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Research Paper

The Number of 1-Nearly Independent Edge Subsets

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Abstract

Let $G = (V(G), E(G))$ be a graph with the set of vertices $V(G)$ and the set of edges $E(G)$. A subset S of $E(G)$ is called a k-nearly independent edge subset if there are exactly k pairs of elements of S that share a common end. $Z_k(G)$ is the number of such subsets. This paper studies Z_1. Various properties of Z_1 are discussed. We characterize the two n-vertex trees with the smallest Z_1, as well as the one with the largest value. A conjecture on the n-vertex tree with the second-largest Z_1 is proposed.

1 Introduction

A *simple* and *undirected graph* G is an ordered pair of sets $G = (V(G), E(G))$, where $V(G)$ is a set of objects called *vertices*, and $E(G)$ is a (possibly empty) set of unordered pairs of elements of $V(G)$ called *edges*. The *order* and *size* of G are $|V(G)|$ and $|E(G)|$, respectively. For simplicity, we write $|G|$ instead of $|V(G)|$. For graph theory notation and terminology, we generally follow [1].

An *independent edge subset* of a graph $G = (V(G), E(G))$ is a subset I of $V(G)$ with the property that if e_1 and e_2 are two edges in I, then e_1 and e_2 are not adjacent in G; that is, e_1 and e_2 do not share a common end in G. Similarly, as already defined in [2], $\sigma_1(G)$ counts the number of independent subsets S of $V(G)$ such that the subgraph induced by S in G contains only one edge. The number of independent edge subsets of a graph has been extensively studied in the literature. See the survey [3], where it is called the *Hosoya index*. The name Hosoya comes from the Japanese chemist, Haruo Hosoya [4] who was the first person to introduce this index in 1971. He showed that there is a correlation between the boiling points of paraffins (saturated hydrocarbons) and the Hosoya index.

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In a series of papers [5–10], the application of the Hosoya index was revealed in showing the structure-dependence of the total π-electron energy of chemical molecules. This boosted the interest of many mathematicians to study the number of independent edge subsets. Established results include classes of graphs that contain elements that are not molecular graphs. In [11], the family of trees with a given degree sequence is studied, and the element which has the minimum number of independent edge subsets is fully characterized. The result implies as corollaries characterizations of trees with the smallest number of independent edge subsets in various other classes like trees with a fixed order, or with fixed order and given maximum degree.

This paper proposes a generalisation of the number of independent edge subsets. For an integer $k \geq 1$, we define a *k-nearly independent edge subset* of a graph G with vertex set $V(G)$ and edge set $E(G)$ as a subset I of $E(G)$ that contains exactly k pairs of adjacent edges. Denote by $Z_k(G)$ the number of k-nearly independent edge subsets of G. $Z_0(G)$ is the number of independent edge subsets of G. The main focus of this paper is to study Z_1. For the classes of graphs we investigated, the behavior of Z_1 seems to have a lot in common with that of Z_0. Among all trees of order n, the star $K_{1,n-1}$ minimises both Z_0 and Z_1, while the path P_n maximises both Z_0 and Z_1. In [2] similar comparison made between σ_1 and the usual number of independent vertex subsets shows a considerable difference.

The rest of the paper is structured as follows. Section 2 is a preliminary, where we present basic useful facts about Z_1. There, we discuss the effect of adding or removing an edge, we provide recursive formulas for Z_1 as well as an explicit formula for Z_1 of paths. These are used in Section 3 to characterize the two trees with order n and smallest Z_1. In Section 4, we proved that the path P_n is the forest of order n that has the largest Z_1. A conjecture on the forest with the second-largest Z_1 is also provided there.

2 Preliminary

This section consists of a few technical tools that will be needed in other sections. Since we are introducing Z_1, we also include some properties that we do not use much, but we expect to be useful for further studies of Z_1.

Let G be a graph with vertex set $V(G)$, edge set $E(G)$, order $n = |V(G)|$ and size $m = |E(G)|$. We denote the degree of a vertex v in G by $\deg_G(v)$. For a subset S of vertices of a graph G, we denote by $G - S$ the graph obtained from G by deleting the vertices in S and all edges incident to them. If $S = \{v\}$, then we simply write $G - v$ rather than $G - \{v\}$.

For positive integers r and s, we denote by $K_{r,s}$ the complete bipartite graph with partite sets X and Y such that $|X| = r$ and $|Y| = s$. A complete bipartite graph $K_{1,n-1}$ is also called a *star*. We use the typical notations P_n, C_n, and K_n for the path of order n, the cycle of order n and the complete graph of order n, respectively.

2.1 Effect of an edge or vertex removal or addition

Suppose that u and v are non-adjacent vertices in a graph G. If $H = G + uv$ is the graph obtained from G by adding the edge uv, then $Z_1(H) \geq Z_1(G)$. Adding the edge uv does not affect the adjacency of the already existing edges. The inequality is strict if and only if $G-u-v$ contains a P_3 or at least one of u and v is not isolated. These are the only situations where the newly added edge is contained in at least one new set of 1-nearly independent edges. For small graphs like $2K_1$ (two vertices with no edge), it is possible that the newly added edge is not contained in a 1-nearly independent edge subset. In this case Z_1 will not increase. It follows from this that for any graph G with n vertices, we have:

$$Z_1(G) \leq Z_1(K_n),$$

with equality occur only if the two compared graphs are the same or $n < 3$. The edgeless graph has the smallest Z_1 which is 0.

An isolated vertex does not affect the value of Z_1. If $\deg_G(v) = 0$, then $Z_1(G) = Z_1(G-v)$. If $\deg_G(v) \geq 2$, then $Z_1(G) > Z_1(G-v)$. In this case, at least one possibility of a P_3 subtree of G is lost and hence at least one 1-nearly independent edge subsets. We still have $Z_1(G) > Z_1(G-v)$ if we remove a vertex v of degree 1 that is attached to a vertex of degree at least 2, as we then lose at least one P_3 containing v. If v is contained in P_2 component of G, then $Z_1(G) \geq Z_1(G-v)$, with strict inequality if $G - N_G[v]$ contains a P_3.

2.2 Relation between σ_1 and Z_1

The line graph $L(G)$ of G is the graph with the set of vertices $E(G)$, and such that two different elements e and e' of $E(G)$ are adjacent in $L(G)$ if they have a common end in G. We state, without proof, the following straightforward lemma.

Lemma 2.1. *For any graph G, we have $Z_1(G) = \sigma_1(L(G))$.*

2.3 Explicit formulas for Z_1 of some graphs

It is convenient to set $Z_1(P_t) = 0$ whenever $t \leq 2$ and $Z_0(P_t) = 1$ whenever $t \leq 1$. Let $\alpha = \frac{1+\sqrt{5}}{2}$ and $\beta = \frac{1-\sqrt{5}}{2}$. Then, we have $\alpha + \beta = 1$, $\alpha - \beta = \sqrt{5}$, $\alpha \cdot \beta = -1$. The following formulas are well known, see for example [12] and [3].

Theorem 2.2 (cf. [12])**.** *For $n \in \mathbb{N}$, we have:*

$$Z_0(P_n) = \frac{1}{\sqrt{5}} \left(\alpha^{n+1} - \beta^{n+1}\right). \tag{1}$$

Theorem 2.3 (cf. [3])**.** *If $G_1, G_2, \ldots, G_r$ are the connected components of a graph G, then*

$$Z_0(G) = Z_0\left(\bigcup_{i=1}^{r} G_i\right) = \prod_{i=1}^{r} Z_0(G_i). \tag{2}$$

The following results have been recently established [2].

$$\sigma_1(P_n) = \frac{1}{5}\left[(n-1)\left(\alpha^n + \beta^n\right) + \frac{2}{\sqrt{5}}\left(\alpha^{n-1} - \beta^{n-1}\right)\right],$$

and

$$\sigma_1(C_n) = \frac{n}{\sqrt{5}}\left(\alpha^{n-2} - \beta^{n-2}\right).$$

Thanks to Lemma 2.1, we also have:

$$Z_1(P_n) = \sigma_1(L(P_n)) = \sigma_1(P_{n-1}) = \frac{1}{5}\left[(n-2)\left(\alpha^{n-1} + \beta^{n-1}\right) + \frac{2}{\sqrt{5}}\left(\alpha^{n-2} - \beta^{n-2}\right)\right],$$

and

$$Z_1(C_n) = \sigma_1(L(C_n)) = \sigma_1(C_n) = \frac{n}{\sqrt{5}}\left(\alpha^{n-2} - \beta^{n-2}\right).$$

2.4 Recursive formula

We denote by $\mathbb{P}_G(v)$ the set of P_3 subtrees in G that contain the vertex v. If there is no risk of confusion, we simply use $\mathbb{P}(v)$.

Lemma 2.4. *For any vertex z in a graph G, we have*

$$Z_1(G) = Z_1(G-z) + \sum_{v \in N_G(z)} Z_1(G-z-v) + \sum_{P \in \mathbb{P}_G(z)} Z_0(G-P). \tag{3}$$

Proof. $Z_1(G-z)$ counts all the 1-nearly independent edge subsets that do not contain z. $\sum_{v \in N_G(z)} Z_1(G-z-v)$ counts all those that contain z in a P_2. $\sum_{P \in \mathbb{P}_G(z)} Z_0(G-P)$ counts those that contain z in a P_3. ■

A *pseudo-leaf* of a forest T is a vertex that is not isolated and has at most one neighbour that is not a leaf (a vertex of degree 1). We often use (3) for z being a leaf attached to a pseudo leaf v with degree d and neighbour u of largest degree, so that it becomes

$$Z_1(G) = Z_1(G-z) + Z_1(G-z-v) + Z_0(G-N_G(v)) + (d-2)Z_0(G-(N_G[v] \setminus \{u\}).$$

3 Trees of order n with small Z_1

This section characterizes the two trees of order $n \geq 9$ that have the smallest Z_1. First, we show that the n-vertex tree with smallest Z_1 is only the star if $n \geq 9$.

Theorem 3.1. *Among all connected graphs, in particular trees, T of order $n \geq 9$ we have $Z_1(T) \geq Z_1(K_{1,n-1})$, with equality if and only if T is $K_{1,n-1}$.*

Proof. As discussed in Subsection 2.1, Removing an edge from a connected graph of order $n \geq 9$ decreases Z_1. Hence, we can restrict this proof to the case where T is a tree.

The basis cases corresponding to $n = 9$ and 10 can be seen in Section 5. Suppose that the claim holds for $n = k$, for some $k \geq 10$. Now consider the case of $n = k+1$. Let v be a pseudo-leaf of degree d in T, z a leaf neighbour of v and u a neighbor of v with the largest degree that might possibly be not a leaf. If $d = n-1$, then $T \cong K_{1,n-1}$. So, we may assume that $d \leq n-2$. Thus, we have:

$$\begin{aligned}
Z_1(T) &= Z_1(T-z) + Z_1(T-v-z) + Z_0(T-z-v-u) + (d-2)Z_0(T-N[v] \setminus \{u\}) \\
&= Z_1(T-z) + Z_1(T-N[v] \setminus \{u\}) + Z_0(T-N[v]) + (d-2)Z_0(T-N[v] \setminus \{u\}) \\
&\geq Z_1(K_{1,(n-1)-1}) + Z_1(K_{1,(n-d-1)}) + Z_0(K_{1,n-(d+1)-1}) + (d-2)Z_0(K_{1,(n-d-1)}) \\
&= \frac{(n-2)(n-3)}{2} + \frac{(n-d-1)(n-d-2)}{2} + n-(d+1)-1+1 \\
&\quad + (d-2)(n-d-1+1) \\
&= -\frac{d^2}{2} + n^2 + \frac{5d}{2} - 5n + 3.
\end{aligned}$$

Hence,

$$\begin{aligned}
Z_1(T) - Z_1(K_{1,n-1}) &\geq -\frac{d^2}{2} + n^2 + \frac{5d}{2} - 5n + 3 - \frac{(n-1)(n-2)}{2} \\
&= -\frac{d^2}{2} + \frac{n^2}{2} + \frac{5d}{2} - \frac{7n}{2} + 2 \\
&= \frac{n^2}{2} - \frac{7n}{2} + 2 - \left(\frac{d^2}{2} - \frac{5d}{2}\right).
\end{aligned}$$

However,

$$\frac{d^2}{2} - \frac{5d}{2} \leq \frac{(n-2)^2}{2} - \frac{5(n-2)}{2} = \frac{n^2}{2} - \frac{9n}{2} + 7.$$

Thus,

$$\begin{aligned} Z_1(T) - Z_1(K_{1,n-1}) &\geq \frac{n^2}{2} - \frac{7n}{2} + 2 - \left(\frac{d^2}{2} - \frac{5d}{2}\right) \\ &\geq \frac{n^2}{2} - \frac{7n}{2} + 2 - \left(\frac{n^2}{2} - \frac{9n}{2} + 7\right) = n - 5 > 0, \qquad \text{since } n > 5, \end{aligned}$$

this compeletes the proof. ■

We use similar techniques to find the tree with second-minimum Z_1. Let B_n^k be the tree of order n obtained from a path, P_k, of order k by adding $n-k$ new vertices and then joining them to exactly one end-vertex of P_k. Such a tree is usually called a broom. B_n^3 is the only n-vertex tree with degree sequence $(n-2, 2, 1, \ldots, 1)$.

Theorem 3.2. *Among all trees $T \neq K_{1,n-1}$ of order $n \geq 9$ we have $Z_1(T) \geq Z_1(B_n^3)$, with equality if and only if T is B_n^3.*

Proof. Note that

$$\begin{aligned} Z_1(B_n^3) &= Z_1(K_{1,n-2}) + Z_1(K_{1,n-3}) + 1 \\ &= \frac{(n-2)(n-3) + (n-3)(n-4) + 2}{2} = (n-3)^2 + 1. \end{aligned}$$

The basis cases corresponding to $n = 9$ and 10 can be seen in Section 5. Suppose that the claim holds for $n = k$, for some $k \geq 10$. Now consider the case of $n = k+1$. Let v be a pseudo-leaf of degree d in T, z a leaf neighbour of v and u a neighbor of v with largest degree that might possibly be not a leaf. If $T - z$ is a star, then T is B_n^3, and there would be nothing left to prove. Hence, we can assume that $T - z$ is not a star. Since $T \neq K_{1,n-1}$, we must have $n \geq d+2$. For $n = d+2$ the graph T is isomorphic to B_n^3. So, we can consider $n \geq d+3$. Thus, we have:

$$\begin{aligned} Z_1(T) =& Z_1(T-z) + Z_1(T-v-z) + Z_0(T-z-v-u) + (d-2)Z_0(T - N[v] \setminus \{u\}) \\ =& Z_1(T-z) + Z_1(T - N[v] \setminus \{u\}) + Z_0(T - N[v]) + (d-2)Z_0(T - N[v] \setminus \{u\}) \\ \geq& Z_1(B_{n-1}^3) + Z_1(K_{1,(n-d-1)}) + Z_0(K_{1,n-(d+1)-1}) + (d-2)Z_0(K_{1,(n-d-1)}) \\ =& (n-3-1)^2 + 1 + \frac{(n-d-1)(n-d-2)}{2} + n - (d+1) - 1 + 1 \\ &+ (d-2)(n-d-1+1) \\ =& -\frac{d^2}{2} + \frac{3n^2}{2} + \frac{5d}{2} - \frac{21n}{2} + 17. \end{aligned}$$

Hence,

$$\begin{aligned} Z_1(T) - Z_1(B_n^3) &\geq -\frac{d^2}{2} + \frac{3n^2}{2} + \frac{5d}{2} - \frac{21n}{2} + 17 - (n-3)^2 - 1 \\ &= \frac{n^2}{2} - \frac{9n}{2} + 7 - \left(\frac{d^2}{2} - \frac{5d}{2}\right). \end{aligned}$$

However,

$$\frac{d^2}{2} - \frac{5d}{2} \leq \frac{(n-3)^2}{2} - \frac{5(n-3)}{2} = \frac{n^2}{2} - \frac{11n}{2} + 12.$$

Thus,

$$\begin{aligned} Z_1(T) - Z_1(B_n^3) &\geq \frac{n^2}{2} - \frac{9n}{2} + 7 - \left(\frac{d^2}{2} - \frac{5d}{2}\right) \\ &\geq \frac{n^2}{2} - \frac{9n}{2} + 7 - \left(\frac{n^2}{2} - \frac{11n}{2} + 12\right) \\ &= n - 5 > 0, \qquad \text{since } n > 5, \end{aligned}$$

this completes the proof. ∎

4 Forest with maximum Z_1

In this section we show that P_n is the tree of order $n \geq 9$ that has the largest Z_1. We also attempted to determine the one that has the second-largest Z_1. We only managed to prove that it has to be a tripod (a tree with only three leaves). Based on a computational check for small values of n, a conjecture describing the full characterization is provided.

We start with a few technical lemmas.

Lemma 4.1. *Let n be an integer.*

i) If $n \geq 0$, we have $Z_0(P_n) \geq n$.

ii) If $n \geq 4$, we have $Z_0(P_n) \geq n + 1$.

iii) If $n \geq 3$, we have $Z_1(P_n) \geq n - 2$.

Proof. For $n = 0, 1, 2$, we have $Z_0(P_0) = 1 \geq 0$, $Z_0(P_1) = 1 \geq 1$ and $Z_0(P_2) = 2 \geq 2$. Suppose that i) holds for $n = k \geq 2$, then for $n = k + 1 \geq 3$ we have:

$$Z_0(P_n) = Z_0(P_{k+1}) = Z_0(P_k) + Z_0(P_{k-1}) \geq k + k - 1 \geq k + 1,$$

since $k \geq 2$, thereby proving i). For $n = 4, 5$, we have $Z_0(P_4) = 5 \geq 4+1$ and $Z_0(P_5) = 7 \geq 5+1$. If $Z_0(P_n) \geq n + 1$ for all $4 \leq n \leq k$ for some $k \geq 5$, then

$$Z_0(P_{k+1}) = Z_0(P_k) + Z_0(P_{k-1}) \geq k + 1 + k - 1 + 1 \geq (k + 1) + 1.$$

This proves ii). The proof of iii), namely $Z_1(P_n) \geq n - 2$ follows from the fact that P_n has at least $n - 2$ copies of P_3. ∎

Lemma 4.2. *For any integers n and d with $n \geq d + 1$ and $d \geq 5$, we have:*

$$(d-1)Z_0(P_{n-d}) + Z_1(P_{n-d}) \leq Z_0(P_{n-3}) + Z_1(P_{n-2}).$$

Proof. We proceed by induction on n. For $n = d + 1 \geq 4$, using Lemma 4.1 we have

$$(d-1)Z_0(P_1) + Z_1(P_1) = d - 1 \leq d + 1 - 3 + 1 \leq Z_0(P_{d+1-3}) + Z_1(P_{d+1-2}),$$

for $d \geq 5$. For $n = d + 2 \geq 5$, using Lemma 4.1 we have:

$$(d-1)Z_0(P_2) + Z_1(P_2) = 2(d-1) \leq d - 1 + 1 + d - 2 \leq Z_0(P_{d+2-3}) + Z_1(P_{d+2-2}),$$

for $d \geq 5$. Suppose that the claim holds for $n = k \geq d + 2$. Now consider the case of $n = k + 1$. Then we have:

$$\begin{aligned}
&Z_0(P_{n-3}) + Z_1(P_{n-2}) \\
&= Z_0(P_{n-4}) + Z_0(P_{n-5}) + Z_1(P_{n-3}) + Z_1(P_{n-4}) + Z_0(P_{n-5}) \\
&= Z_0(P_{(n-1)-3}) + Z_0(P_{(n-2)-3}) + Z_1(P_{(n-1)-2}) + Z_1(P_{(n-2)-2}) + Z_0(P_{n-5}) \\
&\geq (d-1)Z_0(P_{n-1-d}) + Z_1(P_{n-1-d}) + (d-1)Z_0(P_{n-2-d}) + Z_1(P_{n-2-d}) + Z_0(P_{n-3-d}) \\
&= (d-1)Z_0(P_{n-d}) + Z_0(P_{n-d}),
\end{aligned}$$

as required. ■

Lemma 4.3. *For any integer $n \geq 7$, we have:*

$$Z_1(P_{n-3}) + Z_0(P_{n-4}) + Z_0(P_{n-3}) \leq Z_1(P_{n-2}) + Z_0(P_{n-3}).$$

Proof. We proceed by induction on $n \geq 7$. If $n = 7$, we have:

$$Z_1(P_4) + Z_0(P_3) + Z_0(P_4) = 2 + 3 + 5 \leq 5 + 5 = Z_1(P_5) + Z_0(P_4).$$

If $n = 8$, we have:

$$Z_1(P_5) + Z_0(P_4) + Z_0(P_5) = 5 + 5 + 7 \leq 10 + 7 = Z_1(P_6) + Z_0(P_5).$$

For the induction assumption, suppose that the inequality holds for $n = k \geq 8$. Suppose now that $n = k + 1$. Then we have

$$\begin{aligned}
&Z_1(P_{n-3}) + Z_0(P_{n-4}) + Z_0(P_{n-3}) \\
&= Z_1(P_{n-4}) + Z_1(P_{n-5}) + Z_0(P_{n-6}) + Z_0(P_{n-5}) + Z_0(P_{n-6}) + Z_0(P_{n-4}) + Z_0(P_{n-5}) \\
&= Z_1(P_{n-4}) + Z_0(P_{n-5}) + Z_0(P_{n-4}) + Z_1(P_{n-5}) + Z_0(P_{n-6}) + Z_0(P_{n-5}) + Z_0(P_{n-6}) \\
&= Z_1(P_{(n-1)-3}) + Z_0(P_{(n-1)-4}) + Z_0(P_{(n-1)-3}) + \\
&\qquad + Z_1(P_{(n-2)-3}) + Z_0(P_{(n-2)-4}) + Z_0(P_{(n-2)-3}) + Z_0(P_{n-6}) \\
&\leq Z_1(P_{(n-1)-2}) + Z_0(P_{(n-1)-3}) + Z_1(P_{(n-2)-2}) + Z_0(P_{(n-2)-3}) + Z_0(P_{(n-2)-3}) \\
&= Z_1(P_{n-2}) + Z_0(P_{n-3}).
\end{aligned}$$

as required. ■

Lemma 4.4. *For any integer $n \geq 7$, we have:*

$$Z_1(P_{n-4}) + Z_0(P_{n-5}) + 2Z_0(P_{n-4}) \leq Z_1(P_{n-2}) + Z_0(P_{n-3}).$$

Proof. We proceed by induction on $n \geq 7$. For $n = 7$, we have

$$Z_1(P_3) + Z_0(P_2) + 2Z_0(P_3) = 1 + 2 + 2 \times 3 \leq 5 + 5 = Z_1(P_5) + Z_0(P_4).$$

For $n = 8$, we have:

$$Z_1(P_4) + Z_0(P_3) + 2Z_0(P_4) = 2 + 3 + 2 \times 5 \leq 10 + 7 = Z_1(P_6) + Z_0(P_5).$$

For the induction assumption, suppose that the inequality holds for $n = k \geq 8$. Suppose now that $n = k + 1$. Then we have:

$$\begin{aligned}
&Z_1(P_{n-4}) + Z_0(P_{n-5}) + 2Z_0(P_{n-4}) \\
&= Z_1(P_{n-5}) + Z_1(P_{n-6}) + Z_0(n-7) + Z_0(P_{n-6}) + Z_0(P_{n-7}) + 2Z_0(P_{n-5}) + 2Z_0(P_{n-6}) \\
&= Z_1(P_{n-5}) + Z_0(P_{n-6}) + 2Z_0(P_{n-5}) + Z_1(P_{n-6}) + Z_0(P_{n-7}) + 2Z_0(P_{n-6}) + Z_0(P_{n-7}) \\
&= Z_1(P_{(n-1)-4}) + Z_0(P_{(n-1)-5}) + 2Z_0(P_{(n-1)-4}) \\
&\qquad + Z_1(P_{(n-2)-4}) + Z_0(P_{(n-2)-5}) + 2Z_0(P_{(n-2)-4}) + Z_0(P_{(n-3)-4}) \\
&\leq Z_1(P_{(n-1)-2}) + Z_0(P_{(n-1)-3}) + Z_1(P_{(n-2)-2}) + Z_0(P_{(n-2)-3}) \\
&= Z_1(P_{n-2}) + Z_0(P_{n-3}),
\end{aligned}$$

as required. ■

Since adding an edge can only increase Z_1 or keep it unchanged, for any forest F, there is a tree T of the same order such that $Z_1(T) \geq Z_1(F)$. The following lemma is well-known.

Lemma 4.5 ([13])**.** *For any forest F with order n we have $Z_0(F) \leq Z_0(P_n)$.*

We are now ready to present a proof of a characterization of the forest of order $n \geq 9$ that has the largest Z_1.

Theorem 4.6. *Among all forests F of order $n \geq 9$, we have $Z_1(F) \leq Z_1(P_n)$, with equality if and only if F is P_n.*

Proof. We use an induction on n. The base cases of $n = 9, 10$ can be seen on the Section 5. Suppose that the claim holds for $n = k \geq 10$. We now consider the case of $n = k + 1$. Suppose that v is a pseudo-leaf of F of degree d. Let u be a neighbor of v having the largest degree. If v has a neighbour that is not a leaf, then it is u. Let z be a leaf neighbour of v.

Case 1: Suppose that $d = 2$. With the use of Lemma 4.5, we have:

$$\begin{aligned}
Z_1(F) &= Z_1(F - z) + Z_1(F - z - v) + Z_0(F - v - u - z) \\
&\leq Z_1(P_{n-1}) + Z_1(P_{n-2}) + Z_0(P_{n-3}) = Z_1(P_n).
\end{aligned}$$

Case 2: Suppose that $d = 3$. Let x be the leaf adjacent to v other than z. Then, using Lemma 4.3, we have:

$$\begin{aligned}
Z_1(F) &= Z_1(F - z) + Z_1(F - z - v) + Z_0(F - v - u - z) + Z_0(F - v - x - z) \\
&= Z_1(F - z) + Z_1(F - z - v - x) + Z_0(F - v - u - z - x) + Z_0(F - v - x - z) \\
&\leq Z_1(P_{n-1}) + Z_1(P_{n-3}) + Z_0(P_{n-4}) + Z_0(P_{n-3}) \\
&\leq Z_1(P_{n-1}) + Z_1(P_{n-2}) + Z_0(P_{n-3}) = Z_1(P_n).
\end{aligned}$$

Case 3: Suppose that $d = 4$. Let x and y be the two leaves adjacent to v other than z. Then, using Lemma 4.4, we have:

$$\begin{aligned}
Z_1(F) &= Z_1(F - z) + Z_1(F - z - v) + Z_0(F - v - u - z) \\
&\qquad\qquad + Z_0(F - v - x - z) + Z_0(F - v - y - z) \\
&= Z_1(F - z) + Z_1(F - z - v - x - y) \\
&\qquad\qquad + Z_0(F - v - u - z - x - y) + 2Z_0(F - v - x - z - y) \\
&\leq Z_1(P_{n-1}) + Z_1(P_{n-4}) + Z_0(P_{n-5}) + 2Z_0(P_{n-4}) \\
&\leq Z_1(P_{n-1}) + Z_1(P_{n-2}) + Z_0(P_{n-3}) = Z_1(P_n).
\end{aligned}$$

Case 4: Suppose that $d \geq 5$. By counting the 1-nearly independent edge subsets without v, with v in a P_2 and then with v in a P_3, we have:

$$\begin{aligned}
&Z_1(F)\\
&= Z_1(F-z) + Z_1(F-(N[v]\setminus\{u\})) + Z_0(F-N[v]) + (d-2)Z_0(F-(N(v)\setminus\{u\}))\\
&\leq Z_1(F-z) + Z_1(F-(N[v]\setminus\{u\})) + (d-1)Z_0(F-(N[v]\setminus\{u\}))\\
&\leq Z_1(P_{n-1}) + Z_1(P_{n-d}) + (d-1)Z_0(P_{n-d})\\
&\leq Z_1(P_{n-1}) + Z_1(P_{n-2}) + Z_0(P_{n-3}) \qquad \text{(using Lemma 4.2)}\\
&= Z_1(P_n),
\end{aligned}$$

this completes the proof. ■

From now, we aim to find out which n-vertex tree has the second-largest Z_1. A series of lemmas is needed. We write $[T_1,\dots,T_j]$ for the rooted tree, where the branches of the root vertex v are the rooted trees $T_1,\dots,T_j$, such that the root of each of $T_1,\dots,T_j$ is adjacent to v. The following lemma is well-known under the name of Ironing Lemma. It means that replacing a non-path branch by a path branch increases Z_0.

Lemma 4.7 ([14])**.** *For any rooted tree $T_1,\dots,T_j$, we have*

$$Z_0([T_1,\dots,T_j]) < Z_0([P_{|T_1|},T_2,\dots,T_j]),$$

if T_1 is not a path rooted at one of its end-vertices.

We now provide an ironing lemma for Z_1. Replacing a branch that is not a path by a path of the same order increases Z_1.

Lemma 4.8. *For any rooted trees $T_1,\dots,T_j$, we have*

$$Z_1([T_1,\dots,T_j]) < Z_1([P_{|T_1|},T_2,\dots,T_j]),$$

if T_1 is not a path rooted at one of its end-vertices.

Proof. We proceed by induction on j. If $j=1$, then $[P_{|T_1|}] = P_{|T_1|+1}$ and the claim holds by Theorem 4.6. Suppose that the claim holds whenever $j=k$ for some $k \geq 1$ and let us consider the case where $j=k+1$. Let v be the root of $T=[T_1,\dots,T_j]$ and v_i is the neighbour of v in T_i for any i. Suppose that T_1 is not a path rooted at one of its end-vertices. Then $|T_1| \geq 3$. In the equation below, we use Lemmas 2.4 and 4.7 and the induction assumption to replace T_1

with $P_{|T_1|}$.

$$
\begin{aligned}
&Z_1(T)\\
&= Z_1(T-v_2) + Z_1((T_2-v_2)\cup(T-T_2-v)) + \sum_{x\in N_{T_2}(v_2)} Z_1(T-v_2-x)\\
&+ \sum_{i\in\{1,3,4,\dots,\ell\}} Z_0(T-v_2-v-v_i) + \sum_{x\in N_{T_2}(v_2)} Z_0(T-x-v_2-v)\\
&+ \sum_{P\in\mathbb{P}_{T_2}(v_2)} Z_0(T-P)\\
&= Z_1([T_1,T_3,T_4,\dots,T_j])Z_0(T_2-v_2) + Z_0([T_1,T_3,T_4,\dots,T_j])Z_1(T_2-v_2)\\
&+ Z_1(T_2-v_2)Z_0(T_1)\prod_{i=3}^{j} Z_0(T_i) + Z_0(T_2-v_2)Z_1(T_1)\prod_{i=3}^{j} Z_0(T_i)\\
&+ Z_0(T_2-v_2)Z_0(T_1)Z_1(\bigcup_{i=3}^{j} T_i) + \sum_{x\in N_{T_2}(v_2)} Z_1(T_2-v_2-x)Z_0([T_1,T_3,T_4,\dots,T_j])\\
&+ Z_0(T_2-v_2-x)Z_1([T_1,T_3,T_4,\dots,T_j])\\
&+ Z_0(T_1-v_1)Z_0(T-T_1-v_2-v) + \sum_{i\in\{3,4,\dots,\ell\}} Z_0(T_1)Z_0(T-T_1-v_2-v-v_i)\\
&+ \sum_{x\in N_{T_2}(v_2)} Z_0(T_1)Z_0(T-T_1-x-v_2-v) + \sum_{P\in\mathbb{P}_{T_2}(v_2)} Z_0(T_2-P)Z_0(T_1)Z_0(T-T_1-T_2)\\
&< Z_1([P_{|T_1|},T_3,T_4,\dots,T_j])Z_0(T_2-v_2) + Z_0([P_{|T_1|},T_3,T_4,\dots,T_j])Z_1(T_2-v_2)\\
&+ Z_1(T_2-v_2)Z_0(P_{|T_1|})\prod_{i=3}^{j} Z_0(T_i) + Z_0(T_2-v_2)Z_1(P_{|T_1|})\prod_{i=3}^{j} Z_0(T_i)\\
&+ Z_0(T_2-v_2)Z_0(P_{|T_1|})Z_1(\bigcup_{i=3}^{j} T_i) + \sum_{x\in N_{T_2}(v_2)} Z_1(T_2-v_2-x)Z_0([P_{|T_1|},T_3,T_4,\dots,T_j])\\
&+ Z_0(T_2-v_2-x)Z_1([P_{|T_1|},T_3,T_4,\dots,T_j]) + Z_0(P_{|T_1-v_1|})Z_0(T-T_1-v_2-v)\\
&+ \sum_{i\in\{3,4,\dots,\ell\}} Z_0(P_{|T_1|})Z_0(T-T_1-v_2-v-v_i) + \sum_{x\in N_{T_2}(v_2)} Z_0(P_{|T_1|})Z_0(T-T_1-x-v_2-v)\\
&+ \sum_{P\in\mathbb{P}_{T_2}(v_2)} Z_0(T_2-P)Z_0(P_{|T_1|})Z_0(T-T_1-T_2) = Z_1([P_{|T_1|},T_2,\dots,T_j]),
\end{aligned}
$$

this compelets the proof. ■

In view of Lemma 4.8, we can restrict to star-like trees when trying to find trees of given number of vertices and second-largest Z_1. A star-like tree is a tree with at most one vertex of degree greater than 2. We write $[P_{n_1},\dots,P_{n_k}]$ for the star-like tree with $n_1+\cdots+n_k+1$ vertices, k branches where the i-th branches have length n_i for all i.

In the following lemma, we replace two path branches with a single path rooted at one of its ends.

Lemma 4.9. *For any positive integers $n_1 \geq \cdots \geq n_j$ and $j \geq 3$, we have:*

$$Z_1([P_{n_1},\dots,P_{n_j}]) < Z_1([P_{n_1+n_2},P_{n_3},\dots,P_{n_j}]).$$

Proof. We use induction on the order $n = n_1 + \cdots + n_j + 1$. If $n = j + 1$, then $[P_{n_1}, \ldots, P_{n_j}]$ is a star and $[P_{n_1+n_2}, P_{n_3}, \ldots, P_{n_j}]$ is not a star. The desired inequality holds by Theorem 3.1.

Suppose that the inequality $Z_1([P_{n_1}, \ldots, P_{n_j}]) < Z_1([P_{n_1+n_2}, P_{n_3}, \ldots, P_{n_j}])$ holds whenever $n = n_1 + \cdots + n_j + 1 = k$ for some $k \geq j + 1$. Now consider the case where $n = k + 1 \geq j + 2$ Then $n_1 \geq 2$. Suppose that $n_1 > 2$. Using Lemma 2.4, we have:

$$Z_1([P_{n_1}, \ldots, P_{n_j}]) = Z_1([P_{n_1-1}, \ldots, P_{n_j}]) + Z_1([P_{n_1-2}, \ldots, P_{n_j}]) + Z_0([P_{n_1-3}, \ldots, P_{n_j}]),$$

and

$$\begin{aligned} Z_1([P_{n_1+n_2}, P_{n_3}, \ldots, P_{n_j}]) = {} & Z_1([P_{n_1+n_2-1}, P_{n_3}, \ldots, P_{n_j}]) + Z_1([P_{n_1+n_2-2}, P_{n_3}, \ldots, P_{n_j}]) \\ & + Z_0([P_{n_1+n_2-3}, P_{n_3}, \ldots, P_{n_j}]). \end{aligned} \tag{4}$$

By Lemma 4.7, we know that

$$Z_0([P_{n_1+n_2-3}, P_{n_3}, \ldots, P_{n_j}]) > Z_0([P_{n_1-3}, P_{n_2-3}, \ldots, P_{n_j}]).$$

By the induction assumption, we know that

$$Z_1([P_{n_1-1}, \ldots, P_{n_j}]) < Z_1([P_{n_1+n_2-1}, P_{n_3}, \ldots, P_{n_j}]),$$

and

$$Z_1([P_{n_1-2}, \ldots, P_{n_j}]) < Z_1([P_{n_1+n_2-2}, P_{n_3}, \ldots, P_{n_j}]).$$

Hence, we have:

$$Z_1([P_{n_1}, \ldots, P_{n_j}]) < Z_1([P_{n_1+n_2}, P_{n_3}, \ldots, P_{n_j}]),$$

as we aimed to prove.

Now suppose that $n_1 = 2$. (4) still holds, while

$$Z_1([P_{n_1}, \ldots, P_{n_j}]) = Z_1([P_{n_1-1}, \ldots, P_{n_j}]) + Z_1([P_{n_1-2}, \ldots, P_{n_j}]) + Z_0\left(\bigcup_{i=2}^{j} P_{n_i}\right).$$

Note that $n_1 - 2 = 0, n_1 + n_2 - 2 = n_2$ and hence

$$[P_{n_1-2}, \ldots, P_{n_j}] = [P_{n_2}, \ldots, P_{n_j}] = [P_{n_1+n_2-2}, \ldots, P_{n_j}].$$

Moreover, $\bigcup_{i=2}^{j} P_{n_i}$ can be obtained from $[P_{n_1+n_2-3}, P_{n_3}, \ldots, P_{n_j}] = [P_{n_2-1}, P_{n_3}, \ldots, P_{n_j}]$ by removing all edges incident to the branching vertex except the one connecting it to P_{n_2}. Thus we have:

$$Z_0([P_{n_1+n_2-3}, P_{n_3}, \ldots, P_{n_j}]) > Z_0\left(\bigcup_{i=2}^{j} P_{n_i}\right).$$

By the induction assumption, we know that

$$Z_1([P_{n_1-1}, \ldots, P_{n_j}]) < Z_1([P_{n_1+n_2-1}, P_{n_3}, \ldots, P_{n_j}]),$$

and

$$Z_1([P_{n_1-2}, \ldots, P_{n_j}]) = Z_1([P_{n_1+n_2-2}, P_{n_3}, \ldots, P_{n_j}]).$$

Hence, we again have:

$$Z_1([P_{n_1}, \ldots, P_{n_j}]) < Z_1([P_{n_1+n_2}, P_{n_3}, \ldots, P_{n_j}]),$$

as desired. ∎

The following theorem follows immediately from Lemmas 4.8 and 4.9. It reduces the set of candidates to that of tripods.

Theorem 4.10. *If a tree T has order $n \geq 4$, and for any n-vertex tree H, we have $Z_1(P_n) > Z_1(T) \geq Z_1(H)$, then*

$$T \in \{[P_{n_1}, P_{n_2}, P_{n_3}] : n_1 + n_2 + n_3 = n - 1\}.$$

Section 5 suggest that the n-vertex trees with second-largest Z_1 is $[P_1, P_1, P_{n-3}]$ for $n = 9$, and it is $[P_3, P_3, P_{n-7}]$ for $n = 10$. Further computational check showed that we have $[P_1, P_1, P_{n-3}]$ again for $n = 11$, but for $12 \leq n \leq 20$ we always have $[P_3, P_3, P_{n-7}]$. Hence, the following conjecture.

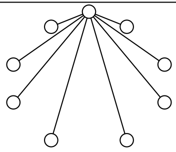
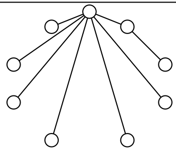
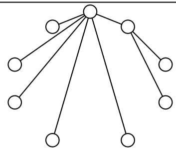
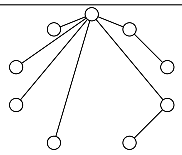
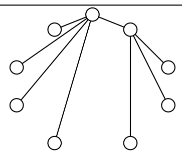
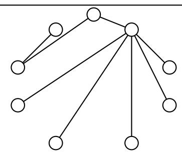
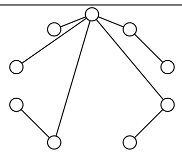
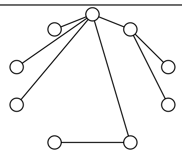
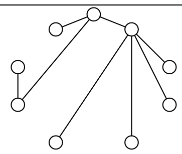
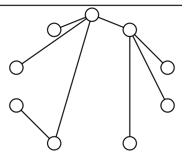
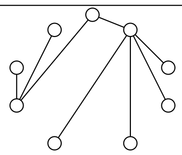
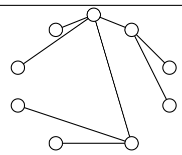
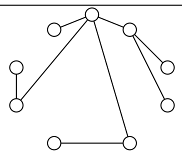
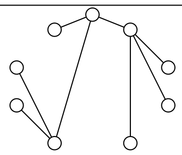
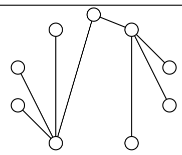
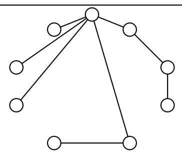
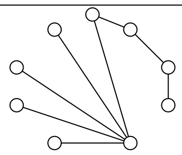
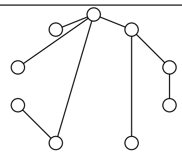
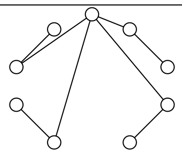
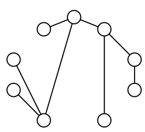
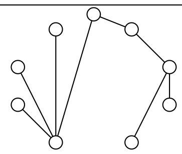
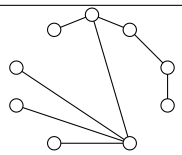
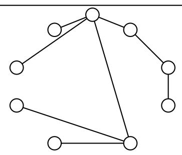
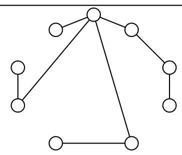
Conjecture 4.11. *Among all forest $F \neq P_n$ of order $n \geq 12$ we have $Z_1(F) \leq Z_1([P_3, P_3, P_{n-7}])$, with equality if and only if F is $[P_3, P_3, P_{n-7}]$.*

The fact that $[P_3, P_3, P_{n-7}]$ is not the tripod with largest Z_0 [15] is part of the reason why proving Conjecture 4.11 is challenging.

5 Appendix

In this appendix, we exhaustively compute $Z_1(T)$, where T is any tree of order n, where $9 \leq n \leq 10$. The trees of order $n = 9$ are in Table 1. Those of order $n = 10$, are in in Table 2.

Table 1: Z_1 of trees of order $n = 9$.

T	$\mathbf{Z_1(T)}$	**T**	$\mathbf{Z_1(T)}$	**T**	$\mathbf{Z_1(T)}$
	28		37		43
	45		46		47
	50		50		51
	52		53		54
	55		55		55
	55		55		55
	56		58		59
	59		59		59

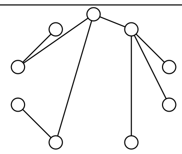
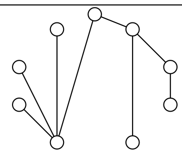
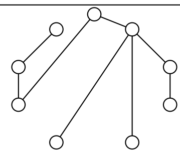
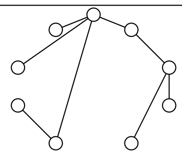
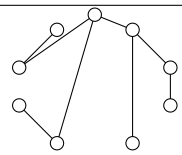
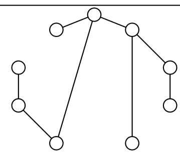
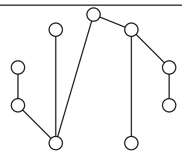
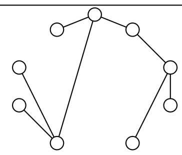
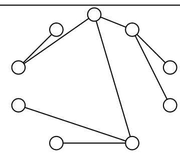
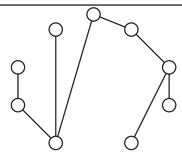
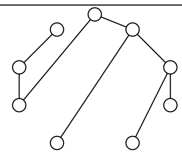
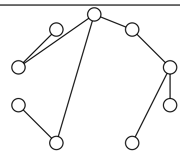
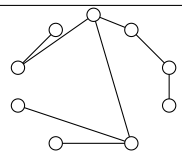
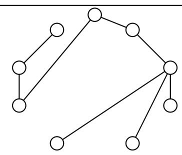
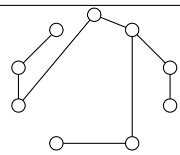
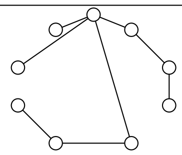
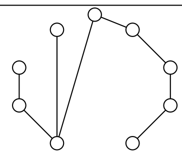
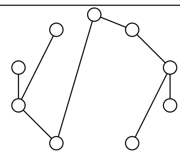
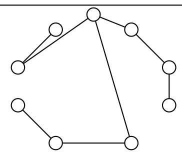
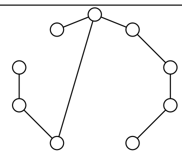
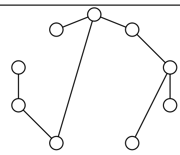
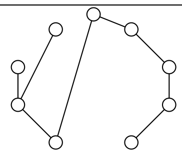
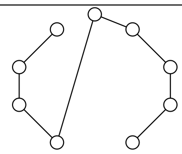
T	$\mathbf{Z_1(T)}$	**T**	$\mathbf{Z_1(T)}$	**T**	$\mathbf{Z_1(T)}$
	60		60		60
	60		61		62
	62		62		63
	63		63		64
	64		64		65
	65		66		67
	67		68		68
	69		71		

Table 2: Z_1 of trees of order $n = 10$.

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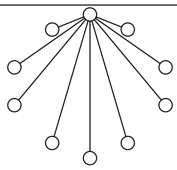
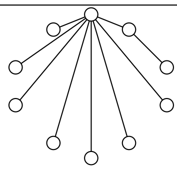
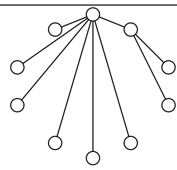
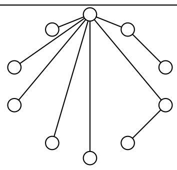
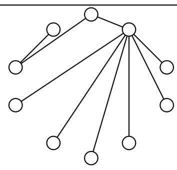
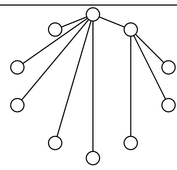
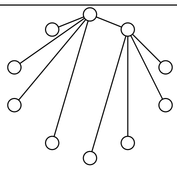
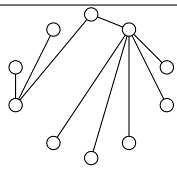
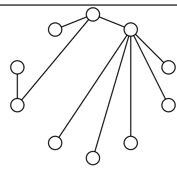
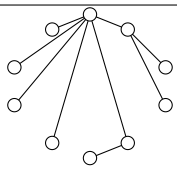
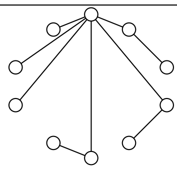
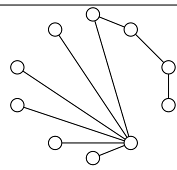
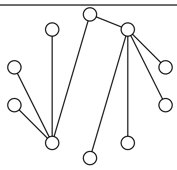
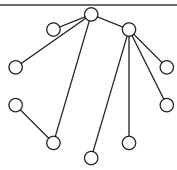
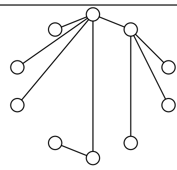
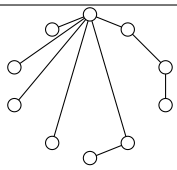
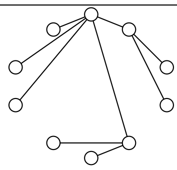
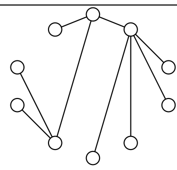
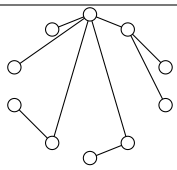
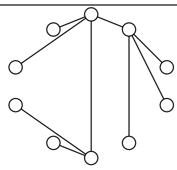
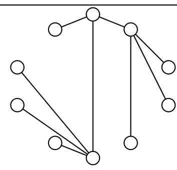
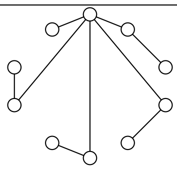
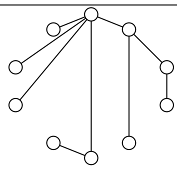
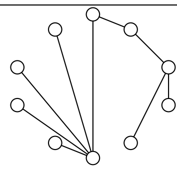
	36		50		60
	65		65		66
	68		75		75
	75		78		80
	80		80		80
	82		84		84
	87		87		87
	88		88		89

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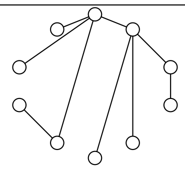
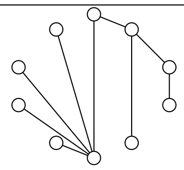
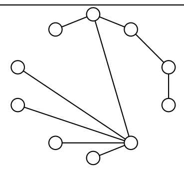
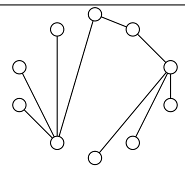
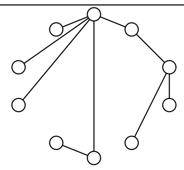
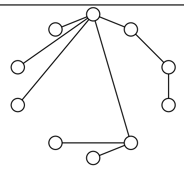
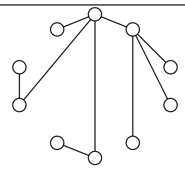
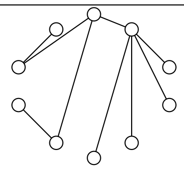
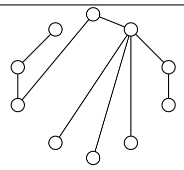
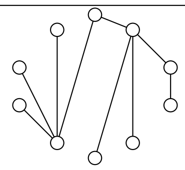
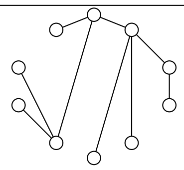
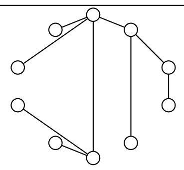
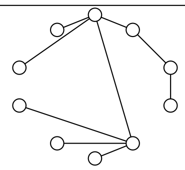
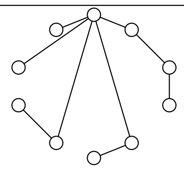
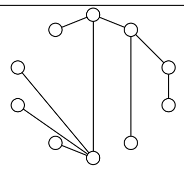
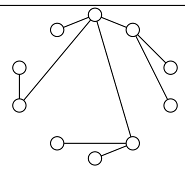
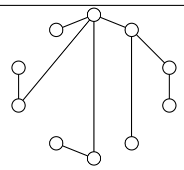
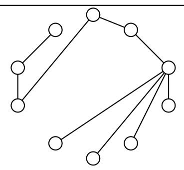
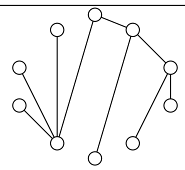
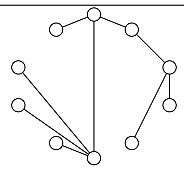
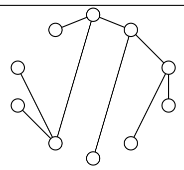
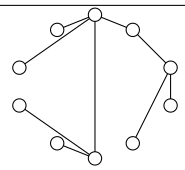
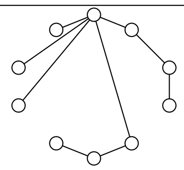
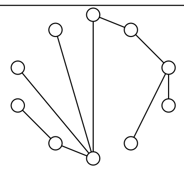
	90		91		91
	92		92		92
	92		93		95
	95		95		95
	95		95		96
	96		97		98
	99		99		100
	100		101		102

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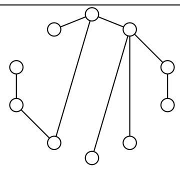
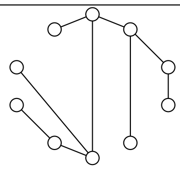
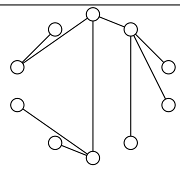
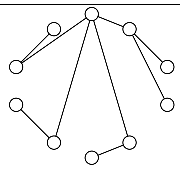
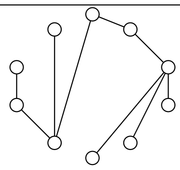
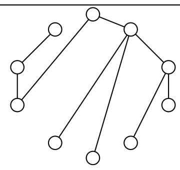
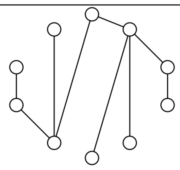
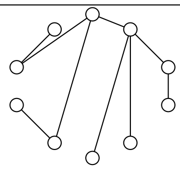
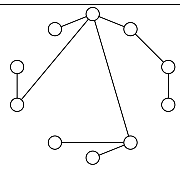
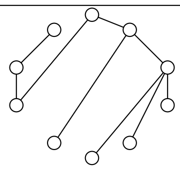
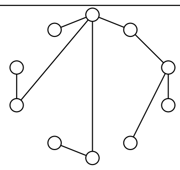
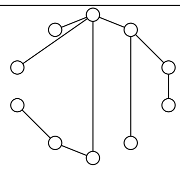
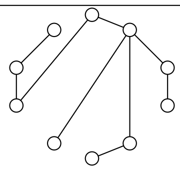
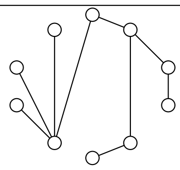
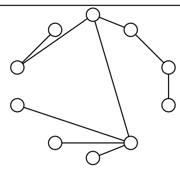
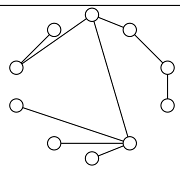
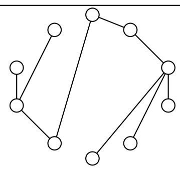
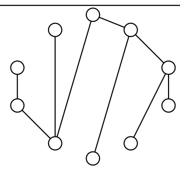
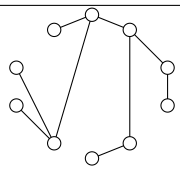
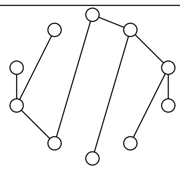
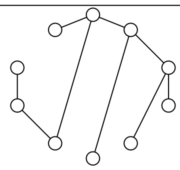
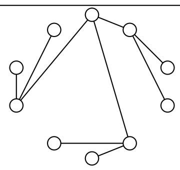
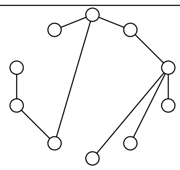
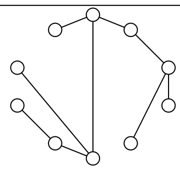
	102		102		102
	102		103		103
	103		103		103
	104		104		104
	105		105		106
	106		107		107
	107		108		108
	108		109		109

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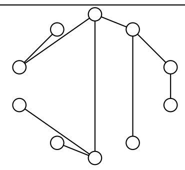
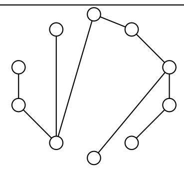
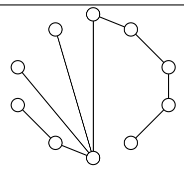
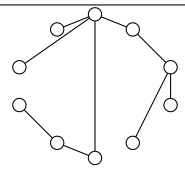
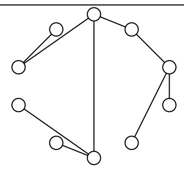
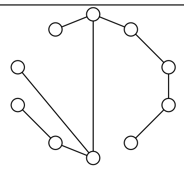
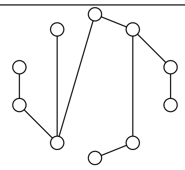
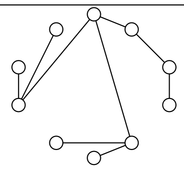
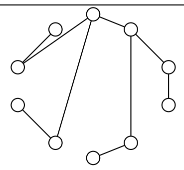
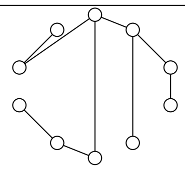
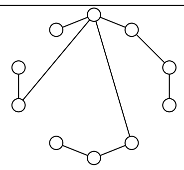
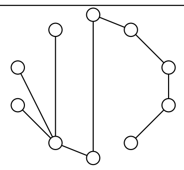
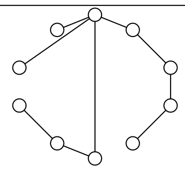
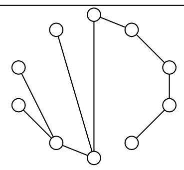
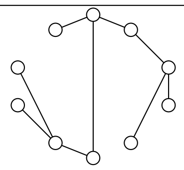
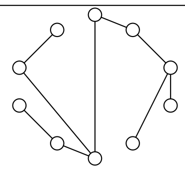
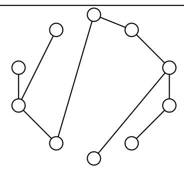
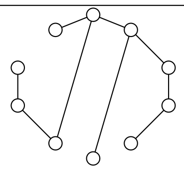
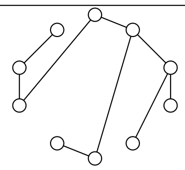
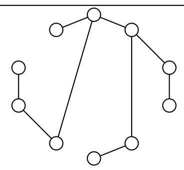
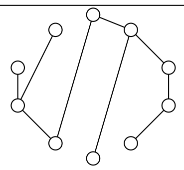
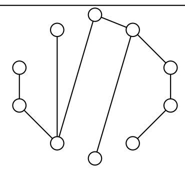
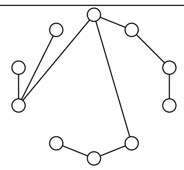
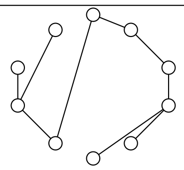
	109		110		110
	110		110		111
	111		111		112
	112		112		113
	113		115		115
	115		116		116
	116		116		117
	117		117		118

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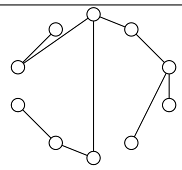
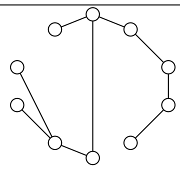
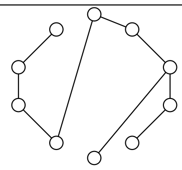
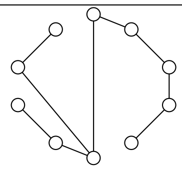
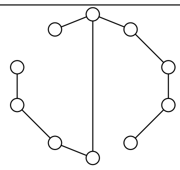
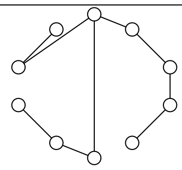
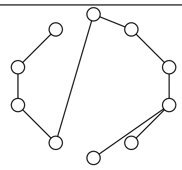
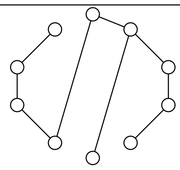
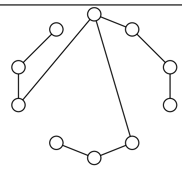
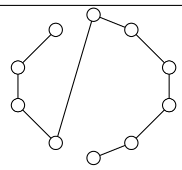
	118		119		120
	120		121		121
	125		125		126
	130				

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Conflicts of Interest. The authors declare that they have no conflicts of interest regarding the publication of this article.

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