Computational and Applied Mathematics (2026) 45:102
https://doi.org/10.1007/s40314-025-03545-9

The subpath number of cactus graphs

Martin Knor[1,6] · Jelena Sedlar[2,4] · Riste Škrekovski[3,4,5,6] · Yu Yang[6]

Received: 21 March 2025 / Revised: 3 July 2025 / Accepted: 14 November 2025

Abstract
The subpath number of a graph G is defined as the total number of subpaths in G, and it is closely related to the number of subtrees, a well-studied topic in graph theory. This paper is a continuation of our previous paper Knor et al. (Knor M, Sedlar J, Škrekovski R, et al (2026) Invitation to the subpath number[J]. Appl Math Comput 509:129646), where we investigated the subpath number and identified extremal graphs within the classes of trees, unicyclic graphs, bipartite graphs, and cycle chains. Here, we focus on the subpath number of cactus graphs and characterize all maximal and minimal cacti with n vertices and k cycles. We prove that maximal cacti are cycle chains in which all interior cycles are triangles, while the two end-cycles differ in length by at most one. In contrast, the minimal cacti consist of k cycles, all of which are end-triangles, with the subgraph induced by the remaining vertices forming a forest. By comparing extremal cacti with respect to the subpath number to those that are extremal for the subtree number and the Wiener index, we demonstrate that the subpath number does not correlate with either of these quantities, as their corresponding extremal graphs differ.

Keywords Subpath number · Cactus graphs · Extremal graphs · Cycle chains · Wiener index · Subtree number

Mathematics Subject Classification 05C30 (Enumeration in graph theory) · 05C35 (Extremal problems in graph theory) · 05C12 (Distance in graphs) · 05C05 (Trees)

1 Introduction

The number of non-empty subtrees, denoted by $N(G)$, in a graph G was first studied in the context of trees (Székely and Wang 2005). Various properties of $N(G)$ have been explored

✉ Yu Yang
yangyu@pdsu.edu.cn

1 Slovak University of Technology, Bratislava, Slovakia

2 University of Split, Faculty of Civil Engineering, Architecture and Geodesy, Split, Croatia

3 University of Ljubljana, FMF, Ljubljana, Slovenia

4 Faculty of Information Studies, Novo Mesto, Slovenia

5 Rudolfovo - Science and Technology Centre, Novo Mesto, Slovenia

6 School of Software, Pingdingshan University, Pingdingshan, China

Published online: 15 December 2025

for several subclasses of trees (Kirk and Wang 2008; Székely and Wang 2007; Zhang et al. 2013), and more recently, research on the number of subtrees has been extended to certain classes of general graphs (Li et al. 2022; Xu et al. 2021). For further interesting results on this topic, we refer the reader to Czabarka et al. (2009); Yang et al. (2021, 2020, 2022). The subtree number can attain extremely high values, making its exact evaluation challenging.

Motivated by this, in our previous paper (Knor et al. 2025) we studied the subpath number of G which is defined as the total number of all subpaths in G, including those of zero length. The subpaths are here defined to be any subgraph of G which is a path. Since every path is a tree, and not every tree is a path, the subpath number is obviously smaller than the subtree number, so it should be more tractable. On the other hand, this quantity is still challenging due to the result from Yamamoto (2009), where it is established that the complexity of counting subpaths is $\#P$-hard.

In our previous paper, we established several preliminary results for the subpath number, such as the exact value of the subpath number for trees and unicyclic graphs, as well as its behavior under edge insertion, which led to identifying the extremal graphs among all connected graphs on n vertices. Additionally, we examined bipartite graphs and cycle chains, determining the extremal graphs within each of these families. Moreover, for cycle chains, we provided an exact formula for the subpath number.

The Wiener index $W(G)$ of a graph G is defined as the sum of the distances over all pairs of vertices in G. Introduced in Wiener's seminal paper (Wiener 1947), it was originally shown to correlate with the chemical properties of certain molecular compounds. Since then, the Wiener index has become one of the most extensively studied indices in chemical graph theory; for an overview of key results, we refer the reader to the surveys (Knor et al. 2016, 2024). Interestingly, a "negative" correlation has been observed between the number of subtrees and the Wiener index: in many graph classes, the graph that maximizes the number of subtrees also minimizes the Wiener index, and vice versa. This phenomenon has been noted in several graph families, including cactus graphs (Xu et al. 2022), i.e. graphs in which all cycles are edge disjoint.

Motivated by these observations, in this paper, we investigate the behavior of the subpath number in the class of cactus graphs, where both the number of vertices and the number of cycles are prescribed. We fully characterize the cacti that minimize and maximize the subpath number. Furthermore, we demonstrate that the subpath number does not exhibit a direct correlation with either the Wiener index or the subtree number, as the extremal cactus graphs with respect to the subpath number differ from those in the other two cases. This suggests that the subpath number is an interesting graph invariant worthy of independent study.

2 Preliminaries

A graph $G' = (V', E')$ is a *subgraph* of $G = (V, E)$ if $V' \subseteq V$ and $E' \subseteq E$. A *subpath* of G is any subgraph of G which is a path. For a graph G, the *subpath number* is defined as the number of paths in G, including paths of length 0. The subpath number of a graph G is denoted by $\mathrm{pn}(G)$. Before delving into specific cases, let us first explore some fundamental properties of this quantity.

We begin by considering trees with n vertices. It is well known that every pair of vertices in a tree is connected by a unique path. In a tree T on n vertices there are $\binom{n}{2}$ pairs of two distinct vertices which are end-vertices of the path of length ≥ 1, and there are n vertices each of which is a path of length zero, so the following observation easily follows.

Observation 1 *If T is a tree on n vertices, then* $\mathrm{pn}(T) = \binom{n+1}{2}$.

Since unicyclic graphs are obtained from trees by introducing a single edge, a natural next step is to analyze unicyclic graphs with n vertices. In a unicyclic graph G containing a cycle of length g, removing the edges of the cycle results in precisely g connected components. The following result, established in Knor et al. (2025), provides an explicit formula for the subpath number of such graphs.

Proposition 2 *Let G be a unicyclic graph on n vertices with the cycle C of length g. Denote by $n_1, n_2, \ldots, n_g$ the number of vertices in the components that remain after removing all edges of C. Then,*

$$\mathrm{pn}(G) = n + 2\binom{n}{2} - \binom{n_1}{2} - \binom{n_2}{2} - \cdots - \binom{n_g}{2}.$$

This result immediately allows us to determine the subpath number for cycles on n vertices, as well as the extremal unicyclic graphs.

Corollary 3 *For a cycle on n vertices, we have* $\mathrm{pn}(C_n) = n^2$.

Corollary 4 *Among unicyclic graphs with n vertices,* $\mathrm{pn}(G)$ *attains its maximum value if and only if $G = C_n$, and its minimum value if and only if the only cycle in G is a triangle with two of its vertices having degree two.*

Next, we examine how the subpath number behaves when an edge is removed. The following lemma, established in Knor et al. (2025), formalizes this observation.

Lemma 5 *Let G be a connected graph on n vertices, and let e be an edge of G. Let G' be the graph obtained from G by removing the edge e. Then,*

$$\mathrm{pn}(G') < \mathrm{pn}(G).$$

This result immediately implies the characterization of extremal graphs with respect to the subpath number among all connected graphs with n vertices, as stated in the following theorem from Knor et al. (2025).

Theorem 6 *Let G be a connected graph on n vertices. Then*

$$\binom{n+1}{2} \leq \mathrm{pn}(G) \leq \frac{n!}{2}\sum_{i=0}^{n-1}\frac{1}{i!} + \frac{n}{2},$$

where the lower bound is attained if and only if G is a tree, and the upper bound if and only if $G = K_n$.

3 Maximal cacti with respect to the subpath number

A *cactus graph* is any graph in which all cycles are pairwise edge disjoint. Denote by $\mathcal{C}_{n,k}$ the class of all cactus graphs on n vertices with k cycles. In this section we will characterize cactus graphs from $\mathcal{C}_{n,k}$ with the maximum value of the subpath number. In the next section we will do the same for the minimum value of the subpath number. Once we do that, we can compare the extremal cacti for the subpath number with the extremal cacti for the Wiener index and the number of subtrees. It turns out that the subpath number is not correlated with either of these quantities.

Let us first define two notions we use in this subsection. A *bridge* in a graph G is any edge e of G such that $G - e$ has more connected components than G. A graph is *bridgeless* if it has no bridges. Notice that a bridgeless graph does not contain leaves. In order to characterize cactus graphs from $\mathcal{C}_{n,k}$ with the maximum value of the subpath number, we will use three cactus transformations. In the first transformation we will address bridges of a cactus graph, in the second the incidence structure of the cycles, and in the third the size of the cycles.

Lemma 7 *If a cactus graph $G \in \mathcal{C}_{n,k}$ contains a bridge, then there exists a bridgeless cactus graph $G' \in \mathcal{C}_{n,k}$ such that* $\mathrm{pn}(G') > \mathrm{pn}(G)$.

Proof Let $e = uv$ be a bridge of G such that one of its end-vertices belongs to a cycle C, say $v \in V(C)$. If G has bridges, such an edge e must exist. Let w be the neighbor of v on C, and let G' be the graph obtained from G by removing the edge vw and adding the edge uw instead. Obviously, $G' \in \mathcal{C}_{n,k}$ and G' has one bridge less than G.

Let us prove that $\mathrm{pn}(G') > \mathrm{pn}(G)$. To see this, denote by $\mathcal{P}$ (resp. $\mathcal{P}'$) the set of all paths in G (resp. G'). We partition the set $\mathcal{P}$ into three parts, $\mathcal{P}_1$ contains all paths P of $\mathcal{P}$ such that $uv \in E(P)$ and $vw \in E(P)$, $\mathcal{P}_2$ all paths P of $\mathcal{P}$ with $uv \notin E(P)$ and $vw \in E(P)$, and $\mathcal{P}_3$ all the remaining paths of $\mathcal{P}$. Next, a function $f : \mathcal{P} \to \mathcal{P}'$ is defined as follows:

- If $P \in \mathcal{P}_1$ then $f(P) \in \mathcal{P}'$ is a path obtained from P by replacing subpath uvw by the edge uw. Notice that $f(P)$ contains uw, but not uv.
- If $P \in \mathcal{P}_2$ then $f(P) \in \mathcal{P}'$ is a path obtained from P by replacing the edge vw by the subpath vuw. Notice that $f(P)$ contains both uw and uv.
- If $P \in \mathcal{P}_3$, then $f(P) = P$. Notice that $f(P)$ does not contain uw.

Let us show that f is an injection. For that purpose, let P_1 and P_2 be two distinct paths in $\mathcal{P}$. If $P_1 \in \mathcal{P}_i$ and $P_2 \in \mathcal{P}_j$ for $i < j$, then $f(P_1)$ and $f(P_2)$ differ either in the edge uw or in the edge uv. On the other hand, if P_1 and P_2 belong to the same $\mathcal{P}_i$, then they differ in the part of the path not changed by the function f, so $f(P_1)$ and $f(P_2)$ are distinct in G'. Hence, in all cases we have established $f(P_1) \neq f(P_2)$, so f is an injection.

Let us next show that f is not a surjection. To see this, notice that uv is the only path connecting u and v in G, and $f(u, v) = uv$. On the other hand, there are two paths connecting u and v in G'. Since the function f preserves the end-vertices of a path, this implies that f is not a surjection.

We have established a function f between $\mathcal{P}$ and $\mathcal{P}'$ which is injection, but not surjection, so we can conclude that $|\mathcal{P}| < \left|\mathcal{P}'\right|$ which means $\mathrm{pn}(G) < \mathrm{pn}(G')$. Applying repeatedly this transformation until we obtain a graph without bridges yields the claim of the lemma.

□

The above lemma confirms that, in the case of unicyclic graphs, the subpath number attains the maximum value only for the cycle C_n, which is already established in Corollary 4. In what follows, we will deal with the cacti with at least two cycles.

A vertex v of a bridgeless cactus graph G is an *intersection vertex* if v belongs to at least two cycles of G. Let $\mathcal{V}$ be the set of all intersection vertices of G and let $\mathcal{C}$ be the set of all cycles of G. A *cycle-incidence graph* T_G of a bridgeless cactus graph G is defined as the graph on the set of vertices $\mathcal{V} \cup \mathcal{C}$ such that an intersection vertex $v \in \mathcal{V}$ and a cycle $C \in \mathcal{C}$

are connected by an edge in T_G if v belongs to the cycle C in G. Notice that T_G is a tree and every leaf in T_G is a vertex of $\mathcal{C}$. A *cactus chain* is a bridgeless cactus graph G such that T_G is a path. Notice that every cycle of G has a corresponding vertex in T_G. Hence, we will refer by "cycle" to the cycle of G as well as to the corresponding vertex of T_G.

Lemma 8 *Let $G \in \mathcal{C}_{n,k}$ be a bridgeless cactus graph with $k \geq 2$. If G is not a cactus chain, then there exists a cactus chain $G' \in \mathcal{C}_{n,k}$ such that* $\mathrm{pn}(G') > \mathrm{pn}(G)$.

Proof Since T_G is not a path, it must contain at least one vertex whose degree is at least three. Denote by t such a vertex of T_G. A component of $T_G - t$ which does not contain a vertex of degree ≥ 3 is called a *thread*. Denote by $T_1, T_2, \ldots, T_k$ all the components of $T_G - t$. Notice that t can be chosen so that all components of $T_G - t$, except at most one, are threads. So, we may assume that $T_1, \ldots, T_{k-1}$ are all threads. Since $k \geq 3$, this implies T_1 and T_2 are both threads. For a component T_i of T_G, denote by $V(T_i)$ the set of vertices of G contained in cycles whose corresponding vertices of T_G belong to T_i. Since T_1 and T_2 are both threads, we may assume $|V(T_1)| \leq |V(T_2)|$, as otherwise we can just swapp the labeling of T_1 and T_2.

We now introduce a graph transformation of G into G' which, as we will establish, increases the subpath number. Recall that t is a vertex of T_G. Since $V(T_G) = \mathcal{V} \cup \mathcal{C}$ where $\mathcal{V}$ and $\mathcal{C}$ are disjoint sets, we have either $t \in \mathcal{V}$ or $t \in \mathcal{C}$. If $t \in \mathcal{V}$, then we set $u = t$ and denote by C a cycle of T_k containing u. On the other hand if $t \in \mathcal{C}$, then we denote by u a vertex of T_k incident with t and denote by C the cycle of T_k containing u. Let v and w be the neighbors of u on C in G. Further, let z be a vertex of degree 2 on the cycle in G which corresponds to the leaf of T_1 in T_G. Graph G' is defined as the graph obtained from G by removing edges vu and wu, and adding edges vz and wz instead. Notice that G' belongs to $\mathcal{C}_{n,k}$.

We now show that $\mathrm{pn}(G) < \mathrm{pn}(G')$. For a pair of vertices $x, y \in V(G)$, denote by $\mathrm{pn}_G(x, y)$ the number of paths in G which connect vertices x and y. Denote further $\Delta(x, y) = \mathrm{pn}_{G'}(x, y) - \mathrm{pn}_G(x, y)$, and notice that

$$\mathrm{pn}(G') - \mathrm{pn}(G) = \sum_{x,y \in V(G)} \Delta(x, y).$$

Observe that $\Delta(x, y)$ may be negative only if x belongs to a cycle of T_k and y belongs to a cycle of T_1. Since $|V(T_1)| \leq |V(T_2)|$, there exists an injection $f : V(T_1) \to V(T_2)$. It is sufficient to prove that $\Delta(x, y) + \Delta(x, f(y)) > 0$, for any $x \in V(T_k)$ and $y \in V(T_1)$.

For a pair of vertices $x, y \in V(G)$, we define the corresponding path $P_{x,y}$ in T_G. Assume that x belongs to a cycle C_x of G and y belongs to C_y. If neither x nor y are intersection vertices in G, then $P_{x,y}$ is the path of T_G which connects the cycles C_x and C_y. If x (resp. y) is an intersection vertex of G, then $P_{x,y}$ starts with x (resp. ends with y) in T_G. In other words, if x (resp. y) belongs to more than one cycle of G, then $P_{x,y}$ in T_G may contain only one cycle of G to which x (resp. y) belongs. Next, for a pair of vertices $x, y \in V(G)$, the number $c(x, y)$ is defined as the number of cycles on $P_{x,y}$.

Let us proceed with proving that $\Delta(x, y) + \Delta(x, f(y)) > 0$, for any $x \in V(T_k)$ and $y \in V(T_1)$. Denote by c the number of cycles in T_1. If t is an intersection vertex, we have

$$\begin{aligned}\Delta(x, y) + \Delta(x, f(y)) &\geq 2^{c(x,t)}(2 - 2^c + 2^{c(t,f(y))+c} - 2^{c(t,f(y))}) \\ &= 2^{c(x,t)}\big((2^c - 1)(2^{c(t,f(y))} - 1) + 1\big) > 0.\end{aligned}$$

If t is a cycle, we have

$$\Delta(x, y) + \Delta(x, f(y)) \geq 2^{c(x,t)}(2 - 2^{c+1} + 2^{c+1+c(t,f(y))} - 2^{1+c(t,f(y))})$$

Fig. 1 A pseudo triangle chain PTC(14, 5)

$$= 2^{c(x,t)}(2^c - 1)(2^{1+c(t,f(y))} - 2) > 0,$$

since $c \geq 1$ and $c(t, f(y)) \geq 1$. Hence, we have established that $\mathrm{pn}(G) < \mathrm{pn}(G')$. Notice that the sum of the degrees over all vertices of T_G of degree at least 3 has decreased from G to G', so applying this transformation repeatedly yields a bridgeless cactus chain G'. □

A cycle C of a bridgeless cactus graph G is an *end-cycle* if at most one of its vertices has degree greater than two, otherwise C is an *interior* cycle. Notice that a cactus chain $G \in \mathcal{C}_{n,k}$ with $k \geq 2$ contains precisely two end-cycles. A *pseudo triangle chain,* denoted by $\mathrm{PTC}(n, k)$, is a cactus chain from $\mathcal{C}_{n,k}$ in which every interior cycle is a triangle and the two end-cycles differ in the number of vertices by at most one. This notion is illustrated by Fig. 1.

Lemma 9 *Let* $G \in \mathcal{C}_{n,k}$ *be a bridgeless cactus chain, where* $k \geq 2$. *If* G *is distinct from* $\mathrm{PTC}(n, k)$, *then* $\mathrm{pn}(\mathrm{PTC}(n, k)) > \mathrm{pn}(G)$.

Proof A graph G, since it is a bridgeless cactus chain, may contain interior cycles which are not triangle. On the other hand, all interior cycles of $\mathrm{PTC}(n, k)$ are triangles. Hence, we will first show that a bridgeless cactus chain G which contains interior cycles which are not triangles can be transformed into a bridgeless cactus chain G' with larger value of the subpath number. After that, we will adrress the end-cycles and show that their number of vertices must be balanced, otherwise G is not maximal.

Assume first that there exists an interior cycle C of G which is not a triangle. Notice that in a cactus chain every interior cycle contains precisely two intersection vertices. This implies that C contains precisely two intersection vertices. Notice that C has more than two vertices, so there exists a vertex u on C which is not an intersection vertex. Since u is not an intersection vertex of C and G is bridgeless, it follows that u has precisely two neighbors, denote by v and w, both of which belong to C. Denote by G_1 and G_2 the two connected components of $G - V(C)$, where we may assume the components are denoted so that $|V(G_1)| \leq |V(G_2)|$. Notice that each of the components G_1 and G_2 must contain vertices of precisely one end-cycle of G. Let a be a vertex of the end-cycle of G which is contained in G_1 such that a is not an intersection vertex of G. Denote by b a neighbor of a. Let G' be a graph obtained from G by removing edges uv, uw and ab, and adding edges ua, ub and vw instead. Notice that G' is also a bridgeless cactus chain on n vertices with k cycles.

We wish to establish that $\mathrm{pn}(G) < \mathrm{pn}(G')$. Again, denote $\Delta(x, y) = \mathrm{pn}_{G'}(x, y) - \mathrm{pn}_G(x, y)$ and notice that $\Delta(x, y)$ may be negative only if $x = u$ and $y \in V(G_1)$. Since $|V(G_1)| \leq |V(G_2)|$, there exists an injection $f : V(G_1) \to V(G_2)$. Denote by c the number of cycles in G_1. Notice that for each $y \in V(G_1)$ it holds that

$$\begin{aligned}\Delta(x, y) + \Delta(x, f(y)) &\geq 2 - 2^{c+1} + 2^{c(x,f(y))+c} - 2^{c(x,f(y))} \\ &= (2^c - 1)(2^{c(x,f(y))} - 2) > 0,\end{aligned}$$

since $c \geq 1$ and $c(x, f(y)) \geq 2$. Applying repeatedly this transformation yields a bridgeless cactus chain G' in which all interior cycles are triangles, such that $\mathrm{pn}(G) < \mathrm{pn}(G')$. Assume that cycles of G' are denoted by $C_1, \ldots, C_k$ such that C_1 and C_k are end-cycles, and the pair of cycles C_i and C_{i+1} share an intersection vertex for every $i = 1, \ldots, k-1$. If the end-cycles C_1 and C_k of G' differ in the number of vertices by at most one, we are done. So, let us assume that $|V(C_k)| - |V(C_1)| \geq 2$.

Let u be a vertex of C_k which is not an intersection vertex, and let v and w be the two neighbors of u in G'. Let a be a vertex of C_1 which is not an intersection vertex and let b be a neighbor of a. Denote by G'' the graph obtained from G' by removing edges uv, uw and ab and adding edges vw, ua and ub instead.

We prove that $\mathrm{pn}(G') < \mathrm{pn}(G'')$. Denote $\Delta(x, y) = \mathrm{pn}_{G''}(x, y) - \mathrm{pn}_{G'}(x, y)$ and notice that $\Delta(x, y)$ may be negative only if $x = u$ and $y \in \big(V(C_1) \cup \cdots \cup V(C_{k-1})\big) \setminus V(C_k)$. Since $|V(C_1)| < |V(C_k)|$ and every interior cycle of G' is a triangle, there exists an injection

$$f : V(C_1) \cup \cdots \cup V(C_{k-1}) \to V(C_2) \cup \cdots \cup V(C_k)$$

such that $f(y) \in V(C_{k+1-i})$ if and only if $y \in V(C_i)$. Observe that if y is the intersection vertex of $V(C_i) \cap V(C_{i+1})$ then $f(y)$ is the intersection vertex of C_{k+1-i} with C_{k-i}. Assume that $y \in V(C_i) \setminus \big(V(C_{i+1} \cup V(C_{i-1})\big)$ for $1 \leq i \leq k-1$. Then, $\mathrm{pn}_{G'}(x, y) = 2^{k-(i-1)}$ and $\mathrm{pn}_{G''}(x, y) = 2^i$. Also, it holds that $\mathrm{pn}_{G'}(x, f(y)) = 2^{k-(k+1-i-1)}$ and $\mathrm{pn}_{G''}(x, y) = 2^{k+1-i}$. Hence, we have

$$\Delta(x, y) + \Delta(x, f(y)) = 2^i - 2^{k-(i-1)} + 2^{k+1-i} - 2^{k-(k+1-i-1)} = 0.$$

Now assume that $y \in V(C_i) \cap V(C_{i-1})$ for $2 \leq i \leq k-1$. Then $\mathrm{pn}_{G'}(x, f(y)) = 2^{k-(k+1-i)}$ and $\mathrm{pn}_{G''}(x, f(y)) = 2^{k+1-i}$. Hence, we have

$$\Delta(x, y) + \Delta(x, f(y)) = 2^{i-1} - 2^{k-(i-1)} + 2^{k+1-i} - 2^{k-(k+1-i)} = 0.$$

Also, $|V(C_1)| < |V(C_k)|$ implies that f is not a surjection, so there exists a vertex $z \in V(C_k)$ which is not in the image of f. For such a vertex z, we have

$$\Delta(u, z) = 2^k - 2 > 0,$$

since $k > 2$. We conclude that $\mathrm{pn}(G') < \mathrm{pn}(G'')$. Applying this transformation repeatedly yields the graph $\mathrm{PTC}(n, k)$, and we are done. □

Lemmas 7–9 immediately yield the following result.

Theorem 10 *The graph* $\mathrm{PTC}(n, k)$ *uniquely maximizes the subpath number among all cacti on n vertices with* $k \geq 2$ *cycles.*

By Theorem 10, it is useful to calculate the subpath number of $\mathrm{PTC}(n, k)$.

Lemma 11 *The subpath number of* $\mathrm{PTC}(n, k)$ *equals*

$$(n^2 - 4kn + 14n + 4k^2 - 28k + 49)2^{k-2} + \tfrac{1}{2}(n^2 - 4kn - 6n + 4k^2 - 4k + 7) + \delta,$$

where $\delta = 0$ *if n is odd, and* $\delta = 1 - 2^{k-2}$ *if n is even.*

Proof Denote by $C_1, C_2, \ldots, C_k$ the cycles in the cactus chain $\mathrm{PTC}(n, k)$, so that C_i and C_{i+1} have a vertex in common, say w_i, where $1 \leq i \leq k-1$. Assume that $|V(C_1)| \geq |V(C_k)|$. Then $|V(C_1)| = n_1 = \lceil \frac{n-2k+5}{2} \rceil$, $|V(C_k)| = n_2 = \lfloor \frac{n-2k+5}{2} \rfloor$, and $|V(C_i)| = 3$ if $2 \leq i \leq k-1$.

We count the number of $u - v$ paths when u and v are in a same cycle, then the number of $u - v$ paths when u and v are in neighboring cycles but not in their intersection, then the number of $u - v$ paths when $u \in V(C_i)$ and $v \in V(C_{i+2})$ but $u, v \notin V(C_{i+1})$, etc. However, we sum the number of paths in the opposite order.

Observe that if $u \in V(C_i)\backslash\{w_i\}$ and $v \in V(C_j)\backslash\{w_{j-1}\}$, where $1 \le i < j \le k$, then $\mathrm{PTC}(n,k)$ contains 2^{j-i+1} paths connecting u with v since in every cycle $C_i, C_{i+1}, \dots, C_j$ we can choose one of the two possibilities of how to traverse it. So we have

$$\begin{aligned}\mathrm{pn}(\mathrm{PTC}(n,k)) &= (n_1-1)(n_2-1)2^k + \sum_{i=1}^{k-2} 2(n_1-1)2^{i+1} + \sum_{i=1}^{k-2} 2(n_2-1)2^{i+1}\\ &\quad + \sum_{i=1}^{k-3} 2\cdot 2\cdot 2^{i+1}(k-2-i) + n_1^2 + n_2^2 + (k-2)3^2 - (k-1),\end{aligned}$$

where the last term $-(k-1)$ appears since in $n_1^2 + n_2^2 + (k-2)3^2$ we counted the paths of length 0 consisting of cut-vertices $w_1, w_2, \dots, w_{k-1}$ twice.

Since $\sum_{i=1}^{t} 2^i = 2^{t+1} - 2$, the sum of the first two sums is $(n_1+n_2-2)(2^{k+1}-8)$. And since $\sum_{i=1}^{t} i\cdot 2^{i-1} = t\cdot 2^{t+1} - (t+1)2^t$, the third sum equals $(k-2)(2^{k+1}-16) - (k-3)2^{k+2} + (k-2)2^{k+1} = 2^{k+2} - 16k + 32$. So the expression for the subpath number of $\mathrm{PTC}(n,k)$ reduces to

$$\begin{aligned}\mathrm{pn}(\mathrm{PTC}(n,k)) &= (n_1-1)(n_2-1)2^k + (n_1+n_2-2)(2^{k+1}-8) + 2^{k+2} - 16k + 32\\ &\quad + n_1^2 + n_2^2 + 8k - 17.\end{aligned}$$

Now if n is odd, we get

$$\begin{aligned}\mathrm{pn}(\mathrm{PTC}(n,k)) &= \left(\frac{n-2k+3}{2}\right)^2 \cdot 2^k + (n-2k+3)(2^{k+1}-8) + 2^{k+2}\\ &\quad + 2\left(\frac{n-2k+5}{2}\right)^2 - 8k + 15,\end{aligned}$$

which reduces to

$$\begin{aligned}\mathrm{pn}(\mathrm{PTC}(n,k)) &= (n^2 - 4kn + 14n + 4k^2 - 28k + 49)2^{k-2}\\ &\quad + \tfrac{1}{2}(n^2 - 4kn - 6n + 4k^2 - 4k + 7).\end{aligned}$$

On the other side when n is even, we get

$$\begin{aligned}\mathrm{pn}(\mathrm{PTC}(n,k)) &= \left(\frac{n-2k+4}{2}\right)\left(\frac{n-2k+2}{2}\right) \cdot 2^k + (n-2k+3)(2^{k+1}-8) + 2^{k+2}\\ &\quad + \left(\frac{n-2k+6}{2}\right)^2 + \left(\frac{n-2k+4}{2}\right)^2 - 8k + 15,\end{aligned}$$

which reduces to

$$\begin{aligned}\mathrm{pn}(\mathrm{PTC}(n,k)) &= (n^2 - 4kn + 14n + 4k^2 - 28k + 48)2^{k-2}\\ &\quad + \tfrac{1}{2}(n^2 - 4kn - 6n + 4k^2 - 4k + 9).\end{aligned}$$

□

4 Minimal cacti with respect to the subpath number

After we have characterized maximal cacti from $\mathcal{C}_{n,k}$ with respect to the subpath number, our next goal is to establish minimal cacti in the same class. We will use the same approach

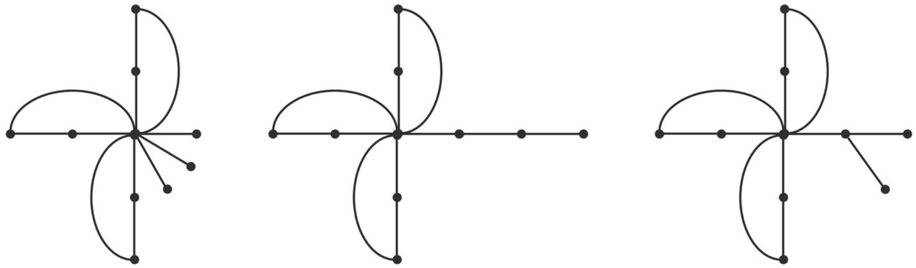

Fig. 2 The figure shows three distinct cactus graphs from $\mathcal{C}_{10,3}$. All these graphs minimize the subpath number in $\mathcal{C}_{10,3}$.

of graph transformation, in a way that we will first address the size of cycles of G by the transformation inverse to the one of Lemma 7, which creates additional bridges. Then we will address the interior cycles of G and thus arrive to all the minimal cacti in $\mathcal{C}_{n,k}$.

Lemma 12 *Let $G \in \mathcal{C}_{n,k}$ be a cactus graph. If G contains a cycle which is not a triangle, then there exists a cactus graph $G' \in \mathcal{C}_{n,k}$ in which every cycle is a triangle such that* $\text{pn}(G) > \text{pn}(G')$.

Proof Let C be a cycle of G which is not a triangle and let uv be an edge of C. Denote by w the other neighbor of u on C. Let G' be the graph obtained from G by removing the edge uv and adding the edge vw. We may consider that the graph G is obtained from G' by removing the edge vw from it and adding the edge uw instead. Then Lemma 7 implies $\text{pn}(G) > \text{pn}(G')$. Applying the transformation repeatedly yields the result. □

An end-cycle of G which is a triangle will be called an *end-triangle*. Observe that end-triangle has only one vertex whose degree is greater than 2. We have reduced the problem of finding minimal cacti to the class of cacti in which every cycle is a triangle. Let us further show that no triangle of minimal cacti can be interior, i.e., minimal cacti have only end-triangles.

Lemma 13 *Let $G \in \mathcal{C}_{n,k}$ be a cactus graph in which every cycle is a triangle. If there exists an interior triangle in G, then there exists a cactus graph $G' \in \mathcal{C}_{n,k}$ in which every cycle is an end-triangle such that* $\text{pn}(G) > \text{pn}(G')$.

Proof Let $C = u_1u_2u_3u_1$ be an interior triangle of G. We may assume that the degrees of the vertices u_1 and u_2 on the cycle C are greater than 2. Denote by G_i the connected component of $G - E(C)$ which contains the vertex u_i, for $i = 1, 2, 3$. Let G' be a graph obtained from G by removing the edge xu_2 and adding the edge xu_1, for every vertex x of G_2 adjacent to u_2. Notice that $\text{pn}_G(a, b)$ increases only if $a = u_2$ and $b \in V(G_2)\setminus\{u_2\}$. But if $b \in V(G_2)\setminus\{u_2\}$ then $\text{pn}_G(b, u_2) + \text{pn}_G(b, u_1) = \text{pn}_{G'}(b, u_1) + \text{pn}_{G'}(b, u_2)$. And since for $a \in V(G_2)\setminus\{u_2\}$ and $b \in V(G_1)\setminus\{u_1\}$ we have $\text{pn}_G(a, b) > \text{pn}_{G'}(a, b)$, we conclude that $\text{pn}(G) > \text{pn}(G')$. Applying the transformation repeatedly yields the result. □

Figure 2 shows three distinct graphs from $\mathcal{C}_{10,3}$ in which every cycle is an end-triangle. In the next theorem we show that all such graphs have the same subpath number, so they all minimize the subpath number.

Theorem 14 *A cactus graph $G \in \mathcal{C}_{n,k}$ has a minimum possible value of the subpath number if and only if every cycle of G is an end-triangle.*

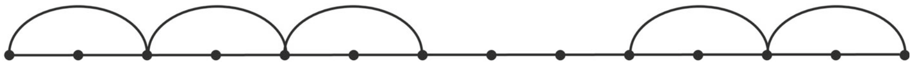

Fig. 3 The balanced saw graph BSG(14, 5)

Proof Lemmas 12 and 13 imply that it is sufficient to establish that all cactus graphs of $\mathcal{C}_{n,k}$ in which every cycle is an end-triangle have the same value of the subpath number. To see this, let $G \in \mathcal{C}_{n,k}$ be such a cactus graph, and let us partition the set of vertices V_1 and V_2, so that V_1 consists of all vertices of cycles in G which have the degree two and $V_2 = V(G)\setminus V_1$. Notice that $\mathrm{pn}_G(x, y) = 1$ if and only if both x and y belong to V_2. Further, $\mathrm{pn}_G(x, y) = 2$ for $x \in V_1$ and either $y \in V_2$ or y belongs to the same triangle as x. Finally, $\mathrm{pn}_G(x, y) = 4$ if $x, y \in V_1$ such that x and y belong to distinct triangles. We conclude that

$$\mathrm{pn}(G) = n + \binom{|V_2|}{2} + 2k + 2\,|V_1|\,|V_2| + 4\binom{k}{2} \cdot 4.$$

Plugging in $|V_1| = 2k$ and $|V_2| = n - 2k$, we obtain

$$\mathrm{pn}(G) = 2k^2 + 2kn - 5k + \frac{1}{2}n^2 + \frac{1}{2}n.$$

Since the expression for $\mathrm{pn}(G)$ depends only on the number of vertices and cycles, we are done. □

Now that we have characterized cactus graphs from $\mathcal{C}_{n,k}$ which maximize and minimize the subpath number, we can summarize our results in the following corollary, which is a direct consequence of Theorems 10 and 14.

Corollary 15 *For a cactus graph $G \in \mathcal{C}_{n,k}$, it holds that*

$$\tfrac{1}{2}(n^2 + 4kn + n + 4k^2 - 10k) \le \mathrm{pn}(G) \le (n^2 - 4kn + 14n + 4k^2 - 28k + 49)2^{k-2} + \tfrac{1}{2}(n^2 - 4kn - 6n + 4k^2 - 4k + 7) + \delta,$$

where $\delta = 0$ if n is odd, and $\delta = 1 - 2^{k-2}$ if n is even. The left inequality is attained if and only if every cycle of G is an end-triangle, and the right inequality is attained if and only if $G = \mathrm{PTC}(n, k)$.

Let us now compare extremal cacti with respect to the subpath number to those with respect to the Wiener index and the number of subtrees. To do that, we first need to introduce some particular cacti from the class $\mathcal{C}_{n,k}$. The *balanced saw* graph $\mathrm{BSG}(n, k)$ is a cactus graph from $\mathcal{C}_{n,k}$ obtained by joining a vertex of an end of a triangle chain with $\lceil k/2\rceil$ cycles to a vertex of a triangle chain with $\lfloor k/2\rfloor$ cycles by a path with $n - 2k - 2$ interior vertices. This notion is illustrated by Fig. 3. A *pseudo friendship* graph $\mathrm{PFG}(n, k)$ is a cactus graph from $\mathcal{C}_{n,k}$ obtained from k triangles, all sharing a common vertex, and $n - 2k - 1$ pendant edges attached to the same vertex. An example of a pseudo friendship graph is the leftmost graph from Fig. 2.

In Liu and Lu (2007); Gutman et al. (2017) the following result on the Wiener index is established.

Theorem 16 *The graph $\mathrm{BSG}(n, k)$ uniquely maximizes and the graph $\mathrm{PFG}(n, k)$ uniquely minimizes the Wiener index among all cacti from $\mathcal{C}_{n,k}$.*

In Li et al. (2022); Liu and Lu (2007) the following result is established regarding the subtree index, which is yet another fact supporting the observation that minimal graphs for the Wiener index maximize the subtree index and vice versa.

Theorem 17 *The graph* $\mathrm{PFG}(n,k)$ *uniquely maximizes and the graph* $\mathrm{BSG}(n,k)$ *uniquely minimizes the subtree index among all cacti from* $\mathcal{C}_{n,k}$.

Comparing extremal graphs from Theorems 16 and 17 with the extremal graphs from Corollary 15, it is observable that the graph $\mathrm{BSG}(n,k)$ which uniquely maximizes the Wiener index is distinct from the graph $\mathrm{PTC}(n,k)$ which uniquely maximizes the subpath number. As for the graph $\mathrm{PFG}(n,k)$ which uniquely minimizes the Wiener index (resp. uniquely maximizes the subtree index), it minimizes the subpath number also, but not uniquely, as there are many more graphs which minimize the subpath number and which are not minimal with respect to the Wiener index, see Fig. 2.

Acknowledgements This work is partially supported by Slovak research grants VEGA 1/0069/23, VEGA 1/0011/25, APVV-22-0005 and APVV-23-0076, by Slovenian Research and Innovation Agency ARIS program P1-0383, project J1-3002, bilateral Croatian-Slovenian project BI-HR/25-27-004 and the annual work program of Rudolfovo, by Project KK.01.1.1.02.0027 co-financed by the Croatian Government and the European Union through the European Regional Development Fund—the Competitiveness and Cohesion Operational Programme, by Croatian Ministry of Science, Education and Youth through the bilateral Croatian-Slovenian project 2025-26 and by the Key Scientific and Technological Project of Henan Province, China (grant nos. 252102521077, 252102240118, 242102521023), China Henan International Joint Laboratory for Multidimensional Topology and Carcinogenic Characteristics Analysis of Atmospheric Particulate Matter (PM2.5).

Data Availability Our manuscript has no associated data.

Declarations

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

References

Czabarka É, Székely L, Wagner S (2009) The inverse problem for certain tree parameters. Discrete Appl Math 157(15):3314–3319

Chen Y, Lin X, Zhang X (2023) The extremal average distance of cubic graphs. J Graph Theory 103(4):713–739

Gutman I, Li S, Wei W (2017) Cacti with n-vertices and t cycles having extremal Wiener index. Discrete Appl Math 232:189–200

Kirk R, Wang H (2008) Largest number of subtrees of trees with a given maximum degree. SIAM J Discrete Math 22:985–995

Knor M, Sedlar J, Škrekovski R, et al (2026) Invitation to the subpath number[J]. Appl Math Comput 509:129646

Knor M, Škrekovski R, Tepeh A (2016) Mathematical aspects of Wiener index. Ars Math Contemp 11:327–352

Knor M, Škrekovski R, Tepeh A (2024) Selected topics on Wiener index. Ars Math Contemp. https://doi.org/10.26493/1855-3974.3077.63a

Li J, Xu K, Zhang T, Wang H, Wagner S (2022) Maximum number of subtrees in cacti and block graphs. Aequat Math 96:1027–1040
Liu H, Lu M (2007) A unified approach to cacti for different indices. MATCH Commun Math Comput Chem 58:193–204
Székely LA, Wang H (2005) On subtrees of trees. Adv Appl Math 34:138–155
Székely LA, Wang H (2007) Binary trees with the largest number of subtrees. Discrete Appl Math 155:374–385
Wiener H (1947) Structural determination of paraffin boiling points. J Amer Chem Soc 69:17–20
Xu K, Li J, Luo Z (2022) Comparative results between the number of subtrees and Wiener index of graphs. RAIRO Oper Res 56:2495–2511
Xu K, Li J, Wang H (2021) The number of subtrees in graphs with given number of cut edges. Discrete Appl Math 304:283–296
Yamamoto M (2009) Approximately counting paths and cycles in a graph. Discrete Appl Math 217:381–387
Yang Y, Li X-X, Jin M-Y, Li L, Wang H, Zhang X-D (2021) Enumeration of subtrees and BC-subtrees with maximum degree no more than k in trees. Theor Comput Sci 892:258–278
Yang Y, Sun X-J, Cao J-Y, Wang H, Zhang X-D (2020) The expected subtree number index in random polyphenylene and spiro chains. Discrete Appl Math 285:483–492
Yang Y, Liu H, Wang H, Zhang X-D, Chen CP (2022) On enumerating algorithms of novel multiple leaf-distance granular regular α-subtrees of trees. Inf Comput 289:104942
Zhang XM, Zhang XD, Gray D, Wang H (2013) The number of subtrees of trees with given degree sequence. J Graph Theory 73:280–295