will be used in the remaining sections, where the PM-trees with diameter $d \leq 7$ are studied. Section 9 discusses the results of this paper and suggests some research problems.

Proposition 4.2. *The spectrum of the (p, q) -double sun is*

$$\{-1^{(p+q-2)}, 1^{(p+q-2)}, -r_1^{(1)}, -r_2^{(1)}, -r_3^{(1)}, r_1^{(1)}, r_2^{(1)}, r_3^{(1)}\}$$

for $p, q \geq 1$, where $\pm r_1, \pm r_2$ and $\pm r_3$ are the roots of the polynomial

$$\lambda^6 - (p + q - 3)\lambda^4 + (pq + p + q + 3)\lambda^2 - 1.$$

Proof. We perform Diagonalize($T, -\lambda$) with the (p, q) -double sun rooted at the vertex of degree $p + 1$ to obtain $\det(A - \lambda I)$. Therefore

$$\phi_{(p,q)\text{-double sun}}(\lambda) = (\lambda^2 - 1)^{p+q-2}[\lambda^6 - (p + q + 3)\lambda^4 + (pq + p + q + 3)\lambda^2 - 1].$$

It is easy to check (say, by substitution) that $\lambda = \pm 1$ are not roots of the sixth degree polynomial and thus the result follows. \square

Lemma 4.3. *Let $T = (V, E)$ be a tree with diameter $d > 3$ and $\ell \geq 1$ non-pendant vertices which are adjacent to quasi-pendant vertices of degree 2. Then T has at least ℓ eigenvalues less than -1 .*

Proof. Let $V' = \{v_1, \dots, v_\ell\} \subset V$ be the $\ell \geq 1$ non-pendant vertices of T having some quasi-pendant neighbor of degree 2. If $\ell \geq 2$, to avoid overcounting, we first need to prove that every quasi-pendant vertex of degree 2 is neither in V' nor has more than one neighbor in V' .

For $\ell \geq 2$, let u be a quasi-pendant vertex of degree 2.

First we show that $u \notin V'$. If $u \in V'$, then u has a quasi-pendant neighbor v of degree 2. Since both u and v have one pendant neighbor each, we have $T \simeq P_4$ with diameter 3, a contradiction. And to see that u cannot have both neighbors in V' we simply notice that one neighbor of u is pendant, another contradiction.

Finally, to prove the desired result, we set the root at some vertex that is neither a pendant nor a quasi-pendant of degree 2 and apply Algorithm 1 with $\alpha = 1$. We notice that this ensures that each vertex in V' is processed after their quasi-pendant neighbor of degree 2 (see Fig. 6 for an illustration).

Initializing Algorithm 1 with $\alpha = 1$ implies that a quasi-pendant vertex u of degree 2 (which has only one pendant child) has its value $d(u) := 1 - \frac{1}{1} = 0$. Now we can process every $v_i \in V'$. We notice that every v_i has children whose value is 0. We choose one such a child u , set $d(u) = 2$, $d(v_i) := -\frac{1}{2}$, and remove the edge with the parent of v_i (if any). Thus the value $d_{v_i} = -1/2$ is permanent and by Theorem 2.3 we have proved the desired result. \square

Next we show an example of Lemma 4.3 represented in Fig. 6, where we set $\alpha = 1$ (to obtain information about $-\alpha$) and we apply Algorithm 1 bottom-up. In this example, we have $\ell = 2$ vertices that satisfy Lemma 4.3 and in fact the tree has 3 eigenvalues less than -1 , because 3 values remain negative after the application of the algorithm.

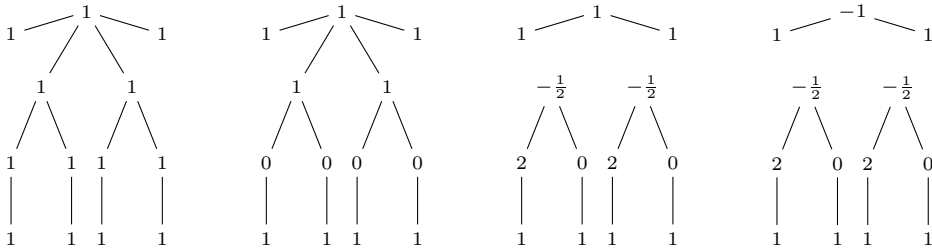


Fig. 6. Application of Lemma 4.3.

Lemma 4.4. *The (p, q) -double sun has exactly two eigenvalues less than -1 .*

Proof. This follows by observing that the application of Algorithm 1 with $\alpha = 1$ on the (p, q) -double sun leaves two negative values. \square

Even though simple, together with Lemma 4.3, the following will be a powerful tool for identifying which PM-trees should be tested as double sun’s cospectral mates.

Lemma 4.5. *In a graph with perfect matching, every quasi-pendant vertex has only one pendant vertex.*

Proof. It suffices to observe that in a graph with perfect matching, all its vertices are matched, and that would not be possible if a quasi-pendant vertex had more than one adjacent pendant vertex. \square

5. PM-trees with diameter 2,3 and 4

In this section we show that trees with diameter 2, 3 and 4 can not be cospectral with the (p, q) -double sun. We use the fact that our target tree, the (p, q) -double sun, is a PM-tree.

Lemma 5.1. *There is no PM-tree with diameter 2.*

Proof. The only tree with diameter 2 is the star $K_{1,n}$, with $n > 1$ and thus its central vertex v has more than one pendant vertex. Now the result follows from Lemma 4.5. \square

Lemma 5.2. *The only PM-tree with diameter 3 is $P_4 \simeq T(1, 1)$.*

Proof. Let T be a tree of diameter 3. Again, applying Lemma 4.5, we see that the only tree having quasi-pendant vertices with a single pendant neighbor each is $T(1, 1)$. \square

Using the same reasoning, follows the result for a diameter 4 tree.

Lemma 5.3. *The only PM-tree with diameter 4 is $T(1, 1, \dots, 1)$.*



Fig. 7. The only PM-trees with $d = 3$ (left) and $d = 4$ (right).

Fig. 7 illustrates the PM-trees with $d = 3$ and $d = 4$. The diameter 4 tree with perfect matching is of particular interest, since it appears as branch at central vertices in PM-trees with greater diameter. On such occasions, we make use of Lemma 4.3 to restrict our possibilities of PM-trees because each branch presenting this form increases the amount of eigenvalues less than -1 by one, since its central vertex is adjacent to quasi-pendant vertices of degree 2.

The following result puts together the above lemmata, concluding that none of the PM-trees with diameter 2, 3 or 4 can be cospectral with the (p, q) -double sun for $p, q \geq 1$.

Proposition 5.4. *The (p, q) -double sun has no cospectral mates among connected graphs with diameters 2, 3 and 4.*

Proof. As before we can restrict ourselves to trees. Now, by Lemma 5.1, there is no PM-tree with diameter 2. As Lemma 5.2 states, the only PM-tree with diameter 3 has 4 vertices, but any cospectral mate with the (p, q) -double sun must have at least 6 vertices, as $p, q \geq 1$ and $n = 2(p + q + 1)$.

Finally we apply Algorithm 1 with $\alpha = 1$ to the tree with diameter 4 together with Theorem 2.3 and we see that $T(1, 1, \dots, 1)$ has a single eigenvalue less than -1 , when it should have exactly two in order to be a possible cospectral mate of the double sun, by Lemma 4.4. \square

6. PM-trees with diameter 5

Not as simple as above, where we can easily see the only possibilities of PM-trees with diameter 2,3 and 4, in this section we determine the PM-trees with diameter 5.

Starting with the general tree with diameter 5, based on Lemma 4.5 our first step is to remove all but one pendant vertex from each quasi-pendant vertex. Next we match all quasi-pendant vertices of degree 2 with their pendant neighbor, which is a consequence of applying Lemma 2.5. This process is represented in Fig. 8.

The reason why we do not match every pendant edge all at once is because some of them could be removed from the tree without changing its diameter or its general form.

Now, we observe that in order to preserve the diameter of the tree we must keep at least one path with maximum length at each central vertex by Observation 2.8 and, therefore, the central vertices can never be removed.

Then we are left with only two possibilities: matching the central edge or not. If we match the central edge, we must remove the pendant edges at each central vertex and

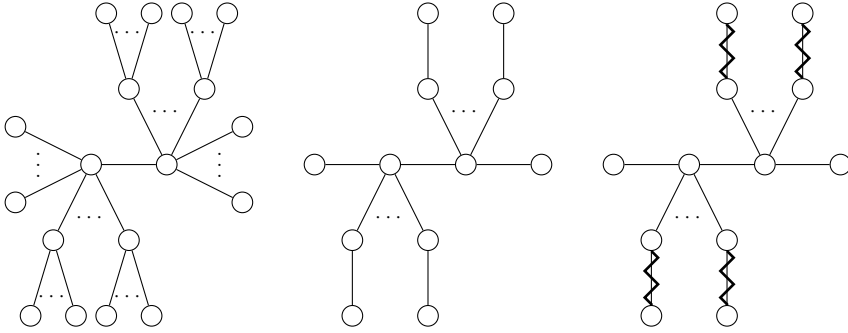


Fig. 8. First steps to build PM-trees with diameter 5.

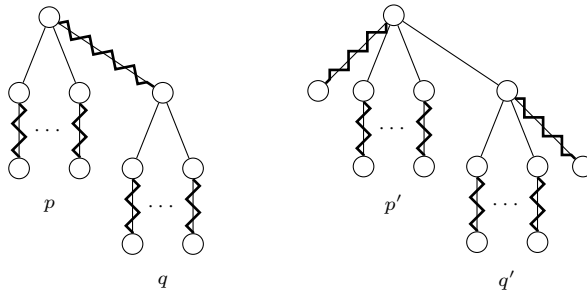


Fig. 9. The only two PM-trees with $d = 5$.

we end up with the double sun. Otherwise, if we do not match the central edge, then we can only match each central vertex with their pendant neighbor and we denote T_5 this PM-tree.

Both possibilities are shown in Fig. 9.

Lemma 6.1. *The only two PM-trees with diameter 5 are the (p, q) -double sun and T_5 .*

The next result shows that T_5 is not cospectral with the double sun. Our method checks the multiplicity of the eigenvalues ± 1 to discard this possibility by the use of Algorithm 1.

Proposition 6.2. *The double sun has no cospectral mates among connected graphs with diameter 5.*

Proof. As before, because we are restricting ourselves to connected graphs, then it follows from Lemma 6.1 that the only possible candidate for cospectrality is the tree T_5 .

First we recall that the multiplicity of the eigenvalues ± 1 of the (p, q) -double sun is $p + q - 2$, where $p, q \geq 1$. In terms of the number of vertices $n = 2(p + q + 1)$, we can translate this multiplicity as $\frac{n}{2} - 3$.

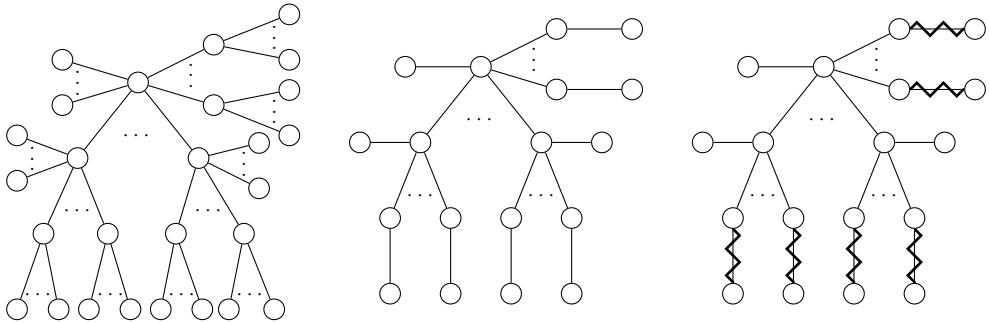


Fig. 10. First steps to build PM-trees with diameter 6.

Let T_5 with $p', q' \geq 1$ quasi-pendant vertices with degree 2 in each central vertex and thus with $n = 2(p' + q' + 2) = 2(p + q + 1)$ vertices.

Using Algorithm 1 on T_5 with $\alpha = 1$, we see that the multiplicity of -1 is $p' + q' - 2 = \frac{n}{2} - 4$, by Theorem 2.3, and we conclude they do not have the same spectrum. \square

From now on, the procedures to determine the PM-trees with diameter 6 and 7 follow the same pattern that we have just seen. Certainly there are many more possibilities of perfect matchings when considering those diameters, but with the help of some previous results we are going to be able to reduce dramatically such cases.

7. PM-trees with diameter 6

In the same way as before, to determine the PM-trees with diameter 6, we start with a general tree and by Lemma 4.5 we prune its pendant vertices, leaving only one at each quasi-pendant vertex. After that, supported by Lemma 2.5, we can match every edge between a quasi-pendant vertex with degree 2 and its pendant neighbor, since they cannot be matched by any other edge. We see this process in Fig. 10.

Looking from the perspective of the central vertex, it can only be matched with some neighbor yet to be matched. There are two ways to do that. The first one is to match the central vertex with its pendant edge, then we must match all other pendant edges left, as there is no other possibility. We call this a *type I* PM-tree with diameter 6. The second way is to match the central vertex u with a non-pendant vertex v , then we must remove both pendant edges incident at u and v since they can no longer be matched, and the remaining pendant edges of the tree are all matched. We call this a *type II* PM-tree with diameter 6. The two resulting trees are illustrated in Fig. 11.

Before we continue, a bit of notation is needed for the two types of diameter 6 PM-trees with central vertex u . For a type I PM-tree with diameter 6, u has $\deg(u) = r + k + 1$ neighbors, where $r \geq 0$ is the number of quasi-pendant vertices with degree 2, $k \geq 2$ is the number of quasi-pendant vertices with degree greater than 2, and the 1 corresponds to the matched pendant edge. We also say that a vertex v_i adjacent to u with $\deg(v_i) > 2$ has $p_i \geq 1$ quasi-pendant neighbors with degree 2, for $1 \leq i \leq k$.

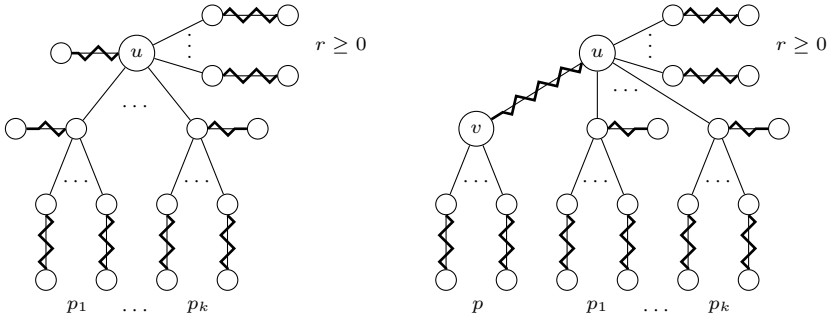


Fig. 11. Type I and type II general PM-trees with diameter 6.

For a type II PM-tree with diameter 6, u has also $\deg(u) = r + k + 1$ neighbors, where we still have $r \geq 0$, but the differences are that $k \geq 1$ and, since its matched edge uv is not pendant, we say that v has $p \geq 1$ quasi-pendant neighbors with degree 2.

Observation 7.1. The reason for the lower restraints at k , p_i and p is only to guarantee the tree’s diameter in each type. More precisely, we need to have at least two paths (with no edge in common) from the central vertex with maximum length. Therefore, the type I tree must have at least two paths with length 3 ($k \geq 2$) and the type II tree must have one path with length 3 containing the central vertex’s matched edge ($p \geq 1$) and at least one more path with the same length ($k \geq 1$). As r has no influence on the diameter, we can have $r = 0$ with no problem.

Thanks to Lemma 4.4, we can determine which PM-trees with diameter 6 are of interest when looking for cospectral mates to the (p, q) -double sun. Its proof uses the notation established for type I and type II PM-trees with diameter 6, as can be easily understood by looking at Fig. 10 together with Observation 7.1 above.

Lemma 7.2. *The only PM-trees with $d = 6$ and two eigenvalues less than -1 are:*

- (i) *the type I tree with $k = 2$ and $r = 0$;*
- (ii) *the type II tree with $k = 1$ and $r = 0$.*

Proof. Let T be a type I PM-tree with diameter 6 and central vertex u , where $\deg(u) = r + k + 1$. As stated in Observation 7.1, we must have $k \geq 2$ in order to maintain the diameter of T , but $r \geq 0$. If $r \geq 1$, then T would have at least $k + 1$ vertices which are adjacent to quasi-pendant vertices of degree 2. Therefore, by Lemma 4.3, T would have $k + 1 \geq 3$ eigenvalues less than -1 , which is not of interest because of Lemma 4.4. So the only way of having (at least) two eigenvalues less than -1 is to assign $k = 2$ and $r = 0$.

Similarly, we now consider a type II PM-tree with diameter 6 but, different from the type I, we have $p \geq 1$ and $k \geq 1$ as restraints to ensure the diameter, and $r \geq 0$ still. Then, by Lemma 4.3, if $r = 0$ we would already have at least $k + 1 \geq 2$ eigenvalues

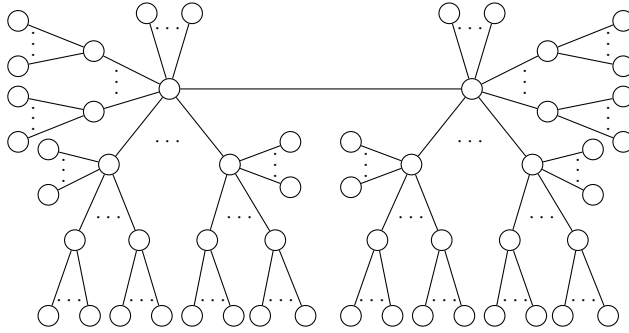


Fig. 13. General tree with diameter 7.

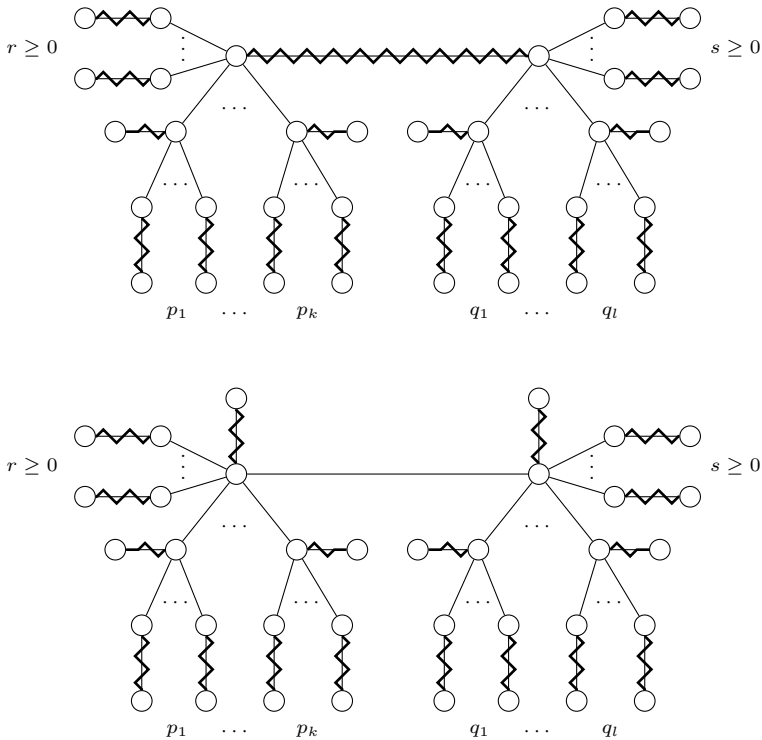


Fig. 14. PM-trees with diameter 7: type I (top) and type II (bottom).

2, since there is no other way of matching them. Observing that the central edge may or may not be matched, we separate our analysis for both cases. If the central edge is matched, we remove the pendant edges at both central vertices and we match all pendant edges remaining. We call this a *type I* PM-tree with diameter 7. The result is represented in Fig. 14 (top).

We set now some notation for the type I trees and future references. We say that the PM-tree with diameter 7 and matched central edge uv has one of its central vertices

u with $\deg(u) = r + k + 1$, where $r \geq 0$ is the number of quasi-pendant vertices with degree 2 and $k \geq 1$ is the number of vertices with degree greater than 2, the other central vertex v has $\deg(v) = s + l + 1$, where s and l are analogous to r and k , respectively, and the number 1 in both degrees represents the central edge. We also say that each vertex $u_i \neq v$ adjacent to u with $\deg(u_i) > 2$ has $p_i \geq 1$ neighbors with degree 2, for $1 \leq i \leq k$. An analogous statement is said about the other central vertex; each vertex $v_i \neq u$ adjacent to v with $\deg(v_i) > 2$ has $q_i \geq 1$ neighbors with degree 2, for $1 \leq i \leq l$. Such restrictions on k, l, p_i and q_i are intended to preserve the diameter of the tree and that is also why r and s can be zero.

Now consider the case when the central edge uv is not matched, then we have 3 possibilities:

- (a) match u and v with their pendant edges;
- (b) match u with its pendant edge and match v with some neighbor v_0 with degree greater than 2;
- (c) match u and v with some neighbors u_0 and v_0 , respectively, with degrees greater than 2;

We notice that case (b) is symmetric in relation to the central edge, that is, it would lead us to the same result if we switch vertices u and v .

In case (a), we simply match all pendant edges and we call this a *type II* PM-tree with diameter 7, as we can see in Fig. 14 (bottom).

Similar to the notation before, we say that the type II PM-tree in case (a) with non-matched central edge uv has the central vertex u with $\deg(u) = r + k + 2$, where $r \geq 0$ is the number of quasi-pendant vertices with degree 2 and $k \geq 1$ is the number of vertices with degree greater than 2, the other central vertex v has $\deg(v) = s + l + 2$, where s and l are analogous to r and k , respectively, and the number 2 in both degrees represents the central and pendant edges at each central vertex. Furthermore, each vertex $u_i \neq v$ adjacent to u with $\deg(u_i) > 2$ has $p_i \geq 1$ neighbors with degree 2, for $1 \leq i \leq k$, and each vertex $v_i \neq u$ adjacent to v with $\deg(v_i) > 2$ has $q_i \geq 1$ neighbors with degree 2, for $1 \leq i \leq l$. We recall that $p_1, \dots, p_k, q_1, \dots, q_l, k, l, r, s$ here have no relation with the ones in the previous (or the following) case(s), so we always make it clear which case we are referring to. We stress that the reason for the restrictions on the parameters is due to the diameter of the tree.

In case (b), we remove only the pendant edges at v and v_0 , and match all pendant edges remaining, as there is nothing else to do. We call this a *type III* PM-tree with diameter 7 and the resulting tree is shown in Fig. 15 (top).

We say that the PM-tree in case (b) and non-matched central edge uv has u with $\deg(u) = r + k + 2$, where $r \geq 0$ is the number of quasi-pendant vertices with degree 2 and $k \geq 1$ is the number of vertices with degree greater than 2. The other central vertex v has $\deg(v) = s + l + 2$, where s is analogous to r , but as much as l represents the same kind of vertices as k , we have $l \geq 0$ because, if $l = 0$ then it does not affect

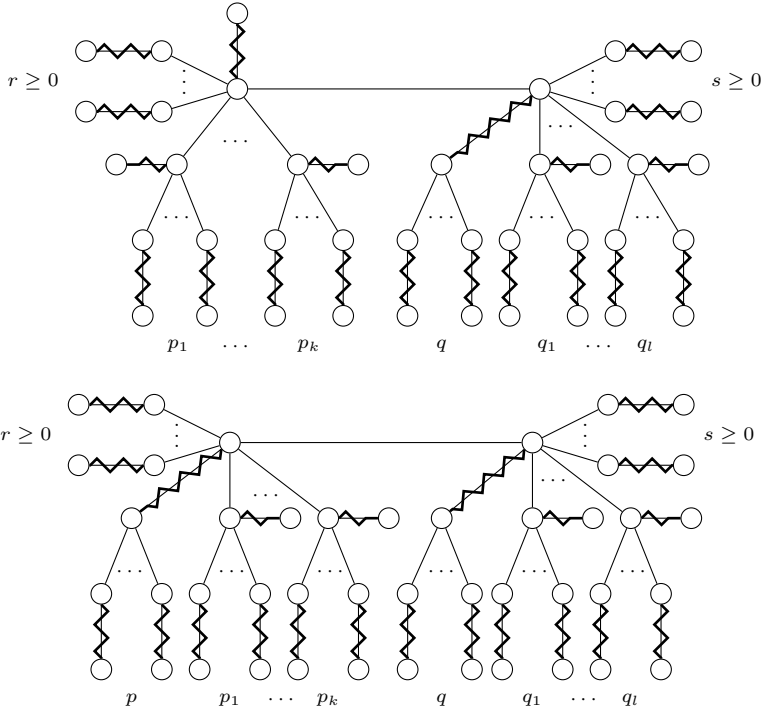


Fig. 15. PM-trees with diameter 7: type III (top) and type IV (bottom).

the diameter of the tree, whereas k must necessarily be positive. The number 2 in both degrees represents the central and matched edges at each central vertex.

Finally, each vertex $u_i \neq v$ adjacent to u with $\deg(u_i) > 2$ has $p_i \geq 1$ neighbors with degree 2, for $1 \leq i \leq k$. Also the vertex v_0 matched to v has $q \geq 1$ neighbors with degree 2 and if $l \geq 1$ then each vertex $v_i \neq u$ adjacent to v with $\deg(v_i) > 2$ has $q_i \geq 1$ neighbors with degree 2, for $1 \leq i \leq l$.

We now turn to case (c), when we must remove the pendant edges at u, v, u_0, v_0 since they cannot be matched anymore and we match the remaining pendant edges. We call this a *type IV* PM-tree with diameter 7 and it is represented in Fig. 15 (bottom).

Here we say that the PM-tree in case (c) and non-matched central edge uv has u with $\deg(u) = r + k + 2$, where $r \geq 0$ is the number of quasi-pendant vertices with degree 2 and $k \geq 0$ is the number of vertices with degree greater than 2 and v with $\deg(v) = s + l + 2$, where s and l are analogous to r and k , respectively. The number 2 in both degrees represents the central and matched edges at each central vertex.

Moreover, the vertex u_0 matched to u has $p \geq 1$ neighbors with degree 2 and if $k \geq 1$ then each vertex $u_i \neq v$ adjacent to u with $\deg(u_i) > 2$ has $p_i \geq 1$ neighbors with degree 2, for $1 \leq i \leq k$. Also the vertex v_0 matched to v has $q \geq 1$ neighbors with degree 2 and if $l \geq 1$ then each vertex $v_i \neq u$ adjacent to v with $\deg(v_i) > 2$ has $q_i \geq 1$ neighbors with degree 2, for $1 \leq i \leq l$. We observe that k and l can be zero because the quantities r and s do not affect the diameter, so they can be zero as well.

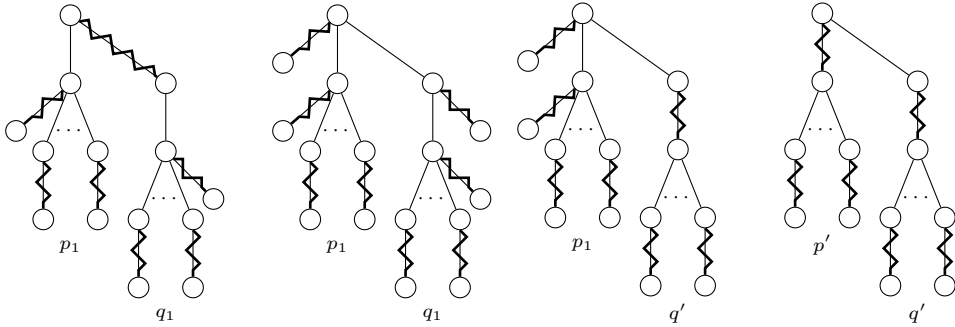


Fig. 16. The four PM-trees of Lemma 8.1, respectively.

The next result reduces the above four types of PM-trees with diameter 7 to just those with exactly two eigenvalues less than -1, thus limiting further our analysis. All the notations used in the proof agree with the ones defined in this section regarding the parameters k, l, r, s, p, q in each case.

Lemma 8.1. *The only PM-trees with $d = 7$ and two eigenvalues smaller than -1 are:*

- (i) *the type I tree with $r, s = 0$ and $k, l = 1$;*
- (ii) *the type II tree with $r, s = 0$ and $k, l = 1$;*
- (iii) *the type III tree with $r, s, l = 0$ and $k = 1$;*
- (iv) *the type IV tree with $r, s, k, l = 0$.*

Proof. We prove case (ii). The other cases are similar. Let T be a type II PM-tree with $d = 7$ and non-matched central edge uv connecting the central vertices u and v , where $\deg(u) = r + k + 2$ and $\deg(v) = s + l + 2$, as depicted in Fig. 14 (bottom). As previously stated, we must have $k, l \geq 1$ to guarantee the diameter, but $r, s \geq 0$.

When applying Lemma 4.3 to T , we begin by identifying V' , i.e., the set of non-pendant vertices adjacent to quasi-pendant vertices of degree 2. At first, since $k, l \geq 1$, we have $|V'| \geq k + l \geq 2$. Additionally, the central vertex $u \in V'$ ($v \in V'$) if and only if $r > 0$ ($s > 0$), but then $|V'| > 2$. By Lemma 4.4, since any cospectral mate with the double sun has also two eigenvalues less than -1, we must have $r = s = 0$ and $k = l = 1$, so that *at least* two eigenvalues are less than -1.

On the other hand, applying Diagonalize to T with $\alpha = 1$ together with Theorem 2.3, we conclude that T has *exactly* two eigenvalues less than -1, as desired. \square

The four types of PM-trees with $d = 7$ that remain to be analyzed are illustrated in Fig. 16.

We now prove that none of the trees of cases (i), (ii) and (iii) are cospectral with the double sun. For this it is sufficient to compute the multiplicity of the eigenvalues ± 1 .

Proposition 8.2. *The double sun has no cospectral mates among type I, type II and type III trees with diameter 7.*

Proof. We recall that the (p, q) -double sun has $n = 2(p + q + 1)$ vertices and the multiplicity of the eigenvalues ± 1 is $p + q - 2 = \frac{n}{2} - 3$. When we apply Algorithm 1 in the cases below, we always root the tree at one of its central vertices. We refer to the trees in cases (i), (ii) and (iii) of Lemma 8.1 as $T_{7(i)}$, $T_{7(ii)}$ and $T_{7(iii)}$, respectively.

First we look at $T_{7(i)}$ with $n = 2(p_1 + q_1 + 3)$ vertices. Applying Algorithm 1 with $\alpha = 1$ followed by Theorem 2.3, we conclude that $T_{7(i)}$ has the eigenvalue -1 with multiplicity $p_1 + q_1 - 1 = \frac{n}{2} - 4$. So $T_{7(i)}$ is not cospectral with the double sun.

Similarly, $T_{7(ii)}$ with $n = 2(p_1 + q_1 + 4)$ vertices. Applying Algorithm 1 with $\alpha = 1$ we find that $T_{7(ii)}$ has the eigenvalue -1 with multiplicity $p_1 + q_1 - 2 = \frac{n}{2} - 6$, by Theorem 2.3. Thus $T_{7(ii)}$ cannot be cospectral with the double sun.

Finally for $T_{7(iii)}$ with $n = 2(p_1 + q' + 3)$ vertices. Applying Algorithm 1 with $\alpha = 1$ together with Theorem 2.3, we determine that $T_{7(iii)}$ has the eigenvalue -1 with multiplicity $p_1 + q' - 2 = \frac{n}{2} - 5$ and thus $T_{7(iii)}$ is also not cospectral with the double sun. \square

For the type IV trees in case (iv) such a method does not work. In fact, we find pairs of cospectral mates among trees of type IV and the (p, q) -double sun. The next result characterizes exactly the parameters (p, q) for which there is a type IV tree cospectral with the double sun.

Proposition 8.3. *Let $3 \leq p \leq q$ be integers and let G be the (p, q) -double sun with $n = 2p + 2q + 2$ vertices. Then G has a type IV tree cospectral mate if and only if*

$$\frac{1}{4}(n - 4 + 2\sqrt{(p - q)^2 + n - 5})$$

is a natural number.

Proof. Here we are with case (iv) of Lemma 8.1, so let $T_{7(iv)}$ be that tree with $n = 2(p' + q' + 2)$ vertices and central edge uv . The method we are using so far does not help us because we find a multiplicity $p' + q' - 1 = \frac{n}{2} - 3$ for its eigenvalue -1 , i.e., it has the same number of eigenvalues -1 (and 1) as the double sun and so we need to compute its characteristic polynomial to see more deeply what its other eigenvalues are.

We point out that $T_{7(iv)}$ has a similar structure as the double sun; both have two stars connected by their centers with a path, making the application of the algorithm somewhat alike. Indeed, when applying Algorithm 1 to $T_{7(iv)}$ rooted at the central vertex u we initialize all the vertices with $-\lambda$ and we obtain $\det(A(T_{7(iv)}) - \lambda I)$. The characteristic polynomial of $T_{7(iv)}$ is given by

$$\begin{aligned} \phi_{T_{7(iv)}}(\lambda) &= (-1)^n \det(A(T_{7(iv)}) - \lambda I) \\ &= (\lambda^2 - 1)^{p'+q'-1} [\lambda^6 - (p' + q' + 4)\lambda^4 + (p'q' + 2p' + 2q' + 4)\lambda^2 - 1]. \end{aligned}$$

Now we look at the remaining polynomial of degree 6 of both the (p, q) -double sun and $T_{7(iv)}$. As $T_{7(iv)}$ and the (p, q) -double sun have the same order n , we have $p' + q' + 1 = p + q$. This implies that the coefficients of λ^4 of the polynomials of both trees are equal. Therefore, $T_{7(iv)}$ and the (p, q) -double sun have the same spectrum if and only if their coefficients of λ^2 coincide, that is, if and only if

$$pq + p + q + 3 = p'q' + 2p' + 2q' + 4. \tag{1}$$

Using the fact that $q' = \frac{n-4-2p'}{2}$ and replacing it into (1) we obtain the following quadratic equation

$$(p')^2 + \left(\frac{4-n}{2}\right)p' + \left(\frac{2pq-n+4}{2}\right) = 0, \tag{2}$$

whose solutions are

$$\frac{1}{4}(n-4 \pm 2\sqrt{(p-q)^2 + n-5}).$$

We notice that, if $p' = \frac{1}{4}(n-4+2\sqrt{(p-q)^2 + n-5})$ is a natural number then $q' = \frac{1}{4}(n-4-2\sqrt{(p-q)^2 + n-5})$ is also natural. Similarly if $p' = \frac{1}{4}(n-4-2\sqrt{(p-q)^2 + n-5})$ is natural, then $q' = \frac{1}{4}(n-4+2\sqrt{(p-q)^2 + n-5})$. Hence, the natural solution $\{p', q'\}$ for (1) gives a cospectral mate $T_{7(iv)}$ of the (p, q) -double sun. Additionally, if (2) does not have a natural solution then the (p, q) -double sun doesn't have a type IV tree as cospectral mate. \square

For instance, following the proof of Proposition 8.3, we find that the $(21, 28)$ -double sun of order $n = 100$ has the same spectrum as the tree $T_{7(iv)}$ with $p' = 18$ and $q' = 30$. Meanwhile, the (p, q) -double sun of order $102 = 2q + 2p + 2$ is DS among connected graphs.

9. Conclusion

We were able to prove that the p -sun is determined by its spectrum among connected graphs and to establish when the (p, q) -double sun is determined by its spectrum among connected graphs and, otherwise, we determine its cospectral mates, thus showing examples of trees which do not fall into Schwenk's theorem that almost every tree has a cospectral mate.

The method used in both cases was mainly supported by the few distinct eigenvalues of their spectra, implying that any cospectral mate should have a not so large maximum diameter, and by considering their nullity and properties involved, therefore not being forced to check every single tree with a fixed diameter, for there are several such trees.

After putting together some results based on Algorithm 1 that shows us the amount of eigenvalues in a given interval, we looked at the few remaining cases of possible cospectral mates and prove the above results.

It is still an open problem to include the disconnected graphs on the analysis, that is, to prove whether or not the p -sun is determined by its spectra and to further characterize the (p, q) -double sun, now among all graphs.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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