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The Bounds of Vertex Padmakar–Ivan Index on k-Trees

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Abstract: The Padmakar–Ivan (PI) index is a distance-based topological index and a molecular structure descriptor, which is the sum of the number of vertices over all edges uv of a graph such that these vertices are not equidistant from u and v. In this paper, we explore the results of PI-indices from trees to recursively clustered trees, the k-trees. Exact sharp upper bounds of PI indices on k-trees are obtained by the recursive relationships, and the corresponding extremal graphs are given. In addition, we determine the PI-values on some classes of k-trees and compare them, and our results extend and enrich some known conclusions.

Keywords: extremal values; PI index; k-trees; distance

1. Introduction

Let G be a simple connected non-oriented graph with vertex set $V(G)$ and edge set $E(G)$. The distance $d(x, y)$ between the vertices $x, y \in V(G)$ is the minimum length of the paths between x and y in G. The oldest and most thoroughly examined molecular descriptor is Wiener index or path number [1], which was first considered in trees by Wiener in 1947 as follows: $W(G) = \sum_{\{x,y\}\subset V(G)} d(x, y)$. Compared to Wiener index, Szeged index was proposed by Gutman [2] in 1994 that, given $xy \in E(G)$, let $n_{xy}(x)$ be the number of vertices $w \in V(G)$ such that $d(x, w) < d(y, w)$, $Sz(G) = \sum_{xy\in E(G)} n_{xy}(x)n_{xy}(y)$. Based on the considerable success of Wiener index and Sz index, Khadikar proposed a new distance-based index [3] to be used in the field of nano-technology, that is edge Padmakar–Ivan (PI_e) index, $PI_e(G) = \sum_{xy\in E(G)}[n_e(x) + n_e(y)]$, where $n_e(x)$ denotes the number of edges which are closer to the vertex x than to the vertex y, and $n_e(y)$ denotes the number of edges which are closer to the vertex y than to the vertex x, respectively.

It is easy to see that the above concept does not count edges equidistant from both ends of the edge $e = xy$. Based on this idea, Khalifeh et al. [4] introduced a new PI index of vertex version that $PI(G) = PI_v(G) = \sum_{xy\in E(G)}[n_{xy}(x) + n_{xy}(y)]$. Note that, in order to obtain a good recursive formulas, we do not consider the vertices x, y for $n_{xy}(x)$ and $n_{xy}(y)$. Thus, $n_{xy}(x) + n_{xy}(y) \le n - 2$.

Nowadays, Padmakar–Ivan indices are widely used in Quantitative Structure–Activity Relationship (QSAR) and Quantitative Structure–Property Relationship (QSPR) [5,6], and there are many interesting results [5,7–26] between graph theory and chemistry. For instances, Klavžar [27] provided PI-partitions and arbitrary Cartesian product. Pattabiraman and Paulraja [28] presented the formulas for vertex PI indices of the strong product of a graph and the complete multipartite graph. Ilić and Milosavljević [29] established basic properties of weighted vertex PI index and some lower and upper bounds on special graphs. Wang and Wei [30] studied vertex PI index on an extention of trees (cacti). In [31], Das and Gutman obtained a lower bound on the vertex PI index of a connected graph in terms of numbers of vertices, edges, pendent vertices, and clique number. Hoji et al. [32] provided exact formulas for the vertex PI indices of Kronecker product of a connected graph G and a complete graph. Since the tree is a basic class of graphs in mathematics and chemistry, and these results indicate that either the stars or the paths attain the maximal or minimal bounds for particular chemical indices, then a natural question is how about the situations for vertex Padmakar–Ivan index?

Because PI index is a distance-based index and not very easy to calculate, we first consider the bipartite graph G with n vertices. Note that the tree is a subclass of bipartite graphs which have no odd cycles. By the definition of $PI(G)$ and the assumption that we do not consider the vertices x, y for $n_{xy}(x)$ and $n_{xy}(y)$, one can obtain that every edge of G has the PI-value as $n-2$. Thus, the following observation is obtained.

Obervation 1. *For a bipartite graph G with n vertices and m edges, $PI(G) = (n-2)m$. In particular, if G is a tree, then $PI(G) = (n-1)(n-2)$.*

Next, we will consider the graphs with odd cycles. In particular, the general tree, k-tree, contains a lot of odd cycles. Then, we are going to consider the PI indices of k-trees and figure out whether or not a k-star or a k-path attains the maximal or minimal bound for PI-indices of k-trees. Our main results are as follows: Theorems 1 and 2 give the exact PI-values of k-stars, k-paths and k-spirals (see Definitions 1–5 below).

Theorem 1. *For any k-star S_n^k and k-path P_n^k with $n = kp + s$ vertices, where $p \geq 0$ is an integer and $s \in [2, k+1]$, we have*

$$(i) PI(S_n^k) = k(n-k)(n-k-1),$$
$$(ii) PI(P_n^k) = \frac{k(k+1)(p-1)(3kp+6s-2k-4)}{6} + \frac{(s-1)s(3k-s+2)}{3}.$$

Theorem 2. *For any k-spiral $T_{n,c}^{k*}$ with $n \geq k$ vertices, where $c \in [1, k-1]$, we have*

$$PI(T_{n,c}^{k*}) = \begin{cases} \frac{(n-k)(n-k-1)(4k-n+2)}{3} & \text{if} \quad n \in [k, 2k-c], \\ \frac{3c(n-2k+c-1)(n-2k+c)+(k-c)(2c^2+3nc-4kc+3kn-4k^2-6k+3n-2)}{3} & \text{if} \quad n \geq 2k-c+1. \end{cases}$$

Theorem 3 proves that k-stars achieve the maximal values of PI-values for k-trees, and Theorem 4 shows that k-paths do not arrive the minimal values and certain PI-values of k-spirals are less than that of k-paths.

Theorem 3. *For any k-tree T_n^k with $n \geq k \geq 1$, we have $PI(T_n^k) \leq PI(S_n^k)$.*

Theorem 4. *For any k-spiral $T_{n,c}^{k*}$ with $n \geq k \geq 1$, we have*

$$\begin{array}{ll} (i) & PI(P_n^k) \geq PI(T_{n,c}^{k*}) \text{ if } c \in [1, \frac{k+1}{2}), \\ (ii) & PI(P_n^k) \leq PI(T_{n,c}^{k*}) \text{ if } c \in [\frac{k+1}{2}, k-1]. \end{array}$$

2. Preliminary

In this section, we first give some notations and lemmas that are crucial in the following sections. As usual, $G = (V, E)$ is a connected finite simple undirected graph with vertex set $V = V(G)$ and edge set $E = E(G)$. Let $|G|$ or $|V|$ be the cardinality of V. For any $S \subseteq V(G)$ and $F \subseteq E(G)$, we use $G[S]$ to denote the subgraph of G induced by S, $G - S$ to denote the subgraph induced by $V(G) - S$ and $G - F$ to denote the subgraph of G obtained by deleting F. $w(G - S)$ is the number of components of $G - S$ and S is a cut set if $w(G - S) \geq 2$. For any $u, v \in V(G)$, P_{uv} is a path connecting u and v, $d(u, v)$ is the distance between u and v, $N(v) = N_G(v) = \{w \in V(G), vw \in E(G)\}$ is the neighborhood of v and $N[v] = N(v) \cup \{v\}$. For any integers a, b with $a \leq b$, the interval $[a, b]$ is the set of all integers between a and b including a, b. In addition, let $[a, b) = [a, b] - \{b\}$ and $(a, b] = [a, b] - \{a\}$. In particular, $[a, b] = \phi$ for $a > b$. $f'(x)$ is a derivative of any differentiable function $f(x)$, where x is the variable. $\lfloor x \rfloor$ is the largest integer that is less than or equal to x; $\lceil x \rceil$ is the smallest integer that is greater than or equal to x. It is clear that d is from 0 to the diameter of graphs. Other undefined notations are referred to [33].

It is commonly known that a chordal graph G with at least three vertices is a triangulated graph and contains a simplicial vertex, whose neighborhood induces a clique. During recent decades, there are many interesting studies related to chordal graphs. In 1969, Beineke and Pippert [7] gave the definition of k-trees, which is a significant subclass of chordal graphs. Now, we just give some definitions about k-trees below.

Definition 1. *For positive integers n, k with $n \geq k$, the k-tree, denoted by T_n^k, is defined recursively as follows: The smallest k-tree is the k-clique K_k. If G is a k-tree with $n \geq k$ vertices and a new vertex v of degree k is added and joined to the vertices of a k-clique in G, then the obtained graph is a k-tree with $n + 1$ vertices.*

Definition 2. *For positive integers n, k with $n \geq k$, the k-path, denoted by P_n^k, is defined as follows: starting with a k-clique $G[\{v_1, v_2 \dots v_k\}]$. For $i \in [k + 1, n]$, the vertex v_i is adjacent to vertices $\{v_{i-1}, v_{i-2} \dots v_{i-k}\}$ only.*

Definition 3. *For positive integers n, k with $n \geq k$, the k-star, denoted by S_n^k, is defined as follows: Starting with a k-clique $G[\{v_1, v_2 \dots v_k\}]$ and an independent set S with $|S| = n - k$. For $i \in [k + 1, n]$, the vertex v_i is adjacent to vertices $\{v_1, v_2 \dots v_k\}$ only.*

Definition 4. *For positive integers n, k, c with $n \geq k$ and $c \in [1, k - 1]$, let $v_1, v_2, \dots, v_{n-c}$ be the simplicial ordering of P_{n-c}^{k-c}. The k-spiral, denoted by $T_{n,c}^{k*}$, is defined as $P_{n-c}^{k-c} + K_c$, which is, $V(T_{n,c}^{k*}) = \{v_1, v_2, \dots, v_n\}$ and $E(T_{n,c}^{k*}) = E(P_{n-c}^{k-c}) \cup E(K_c) \cup \{v_1v_l, v_2v_l, \dots, v_{n-c}v_l\}$, for $l \in [n - c + 1, n]$.*

Definition 5. *Let $v \in V(T_n^k)$ be a vertex of degree k whose neighbors form a k-clique of T_n^k, then v is called a k-simplicial vertex. Let $S_1(T_n^k)$ be the set of all k-simplicial vertices of T_n^k, for $n \geq k + 2$, and set $S_1(K_k) = \phi, S_1(K_{k+1}) = \{v\}$, where v is any vertex of K_{k+1}. Let $G_0 = G, G_i = G_{i-1} - v_i$, where v_i is a k-simplicial vertex of G_{i-1}, then $\{v_1, v_2 \dots v_n\}$ is called a simplicial elimination ordering of the n-vertex graph G.*

In order to consider the PI-value of any k-tree G, let $G' = G \cup \{u\}$ be a k-tree obtained by adding a new vertex u to G. For any $v_1, v_2 \in V(G)$, let $d(v_1, v_2)$ be the distance between v_1 and v_2 in G, $d'(v_1, v_2)$ be the distance between v_1 and v_2 in G'. Now, we define a function that measures the difference of PI-values of any edge relating a vertex from G to G' as follows: $f : \{w \in V(G'), xy \in E(G)\}$ to $\{1, 0\}$ as follows:

$$f(w, xy) = \begin{cases} 0, & \text{if} \quad w = u \text{ and } d'(x, w) = d'(y, w), \\ 0, & \text{if} \quad w \in V(G) \text{ and } d(x, w) - d'(x, w) = d(y, w) - d'(y, w), \\ 1, & \text{if} \quad otherwise. \end{cases}$$

Using the construction of k-trees, we can derive the following lemmas. Note that $PI(xy) = n_{xy}(x) + n_{xy}(y)$ and $PI(xy) \leq n - 2$.

Lemma 1. *Let xy be any edge of a k-tree G with at least $n \geq k + 1$ vertices, then $PI(xy) \leq n - k - 1$.*

Proof. Since every vertex of any k-tree G with at least $k+1$ vertices must be in some $(k+1)$-cliques, which is, $|N(x) \cap N(y)| \geq k-1$ for any $xy \in E(G)$, we have $PI(xy) \leq n-(k-1)-2 = n-k-1$. □

Lemma 2. *Let xy be any edge of a k-tree G with n vertices and $G' = G \cup \{u\}$ be a k-tree obtained by adding u to G. If $w \in V(G)$, then $f(w, xy) = 0$.*

Proof. By adding u to G, since G' is a k-tree, we can get that the distance of any pair of vertices of G will increase at most 1, then $f(w, xy) \leq 1$. If $w \in V(G)$, then there exists a shortest path P_{xw} or P_{yw} such that $u \notin V(P_{xw})$ or $V(P_{yw})$, that is, $f(w, xy) = 0$. □

Lemma 3. *For any k-path G with n vertices, where $n \geq k+2$, let $S_1(G) = \{v_1, v_n\}$ and $\{v_1, v_2, \ldots, v_n\}$ be the simplicial elimination ordering of G, then $d(v_i, v_j) = \lceil \frac{j-i}{k} \rceil$, for $i < j$ and $i, j \in [1, n]$. Furthermore, if $n = kp + s$ with $p \geq 1, s \in [2, k+1]$, then*

$$d(v, v_{kp+s}) = \begin{cases} p+1 & \text{if} \quad v \in \{v_1, v_2, \ldots, v_{s-1}\}, \\ p-i & \text{if} \quad v \in \{v_{ki+s}, v_{ki+s+1}, \ldots, v_{k(i+1)+s-1}\}, i \in [0, p-1]. \end{cases}$$

Proof. If $j - i \leq k$, then v_i, v_j must be in the same $(k+1)$-clique of G, and we have $d(v_i, v_j) = 1$; if $j - i \geq k+1$, then $P_{v_i v_j} = v_i v_{i+k} v_{i+2k} \ldots v_{i+(\lfloor \frac{j-i}{k} \rfloor - 1)k} v_{i+\lfloor \frac{j-i}{k} \rfloor k} v_j$ is one of the shortest paths between v_i and v_j. Thus, $d(v_i, v_j) = \lceil \frac{j-i}{k} \rceil$ and Lemma 3 is proved. □

Lemma 4. *For any k-spiral $T^{k*}_{n,c}$ with n vertices and $v_i, v_j \in V(T^{k*}_{n,c})$ for $i < j$,*

$$d(v_i, v_j) = \begin{cases} 1, & \text{if} \quad j - i \leq k - c, i, j \in [1, n-c], \\ 1, & \text{if} \quad i \text{ or } j \in [n-c+1, n], \\ 2, & \text{if} \quad j - i \geq k - c + 1, i, j \in [1, n-c]. \end{cases}$$

Proof. If $j - i \leq k - c$ with $i, j \in [1, n-c]$, by Definition 4, we can get that v_i, v_j must be in the same $(k+1)$-clique of G and $d(v_i, v_j) = 1$; If i or $j \in [n-c+1, n]$, without loss of generality, say v_i such that $i \in [n-c+1, n]$, then $N[v_i] = V(T^{k*}_{n,c})$, that is, $d(v_i, v_j) = 1$; If $j - i \geq k - c + 1$ with $i, j \in [1, n-c]$, then $v_i \notin N(v_j)$ and $P_{v_i v_j} = v_i v_n v_j$ is one of the shortest paths between v_i and v_j, that is, $d(v_i, v_j) = 2$. Thus, Lemma 4 is proved. □

3. Main Proofs

In this section, we give the proofs of main results by inductions. For a k-tree T^k_n, if $n = k$ or $k+1$, then T^k_n is a k or (k+1)-clique, that is, $PI(T^k_n) = 0$. Thus, all of the theorems are true and we will only consider the case when $n \geq k+2$ below.

Proof of Theorem 1. For (i), let $V(S^k_n) = \{u_1, u_2, \ldots, u_n\}$, $G[\{u_1, \ldots, u_k\}]$ be a k-clique and $N(u_{l_0}) = \{u_1, u_2, \ldots, u_k\}$ for $l_0 \geq k+1$. Just by Definition 3, we can get that for $i, j \in [1, k]$, $N[u_i] = N[u_j] = V(S^k_n)$, then $PI(u_i u_j) = n_{u_i u_j}(u_i) + n_{u_i u_j}(u_j) = 0$; for $i \in [1, k]$ and $l_0 \in [k+1, n]$, $|N[u_i] - N[u_{l_0}]| = n - k - 1$, then $PI(u_i u_l) = n - k - 1$. Thus, we can get $PI(S^k_n) = \sum_{i,j \in [1,k]} PI(u_i u_j) + \sum_{i \in [1,k], l_0 \in [k+1,n]} PI(u_i u_{l_0}) = k(n-k)(n-k-1)$.

For (ii), we will proceed it by induction on $|P^k_n| = n \geq k+2$. If $n = k+2$, let $\{v_1, v_2, \ldots, v_{k+2}\}$ be the simplicial elimination ordering of P^k_{k+2}. By Lemma 3, we can get that $PI(v_1 v_i) = 1, PI(v_i v_{i'}) = 0$ and $PI(v_i v_{k+2}) = 1$ for $i, i' \in [2, k+1]$. Thus, $PI(P^k_{k+2}) = \sum_{i=2}^{k+1} PI(v_1 v_i) + \sum_{i=2}^{k+1} PI(v_i v_{k+2}) = 2k$. Assume that Theorem 1 is true for a k-path with at most $kp + s - 1$ vertices, where $p \geq 1, 2 \leq s \leq k+1$. Let P^k_n be a k-path such that $|P^k_n| = kp + s$, $V(P^k_n) = \{v_1, v_2, \ldots, v_{kp+s}\}$ and $\{v_1, v_2, \ldots, v_{kp+s}\}$ be the simplicial elimination ordering of P_n^k. Set $P_{n-1}^k = P_n^k - \{v_{kp+s}\}$, then $\{v_1, v_2, \ldots, v_{kp+s-1}\}$ is the simplicial elimination ordering of P_{n-1}^k and for any edge $v_iv_j \in E(P_n^k)$, $d(v_i, v_j)$ or $d'(v_i, v_j)$ is the distance of v_i and v_j in P_{n-1}^k or P_n^k, respectively.

Let $\alpha = [\frac{k(k+1)(p-1)(3kp+6s-2k-4)}{6} + \frac{(s-1)s(3k-s+2)}{3}] - [\frac{k(k+1)(p-1)(3kp+6s-2k-10)}{6} + \frac{(s-2)(s-1)(3k-s+3)}{3}] = pk^2 + pk - k^2 - 3k + 2ks - s^2 + 3s - 2$. If we can show that by adding v_{kp+s} to P_{n-1}^k, $PI(P_n^k) = PI(P_{n-1}^k) + \alpha$, then Theorem 1 is true.

Set $w = v_{kp+s}$, $A_1 = \{v_1v_s, v_1v_{s+1}, \ldots, v_1v_{k+1}\}, A_2 = \{v_2v_s, \ldots, v_2v_{k+2}\}, \ldots, A_{s-1} = \{v_{s-1}v_s, \ldots, v_{s-1}v_{k+s-1}\}$ and $B_1 = \{v_1v_2, v_1v_3, \ldots, v_1v_{s-1}\}, B_2 = \{v_2v_3, \ldots, v_2v_{s-1}\}, \ldots, B_{s-2} = \{v_{s-2}v_{s-1}\}, B_{s-1} = \phi$. By Definition 2 and Lemma 3, we have $d'(v_1, v_{kp+s}) = p+1, d'(v_s, v_{kp+s}) = p$ and $d'(v_1, v_{kp+s}) = p+1, d'(v_2, v_{kp+s}) = p+1$, that is, $d'(v_1, v_{kp+s}) \neq d'(v_s, v_{kp+s})$ and $d'(v_1, v_{kp+s}) = d'(v_2, v_{kp+s})$. Thus, $f(w, v_1v_s) = 1$ and $f(w, v_1v_2) = 0$. Similarly, for any edge $v_{h_1}v_{h_2} \in \cup_{i=1}^{s-1} A_i$ with $h_1 < h_2$, we have $d'(v_{h_1}, v_{kp+s}) \neq d'(v_{h_2}, v_{kp+s})$, that is, $f(w, v_{h_1}v_{h_2}) = 1$; For $v_{h_1}v_{h_2} \in \cup_{i=1}^{s-1} B_i$ with $h_1 < h_2$, we have $d'(v_{h_1}, v_{kp+s}) = d'(v_{h_2}, v_{kp+s})$, that is, $f(w, v_{h_1}v_{h_2}) = 0$. Thus, we can get that

$$f(v_{kp+s}, xy) = \begin{cases} 1, & \text{if} \quad xy \in \cup_{i=1}^{s-1} A_i, \\ 0, & \text{if} \quad xy \in \cup_{i=1}^{s-1} B_i. \end{cases}$$

For $t \in [0, p-2]$, set $A_{kt+s} = \{v_{kt+s}v_{k(t+1)+s}\}$, $A_{kt+s+1} = \{v_{kt+s+1}v_{k(t+1)+s}, v_{kt+s+1}v_{k(t+1)+s+1}\}$, $\ldots, A_{k(t+1)+s-1} = \{v_{k(t+1)+s-1}v_{k(t+1)+s}, v_{k(t+1)+s-1}v_{k(t+1)+s+1}, \ldots, v_{k(t+1)+s-1}v_{k(t+2)+s-1}\}$, and $B_{kt+s} = \{v_{kt+s}v_{kt+s+1}, \ldots, v_{kt+s}v_{k(t+1)+s-1}\}, B_{kt+s+1} = \{v_{kt+s+1}v_{kt+s+2}, ..., v_{kt+s+1}v_{k(t+1)+s-1}\}, \ldots, B_{k(t+1)+s-2} = \{v_{k(t+1)+s-2}v_{k(t+1)+s-1}\}, B_{k(t+1)+s-1} = \phi$. For $t = 0$ and by Lemma 3, we have $d'(v_s, v_{kp+s}) = p$, $d'(v_{k+s}, v_{kp+s}) = p-1$ and $d'(v_s, v_{kp+s}) = p, d'(v_{s+1}, v_{kp+s}) = p$, that is, $d'(v_s, v_{kp+s}) \neq d'(v_{k+s}, v_{kp+s})$ and $d'(v_s, v_{kp+s}) = d'(v_{s+1}, v_{kp+s})$. Thus, $f(w, v_sv_{k+s}) = 1$ and $f(w, v_sv_{s+1}) = 0$. similarly, for any edge $v_{h_1}v_{h_2} \in \cup_{i=kt+s}^{k(t+1)+s-1} A_i$ with $h_1 < h_2$, we have $d'(v_{h_1}, v_{kp+s}) \neq d'(v_{h_2}, v_{kp+s})$, that is, $f(w, v_{h_1}v_{h_2}) = 1$; for $v_{h_1}v_{h_2} \in \cup_{i=kt+s}^{k(t+1)+s-1} B_i$ with $h_1 < h_2$, we have $d'(v_{h_1}, v_{kp+s}) = d'(v_{h_2}, v_{kp+s})$, that is, $f(w, v_{h_1}v_{h_2}) = 0$. Thus, we can get that

$$f(v_{kp+s}, xy) = \begin{cases} 1, & \text{if} \quad xy \in \cup_{i=kt+s}^{k(t+1)+s-1} A_i, \\ 0, & \text{if} \quad xy \in \cup_{i=kt+s}^{k(t+1)+s-1} B_i. \end{cases}$$

Next, we consider the edges in the $(k+1)$-clique $P_n^k[N[v_{kp+s}]]$. For any edge $v_{h_1}v_{h_2}$ with $h_1, h_2 \in [k(p-1)+s, kp+s-1]$, we have $d'(v_{h_1}, v_{kp+s}) = d'(v_{h_2}, v_{kp+s}) = 1$, that is, $f(w, v_{h_1}v_{h_2}) = 0$. For any edge v_hv_{kp+s} with $h \in [k(p-1)+s, kp]$, by Lemma 3, we can obtain that $d'(v_1, v_h) = p, d'(v_1, v_{kp+s}) = p+1$, $d'(v_{h-k}, v_h) = 1, d'(v_{h-k}, v_{kp+s}) = 2$ and when $h \neq k(p-1)+s$, $d'(v_{k(p-1)+s}, v_h) = 1, d'(v_{k(p-1)+s}, v_{kp+s}) = 1$, that is, $d'(v_1, v_h) \neq d'(v_1, v_{kp+s})$, $d'(v_{h-k}, v_h) \neq d'(v_{h-k}, v_{kp+s})$ and $d'(v_{k(p-1)+s}, v_h) = d'(v_{k(p-1)+s}, v_{kp+s})$. Similarly, we get that for $j \in [1, p-1]$, $j' \in [1, p]$ and $l \neq h$,

$$\begin{cases} d'(v_l, v_h) \neq d'(v_l, v_{kp+s}) & \text{if} \quad l \in [1, s-1] \cup [h-jk, k(p-j)+s-1], \\ d'(v_l, v_h) = d'(v_l, v_{kp+s}) & \text{if} \quad l \in [k(p-j')+s, h-j'k+k-1] \cup [h+1, kp+s-1]. \end{cases}$$

Thus, if $v_h = v_{k(p-1)+s}$, then $d'(v_l, v_{k(p-1)+s}) \neq d'(v_l, v_{kp+s})$ with $l \in [1, s-1] \cup \{\cup_{j=1}^{p-1} [k(p-1)+s-jk, (p-j)k+s-1]\} = [1, (p-1)k+s-1]$ and $d'(v_l, v_{k(p-1)+s}) = d'(v_l, v_{kp+s})$ with $l \in [(p-1)k+s+1, kp+s]$, that is, $PI(v_{k(p-1)+s}v_{kp+s}) = (p-1)k+s-1$; similarly, we can obtain that $PI(v_{k(p-1)+s+1}v_{kp+s}) = (p-1)(k-1)+s-1; PI(v_{k(p-1)+s+2}v_{kp+s}) = (p-1)(k-2)+s-1; \ldots; PI(v_{kp}v_{kp+s}) = (p-1)s+s-1$.

For any edge v_hv_{kp+s} with $h \in [kp+1, kp+s-1]$, by Lemma 3, we can obtain that $d'(v_{h-k}, v_h) = 1, d'(v_{h-k}, v_{kp+s}) = 2$ and $d'(v_{k(p-1)+s}, v_h) = 1, d'(v_{k(p-1)+s}, v_{kp+s}) = 1$, that is, $d'(v_{h-k}, v_h) \neq$

$d'(v_{h-k}, v_{kp+s})$ and $d'(v_{k(p-1)+s}, v_h) = d'(v_{k(p-1)+s}, v_{kp+s})$. Similarly, we get that for $j'' \in [1, p]$ and $l \neq h$,

$$\begin{cases} d'(v_l, v_h) \neq d'(v_l, v_{kp+s}) & \text{if} \quad l \in [h - j''k, k(p - j'') + s - 1], \\ d'(v_l, v_h) = d'(v_l, v_{kp+s}) & \text{if} \quad l \in [k(p - j'') + s, h - j''k + k - 1] \cup [h + 1, kp + s - 1]. \end{cases}$$

Thus, if $v_h = v_{kp+1}$, then $d'(v_l, v_{kp+1}) \neq d'(v_l, v_{kp+s})$ for $l \in \cup_{j''=1}^{p}[kp + 1 - j''k, k(p - j'') + s - 1]$ and $d'(v_l, v_{kp+1}) = d'(v_l, v_{kp+s})$ with $l \in \{\cup_{j''=1}^{p}[k(p - j'') + s, k(p + 1 - j'')]\} \cup [h + 1, kp + s - 1]$, that is, $PI(v_{kp+1}v_{kp+s}) = (s - 1)p$; similarly, we have $PI(v_{kp+1}v_{kp+s}) = (s - 2)p; \ldots ; PI(v_{kp+s-2}v_{kp+s}) = 2p; PI(v_{kp+s-1}v_{kp+s}) = p$.

Set $w \in V(P_{n-1}^k)$, if $xy \in E(P_n^k)$ with x or $y \neq v_{kp+s}$, by Lemma 2, we have $f(w, xy) = 0$. Thus,

$$\begin{aligned} PI(P_n^k) - PI(P_{n-1}^k) &= \textstyle\sum_{xy \in \cup_{i=1}^{k(p-1)+s-1}(A_i \cup B_i)} f(w, xy) + PI(v_{k(p-1)+s}v_{kp+s}) \\ &\quad + PI(v_{k(p-1)+s+1}v_{kp+s}) + \cdots + PI(v_{kp+s-1}v_{kp+s}) \\ &= [(k + 2 - s) + (k + 3 - s) + \cdots + k] + (1 + 2 + \cdots + k)(p - 1) \\ &\quad + [k(p - 1) + s - 1] + [(k - 1)(p - 1) + s - 1] + [(k - 2)(p - 1) + s \\ &\quad - 1] + \cdots + [s(p - 1) + s - 1] + [(s - 1)p + (s - 2)p + \cdots + 2p + p] \\ &= pk^2 + pk - k^2 - 3k + 2ks - s^2 + 3s - 2 \\ &= \alpha. \end{aligned}$$

Thus, $PI(P_n^k) = \frac{k(k+1)(p-1)(3kp+6s-2k-4)}{6} + \frac{(s-1)s(3k-s+2)}{3}$, for $|P_n^k| = kp + s$ and Theorem 1 is proved. □

Proof of Theorem 2. We will proceed with it by induction on $n \geq k + 2$. If $n = k + 2$, by Definition 4, we have $T_{n,c}^{k*}$ is also a k-path, that is, $PI(T_{n,c}^{k*}) = 2k$. If $n \geq k + 3$, assume that Theorem 2 is true for the k-spiral with at most $n - 1$ vertices, we will consider $T_{n,c}^{k*}$ with n vertices. Let $T_{n,c}^{k*}$ be a k-spiral with $V(T_{n,c}^{k*}) = V(T_{n-1,c}^{k*}) \cup \{v\}$ and $E(T_{n,c}^{k*}) = E(T_{n-1,c}^{k*}) \cup \{vv_{n-1}, vv_{n-2}, \ldots, vv_{n-k}\}$ such that $v_1, v_2, \ldots, v_{n-c-1}$ is the simplicial ordering of P_{n-c-1}^{k-c}, where $T_{n-1,c}^{k*} = P_{n-c-1}^{k-c} + K_c$ with $V(T_{n-1,c}^{k*}) = \{v_1, v_2, \ldots, v_{n-1}\}$ and $E(T_{n-1,c}^{k*}) = E(P_{n-c-1}^{k-c}) \cup E(K_c) \cup \{v_1v_l, v_2v_l, \ldots, v_{n-c-1}v_l\}$ for $l \in [n - c, n - 1]$. For any edge $v_iv_j \in E(T_{n,c}^{k*})$, $d(v_i, v_j)$ or $d'(v_i, v_j)$ is the distance of v_i and v_j in $T_{n-1,c}^{k*}$ or $T_{n,c}^{k*}$, respectively.

For $k + 2 \leq n \leq 2k - c$, let $\gamma = \frac{(n-k)(n-k-1)(4k-n+2)}{3} - \frac{(n-k-1)(n-k-2)(4k-n+3)}{3} = (n - k - 1)(3k - n + 2)$. If we can show that by adding v to $T_{n-1,c}^{k*}$, $PI(T_{n,c}^{k*}) = PI(T_{n-1,c}^{k*}) + \gamma$, then Theorem 2 is true.

Set $w = v$ and let $l \in [n - c, n - 1]$, by Lemma 4, we have $d'(v_l, v) = 1$ and $d'(v_i, v) = 2$ for $i \in [1, n - k - 1]$, that is, $f(w, v_lv_i) = 1$; $d'(v_l, v) = d'(v_i, v) = 1$ for $i \in [n - k, n - 1]$, that is, $f(w, v_lv_i) = 0$. Set $C_1 = \{v_1v_2, v_1v_3, \ldots, v_1v_{n-k-1}\}, C_2 = \{v_2v_3, v_2v_4, \ldots, v_2v_{n-k-1}\}, \ldots, C_{n-k-2} = \{v_{n-k-2}v_{n-k-1}\}, C_{n-k-1} = \phi, D_1 = \{v_1v_{n-k}, v_1v_{n-k+1}, \ldots, v_1v_{k-c+1}\}, D_2 = \{v_2v_{n-k}, v_2v_{n-k+1}, \ldots, v_2v_{k-c+2}\}, \ldots, D_{n-k-1} = \{v_{n-k-1}v_{n-k}, v_{n-k-1}v_{n-k+1}, \ldots, v_{n-k-1}v_{n-c-1}\}$. By Lemma 4, we have $d'(v_1, v) = d'(v_2, v) = 2$ and $d'(v_{n-k}, v) = 1$, that is, $f(w, v_1v_2) = 0$ and $f(w, v_1v_{n-k}) = 1$. Similarly, for $v_{h_1}v_{h_2} \in \cup_{i=1}^{n-k-1}C_i$ with $h_1 < h_2$, we have $d'(v_{h_1}, v) = d'(v_{h_2}, v) = 2$, that is, $f(w, v_{h_1}v_{h_2}) = 0$; for $v_{h_1}v_{h_2} \in \cup_{i=1}^{n-k-1}D_i$ with $h_1 < h_2$, we have $d'(v_{h_1}, v) = 2$ and $d'(v_{h_2}, v) = 1$, that is, $f(w, v_{h_1}v_{h_2}) = 1$. Set $C_{n-k} = \{v_{n-k}v_{n-k+1}, v_{n-k}v_{n-k+2}, \ldots, v_{n-k}v_{n-c-1}\}, C_{n-k+1} = \{v_{n-k+1}v_{n-k+2}, v_{n-k+1}v_{n-k+3}, \ldots, v_{n-k+1}v_{n-c-1}\}, \ldots, C_{n-c-2} = \{v_{n-c-2}v_{n-c-1}\}$. By Lemma 4, we have $d'(v_{n-k}, v) = d'(v_{n-k-1}, v) = 1$, that is, $f(w, v_{n-k}v_{n-k-1}) = 0$. Similarly, for $v_{h_1}v_{h_2} \in \cup_{i=n-k}^{n-c-2}C_i$ with $h_1 < h_2$, we have $d'(v_{h_1}, v) = d'(v_{h_2}, v) = 1$, that is, $f(w, v_{h_1}v_{h_2}) = 0$.

Set $E_1 = \{vv_i, i \in [n - k, n - c - 1]\}$, by Lemma 4, we have $d'(v_i, v) = 2, d'(v_i, v_{n-k}) = 1$ for $i \in [1, n - k - 1]$ and $d'(v_j, v) = d'(v_j, v_{n-k}) = 1$ for $i \in [n - k + 1, n]$. Thus, $PI(v_{n-k}v) = n - k - 1$. Similarly, $PI(v_{n-k+1}v) = PI(v_{n-k+2}v) = \cdots = PI(v_{k-c+1}v) = n - k - 1$. In addition, by Lemma 4, we have $d'(v_i, v) = 2, d'(v_i, v_{k-c+2}) = 1$ for $i \in [2, n - k - 1]$, $d'(v_1, v) = d'(v_1, v_{k-c+2}) = 2$ and $d'(v_j, v) = d(v_j, v_{k-c+2}) = 1$ for $j \in [n - k, n]$. Thus, $PI(v_{k-c+2}v) = n - k - 2$. Similarly, we have $PI(v_{k-c+3}v) = n - k - 3, PI(v_{k-c+4}v) = n - k - 4, \ldots, PI(v_{n-c-1}v) = 1$. Set $E_2 = \{vv_l, l \in$

$[n-c,n-1]\}$, since $N[v_l]-N[v]=n-k-1$, we have $PI(vv_l)=n-k-1$. Set $E_3=\{v_iv_l, i\in[1,n-c-1], l\in[n-c,n-1]\}$, by Lemma 4, we have $d'(v_i,v)=2$ for $i\in[1,n-k-1]$, $d'(v_i,v)=1$ for $i\in[n-k,n-c-1]$, $d'(v_l,v)=1$ for $l\in[n-c,n-1]$. Thus, $f(w,v_iv_l)=1$ for $i\in[1,n-k-1]$ and $f(w,v_iv_l)=0$ for $i\in[n-k,n-c-1]$.

Set $w\in V(T_n^{k*})-\{v\}$, if $xy\in E(T_{n,c}^{k*})$ with x or $y\neq v$, by Lemma 2, we have $f(w,xy)=0$. Thus,

$$\begin{aligned}
PI(T_n^{k*})-PI(T_{n-1}^{k*}) &= \textstyle\sum_{xy\in\cup_{i=1}^{n-c-2}C_i} f(w,xy)+\sum_{xy\in_{i=1}^{n-k-1}D_i} f(w,xy)+\sum_{xy\in E_1\cup E_2} PI(xy)+\\
&\quad \textstyle\sum_{xy\in E_3} f(w,xy)\\
&= 0+[(2k-n-c+2)+(2k-n-c+3)+\cdots+(k-c)]\\
&\quad +[1+2+\cdots+(n-k-2)+(n-k-1)(2k-n-c+2)]\\
&\quad +c(n-k-1)+c(n-k-1)\\
&= (n-k-1)(3k-n+2)\\
&= \gamma,
\end{aligned}$$

and Theorem 2 is proved.

For $n\geq 2k-c+1$, let $\sigma=\frac{3c(n-2k+c-1)(n-2k+c)+(k-c)(2c^2+3nc-4kc+3kn-4k^2-6k+3n-2)}{3}-\frac{3c(n-2k+c-2)(n-1-2k+c)+(k-c)(2c^2+3(n-1)c-4kc+3k(n-1)-4k^2-6k+3n-2)}{3}=k^2-4kc+c^2+2nc-3c+k$. If we can show that by adding v to $T_{n-1,c}^{k*}$, $PI(T_{n,c}^{k*})=PI(T_{n-1,c}^{k*})+\sigma$, then Theorem 2 is proved.

Set $w=v$, by Lemma 4, we have $d'(v_l,v)=1$ for $l\in[n-c,n-1]$, $d'(v_i,v)=2$ for $i\in[1,n-k-1]$ and $d'(v_j,v)=1$ for $j\in[n-k,n-c-1]$. Thus, $f(w,v_lv_i)=1$ and $f(w,v_lv_j)=0$. Set $C_1=\{v_1v_2,v_1v_3,\ldots,v_1v_{k-c+1}\}, C_2=\{v_2v_3,v_2v_4,\ldots,v_2v_{k-c+2}\},\ldots,C_{n-2k+c-1}=\{v_{n-2k+c-1}v_{n-2k+c}, v_{n-2k+c-1}v_{n-2k+c+1},\ldots,v_{n-2k+c-1}v_{n-k-1}\}, C_{n-2k+c}=\{v_{n-2k+c}v_{n-2k+s+1},v_{n-2k+c}v_{n-2k+s+2},\ldots, v_{n-2k+c}v_{n-k-1}\}, C_{n-2k+c+1}=\{v_{n-2k+c+1}v_{n-2k+c+2},v_{n-2k+c+1}v_{n-2k+c+3},\ldots,v_{n-2k+c+1}v_{n-k-1}\},\ldots, C_{n-k-1}=\phi, D_{n-2k+c}=\{v_{n-2k+c}v_{n-k}\}, D_{n-2k+c+1}=\{v_{n-2k+c+1}v_{n-k},v_{n-2k+c+1}v_{n-k+1}\},\ldots,D_{n-k-1} =\{v_{n-k-1}v_{n-k},v_{n-k-1}v_{n-k+1},\ldots,v_{n-k-1}v_{n-c-1}\}$.

By Lemma 4, we can get that $d'(v_1,v)=d'(v_2,v)=2$ and $d'(v_{n-k},v)=1$, that is, $f(w,v_1v_2)=0$ and $f(w,v_1v_{n-k})=1$. Similarly, for $v_{h_1}v_{h_2}\in\cup_{i=1}^{n-k-1}C_i$ with $h_1<h_2$, we have $d'(v_{h_1},v)=d'(v_{h_2},v)=2$, that is, $f(w,v_{h_1}v_{h_2})=0$; for $v_{h_1}v_{h_2}\in\cup_{i=n-2k+c}^{n-k-1}D_i$ with $h_1<h_2$, we have $d'(v_{h_1},v)=2$ and $d'(v_{h_2},v)=1$, that is, $f(w,v_{h_1}v_{h_2})=1$. Set $C_{n-k}=\{v_{n-k}v_{n-k+1},v_{n-k}v_{n-k+2},\ldots,v_{n-k}v_{n-c-1}\}, C_{n-k+1} =\{v_{n-k+1}v_{n-k+2},v_{n-k+1}v_{n-k+3},\ldots,v_{n-k+1}v_{n-c-1}\},\ldots,C_{n-c+2}=\{v_{n-c-2}v_{n-c-1}\}$. By Lemma 4, we can get that $d'(v_{n-k},v)=d'(v_{n-k+1},v)=1$, that is, $f(w,v_{n-k}v_{n-k+1})=0$. Similarly, for $v_{h_1}v_{h_2}\in\cup_{i=n-k}^{n-c-2}C_i$ with $h_1<h_2$, we have $d'(v_{h_1},v)=d'(v_{h_2},v)=1$, that is, $f(w,v_{h_1}v_{h_2})=0$.

Set $E_1=\{vv_i, i\in[n-k,n-c-1]\}$, by Lemma 4, we have $d'(v,v_{n-k-1})=2, d'(v_{n-c-1},v_{n-k-1})=1$, $d'(v,v_i)=d'(v_{n-c-1},v_i)=1$ for $i\in[n-k,n-c-2]\cup[n-c,n-1]$ and $d'(v,v_j)=d(v_{n-c-1},v_j)=2$ for $j\in[1,n-k-2]$. Thus, $PI(vv_{n-c-1})=1$. Similarly, we have $PI(vv_{n-c-2})=2, PI(vv_{n-c-3})=3,\ldots,PI(vv_{n-k})=k-c$. Set $E_2=\{vv_l, l\in[n-c,n-1]\}$, since $N[v_l]-N[v]=n-k-1$, we have $PI(vv_l)=n-k-1$. Set $E_3=\{v_iv_l, i\in[1,n-c-1], l\in[n-c,n-1]\}$, by Lemma 4, we have $d'(v,v_i)=2, d'(v,v_l)=1$ for $i\in[1,n-k-1]$ and $d'(v,v_i)=d'(v,v_l)=1$ for $i\in[n-k,n-c-1]$. Thus, $f(w,v_iv_l)=1$ for $i\in[1,n-k-1]$ and $f(w,v_iv_l)=0$ for $i\in[n-k,n-c-1]$.

Set $w\in V(T_n^{k*})-\{v\}$, if $xy\in E(T_{n,c}^{k*})$ with x or $y\neq v$, by Lemma 2, we have $f(w,xy)=0$. Thus,

$$\begin{aligned}
PI(T_n^{k*})-PI(T_{n-1}^{k*}) &= \textstyle\sum_{xy\in\cup_{i=1}^{n-c-2}C_i} f(w,xy)+\sum_{xy\in_{i=n-2k+c}^{n-k-1}D_i} f(w,xy)+\sum_{xy\in E_1\cup E_2} PI(xy)\\
&\quad \textstyle+\sum_{xy\in E_3} f(w,xy)\\
&= 0+[1+2+3+\cdots+(k-c)]+[1+2+3+\cdots+(k-c)]\\
&\quad +c(n-k-1)+c(n-k-1)\\
&= k^2-4kc+c^2+2nc-3c+k\\
&= \sigma,
\end{aligned}$$

and Theorem 2 is proved. □

Proof of Theorem 3. For $n \geq k+2$, we will proceed it by introduction on $|T_n^k| = n$. If $n = k+2$, T_n^k is also a k-path, that is, $PI(T_n^k) = 2k$. If $n \geq k+3$, assume that Theorem 3 is true for the k-tree with at most $n-1$ vertices, let $v \in S_1(T_n^k)$ and $T_{n-1}^k = T_n^k - v$, by the induction hypothesis, we have $PI(T_{n-1}^k) \leq PI(S_{n-1}^k) = k(n-k-1)(n-k-2)$. By adding back v, let $N(v) = \{x_1, x_2, \ldots, x_k\}$ and $w = v$. Since $T_n^k[v, x_1, x_2, \ldots, x_k]$ is a $(k+1)$-clique, we have $f(w, x_i x_j) = 0$ for $i, j \in [1, k]$. By Lemmas 1 and 2, we can obtain that $PI(vx_i) \leq n-k-1$ with $i \in [1, k]$ and $f(w, xy) \leq 1$ for any edge $xy \in E(T_n^k) - E(T_n^k[v, x_1, x_2, \ldots, x_k])$. Next, set $w \in V(T_n^k) - \{v\}$, by Lemma 2, if $xy \in E(T_n^k)$ with x or $y \neq v$, we have $f(w, xy) = 0$. Since $|E(T_n^k) - E(T_n^k[v, x_1, x_2, \ldots, x_k])| = k(n-k-1)$, we have

$$
\begin{aligned}
PI(T_n^k) &= PI(T_{n-1}^k) + \textstyle\sum_{xy \in E(T_n^k - \{vx_i, i \in [1,k]\})} f(w, xy) + \sum_{i=1}^k PI(vx_i) \\
&\leq PI(S_{n-k}^k) + k(n-k-1) + k(n-k-1) \\
&= k(n-k-1)(n-k-2) + k(n-k-1) + k(n-k-1) \\
&= k(n-k)(n-k-1) \\
&= PI(S_n^k).
\end{aligned}
$$

Thus, this finishes the proof of Theorem 3. □

Proof of Theorem 4. For $k = 1$ and by Fact 1, we can get that every tree with the same vertices has the same PI-value; then, Theorem 4 is obvious; for $k \geq 2$, if $k+2 \leq n \leq 2k-c$, let $n = kp + s$ with $p = 1$ and $s = n-k$, by Theorem 1, we have $PI(P_n^k) - PI(T_{n,c}^{k*}) = \frac{(s-1)s(3k-s+2)}{3} - \frac{(n-k)(n-k-1)(4k-n+2)}{3} = \frac{(n-k-1)(n-k)[3k-(n-k)+2]}{3} - \frac{(n-k)(n-k-1)(4k-n+2)}{3} = 0$, and Theorem 4 is true. If $n \geq 2k-c+1$, $p = \frac{n-s}{k}$ and by Theorems 1 and 2, define the new functions as follows: for $z \geq 2k-c+1$, $1 \leq c \leq k-1$ and $2 \leq s \leq k+1$,

$$
\begin{aligned}
g(z) &= \tfrac{(k+1)(z-s-k)(3z+3s-2k-4)}{6} + \tfrac{s(s-1)(3k-s+2)}{3}, \\
h(z,c) &= c(z-2k+c-1)(z-2k+c) + \tfrac{(k-c)(2c^2+3zc-4kc+3kz-4k^2-6k+3z-2)}{3}, \\
l(z,c) &= g(z) - h(z,c) \\
&= (\tfrac{k}{2} + \tfrac{1}{2} - c)z^2 + (-c^2 + 2c + 4kc - \tfrac{11k^2}{6} - \tfrac{5k}{2} - \tfrac{2}{3})z \\
&+ \tfrac{ks^2}{2} - \tfrac{k^2 s}{6} - \tfrac{ks}{2} + \tfrac{5k^3}{3} + \tfrac{5k^2}{3} + \tfrac{s^2}{2} + \tfrac{4k}{3} - \tfrac{s^3}{3} - 6k^2 c + 3kc^2 - \tfrac{c^3}{3} - 4kc + c^2 - \tfrac{2c}{3}, \\
l_z(z) &= l_z(z,c) \\
&= (k+1-2c)z - c^2 + 2c + 4kc - \tfrac{11k^2}{6} - \tfrac{5k}{2} - \tfrac{2}{3}.
\end{aligned}
$$

Then, it is enough to determine whether or not $l(z,c) \geq 0$ is true. By some calculations, we can obtain the following claim:

Claim 1. *$z_1 = 2k-c+1$, $z_2 = 2k-c+2$ are the two roots of $l(z,c) = 0$ with $c \neq \frac{k+1}{2}$.*

Proof. For any $c \in [1, k-1]$, let $z_1 = 2k-c+1$, $z_2 = 2k-c+2$, and we have $l(2k-c+1, c) = 0$, $l(2k-c+2, c) = 0$. If $c \neq \frac{k+1}{2}$, then Claim is true. □

For fixed $c \in [1, \frac{k+1}{2})$, that is, $\frac{k}{2} + \frac{1}{2} - c > 0$, then the function of $l(z,c)$ about z is open up. Since z is an integer and by Fact 2, we have $l(z,c) \geq 0$ for $z \geq 2k-c+1$ and Theorem 4 is true; if $c = \frac{k+1}{2}$ and $k \geq 1$, we have $l_z(z) = \frac{1-k^2}{12} \leq 0$, that is, $l(z, \frac{k+1}{2})$ is decreasing about z. By the proof of Fact 2, we have $l(2k-c+1, c) = 0$. For $z \geq 2k-c+1$, we can get that $l(z, \frac{k+1}{2}) \leq l(2k-c+1, \frac{k+1}{2}) = 0$ and Theorem 4 is true; for fixed $c \in (\frac{k+1}{2}, k-1]$, that is, $\frac{k}{2} + \frac{1}{2} - c < 0$, then the function of $l(z,c)$ about z is open down. Since z is an integer and by Claim, we can obtain that $l(z,c) \leq 0$ for $z \geq 2k-c+1$ and this finishes the proof of Theorem 4. □

4. Conclusions

We can see that the k-stars attain the maximal values of PI-values for k-trees. One of the guesses is that the k-paths attain the minimal values. Actually, it is not the case and some PI-values of k-spirals is even smaller than that of k-paths. Meanwhile, not all PI-values of k-spirals are less than the values of all other k-trees. This fact indicates an interesting problem—which type of k-trees will achieve the minimum PI-value?

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