Minor-Obstructions for Apex Sub-unicyclic Graphs[1]

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Abstract

A graph is *sub-unicyclic* if it contains at most one cycle. We also say that a graph G is *k-apex sub-unicyclic* if it can become sub-unicyclic by removing k of its vertices. We identify 29 graphs that are the minor-obstructions of the class of 1-apex sub-unicyclic graphs, i.e., the set of all minor minimal graphs that do not belong in this class. For bigger values of k, we give an exact structural characterization of all the cactus graphs that are minor-obstructions of k-apex sub-unicyclic graphs and we enumerate them. This implies that, for every k, the class of k-apex sub-unicyclic graphs has at least $0.34 \cdot k^{-2.5}(6.278)^k$ minor-obstructions.

Keywords: Graph Minors, Obstruction set, Sub-unicyclc graphs.

1 Introduction

A graph is called *unicyclic* [17] if it contains exactly one cycle and is called *sub-unicyclic* if it contains at most one cycle. Notice that sub-unicyclic graphs are exactly the subgraphs of unicyclic graphs.

A graph H is a minor of a graph G if a graph isomorphic to H can be obtained by some subgraph of G after a series of contractions. We say that a graph class $\mathcal{G}$ is *minor-closed* if every minor of every graph in $\mathcal{G}$ also belongs in $\mathcal{G}$. We also define $\mathbf{obs}(\mathcal{G})$, called the *minor-obstruction set* of $\mathcal{G}$, as the set of minor-minimal graphs not in $\mathcal{G}$. It is easy to verify that if $\mathcal{G}$ is minor-closed, then $G \in \mathcal{G}$ iff G excludes all graphs in $\mathbf{obs}(\mathcal{G})$ as a minor. Because of Roberson and Seymour theorem [26], $\mathbf{obs}(\mathcal{G})$ is finite for every minor-closed graph class. That way, $\mathbf{obs}(\mathcal{G})$ can be seen as a *complete characterization* of $\mathcal{G}$ via a finite set of forbidden graphs. The identification of $\mathbf{obs}(\mathcal{G})$

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for distinct minor-closed classes has attracted a lot of attention in Graph Theory (see [1, 22] for related surveys).

There are several ways to construct minor-closed graph classes from others (see [22]). A popular one is to consider the set of all *k-apices* of a graph class $\mathcal{G}$, denoted by $\mathcal{A}_k(\mathcal{G})$, that contains all graphs that can give a graph in $\mathcal{G}$, after the removal of at most k vertices. It is easy to verify that if $\mathcal{G}$ is minor closed, then the same holds for $\mathcal{A}_k(\mathcal{G})$ as well, for every non-negative integer k. It was also proved in [2] that the construction of $\mathbf{obs}(\mathcal{A}_k(\mathcal{G}))$, given $\mathbf{obs}(\mathcal{G})$ and k, is a computable problem.

A lot of research has been oriented to the (partial) identification of the minor-obstructions of the k-apices, of several minor-closed graph classes. For instance, $\mathbf{obs}(\mathcal{A}_k(\mathcal{G}))$ has been identified for $k \in \{1, \ldots, 7\}$ when $\mathcal{G}$ is the set of edgeless graphs [5, 10, 11], and for $k \in \{1, 2\}$ when $\mathcal{G}$ is the set of acyclic graphs [9]. Recently, $\mathbf{obs}(\mathcal{A}_1(\mathcal{G}))$ was identified when $\mathcal{G}$ is the class of outerplanar graphs [7] and when $\mathcal{G}$ is the class of cactus graphs (as announced in [14]). A particularly popular problem is identification of $\mathbf{obs}(\mathcal{A}_k(\mathcal{G}))$ when $\mathcal{G}$ is the class of planar graphs (see e.g., [21, 22, 29]). The best advance on this question was done recently by Jobson and Kézdy [18] who identified all 2-connected minor-obstructions of 1-apex planar graphs (see also [23, 25]). Another recent result is the identification of $\mathbf{obs}(\mathcal{A}_1(\mathcal{P}))$ where $\mathcal{P}$ is the class of all pseudoforests, i.e., graphs where all connected components are sub-unicyclic [20].

A different direction is to upper-bound the size of the graphs $\mathbf{obs}(\mathcal{A}_k(\mathcal{G}))$ by some function of k. In this direction, it was proved in [16] that the size of the graphs in $\mathbf{obs}(\mathcal{A}_k(\mathcal{G}))$ is bounded by a polynomial on k in the case where the $\mathbf{obs}(\mathcal{G})$ contains some planar graph (see also [30]). Another line of research is to prove lower bounds to the size of $\mathbf{obs}(\mathcal{A}_k(\mathcal{G}))$. In this direction Michael Dinneen proved in [8] that, if all graphs in $\mathbf{obs}(\mathcal{G})$ are connected, then $|\mathbf{obs}(\mathcal{A}_k(\mathcal{G}))|$ is exponentially big. To show this, Dinneen proved a more general structural theorem claiming that, under the former connectivity assumption, every connected component of a non-connected graph in $\mathbf{obs}(\mathcal{A}_k(\mathcal{G}))$ is a graph in $\mathbf{obs}(\mathcal{A}_{k'}(\mathcal{G}))$, for some $k' < k$. Another way to prove lower bounds to $|\mathbf{obs}(\mathcal{A}_k(\mathcal{G}))|$ is to completely characterize, for every k, the set $\mathbf{obs}(\mathcal{A}_k(\mathcal{G})) \cap \mathcal{H}$, for some graph class $\mathcal{H}$, and then lower bound $|\mathbf{obs}(\mathcal{A}_k(\mathcal{G}))|$ by counting (asymptotically or exactly) all the graphs in $\mathbf{obs}(\mathcal{A}_k(\mathcal{G})) \cap \mathcal{H}$. This last approach has been applied in [28] when $\mathcal{G}$ is the class of acyclic graphs and $\mathcal{H}$ is the class of outerplanar graphs (see also [13, 19]).

Our results. In this paper we study the set $\mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$ where $\mathcal{S}$ is the class of sub-unicyclic graphs. Certainly the class $\mathcal{S}$ is minor-closed (while this is not the case for unicyclic graphs). It is easy to see that $\mathbf{obs}(\mathcal{S}) = \{2K_3, K_4^-, Z\}$, where $2K_3$ is the disjoint union of two triangles, K_4^- is the complete graph on 4 vertices minus an edge, and Z the *butterfly graph*, obtained by $2K_3$ after identifying two vertices of its triangles (we call the result of this identification *central vertex* of Z).

Our first result is the identification of $\mathbf{obs}(\mathcal{A}_1(\mathcal{S}))$, i.e., the minor-obstruction set of all 1-apices of sub-unicyclic graphs (Section 3). This set contains 29 graphs that is the union of two sets $\mathcal{L}_0$ and $\mathcal{L}_1$, depicted in Figures 1 and 6 respectively. An important ingredient of our proof is the notion of a *nearly-biconnected graph*, that is any graph that is either biconnected or it contains only one cut-vertex joining two blocks where one of them is a triangle. We first prove that $\mathcal{L}_0$ is the set of minor-obstructions in $\mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$ that are not nearly-biconnected. The proof is completed by proving that the nearly-biconnected graphs in $\mathbf{obs}(\mathcal{A}_1(\mathcal{S}))$ are also minor-obstructions for 1-apex pseudoforests, i.e., members of $\mathbf{obs}(\mathcal{A}_1(\mathcal{P}))$. As this set is known from [20], we can identify the remaining obstructions in $\mathbf{obs}(\mathcal{A}_1(\mathcal{S}))$, that is the set $\mathcal{L}_1$, by exhaustive search.

Our second result is an exponential lower bound on the size $\mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$ (Section 4). For this we completely characterize, for every k, the set $\mathbf{obs}(\mathcal{A}_k(\mathcal{S})) \cap \mathcal{K}$ where $\mathcal{K}$ is the set of all cacti (graphs whose all blocks are either edges or cycles). In particular, we first prove that each connected cactus obstruction in $\mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$ can be obtained by identifying non-central vertices of $k+1$ butterfly graphs and then we give a characterization of disconnected cacti in $\mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$ in terms of obstructions in $\mathbf{obs}(\mathcal{A}_{k'}(\mathcal{S}))$ for $k' < k$ (we stress that here the result of Dinneen in [8] does not apply immediately, as not all graphs in $\mathbf{obs}(\mathcal{S})$ are connected).

After identifying $\mathbf{obs}(\mathcal{A}_k(\mathcal{S}))\cap\mathcal{K}$, the next step is to count the number of its elements (Section 5). To that end, we employ the framework of the *Symbolic Method* and the corresponding techniques of *singularity analysis*, as they were presented in [15]. The combinatorial construction that we devise relies critically on the *Dissymmetry Theorem for Trees*, by which one can move from the enumeration of rooted tree structures to unrooted ones (see [3] for a comprehensive account of these techniques, in the context of the *Theory of Species*).

$$|\mathbf{obs}(\mathcal{A}_k(\mathcal{S})) \cap \mathcal{K}| \sim c{\cdot}k^{-5/2} \cdot x^k,$$

where $c \approx 0.33995$ and $x \approx 6.27888$. This provides an exponential lower bound for $|\mathbf{obs}(\mathcal{A}_k(\mathcal{S}))|$.

2 Preliminaries

Sets, integers, and functions. We denote by $\mathbb{N}$ the set of all non-negative integers and we set $\mathbb{N}^+ = \mathbb{N} \setminus \{0\}$. Given two integers p and q, we set $[p,q] = \{p,\dots,q\}$ and given a $k \in \mathbb{N}^+$ we denote $[k] = [1,k]$. Given a set A, we denote by 2^A the set of all its subsets and we define $\binom{A}{2} := \{e \mid e \in 2^A \wedge |e| = 2\}$. If $\mathcal{S}$ is a collection of objects where the operation $\cup$ is defined, then we denote $\bigcup\mathcal{S} = \bigcup_{X\in\mathcal{S}} X$.

Graphs. All the graphs in this paper are finite, undirected, and without loops or multiple edges. Given a graph G, we denote by $V(G)$ the set of vertices of G and by $E(G)$ the set of the edges of G. We refer to the quantity $|V(G)|$ as the *size* of G. For an edge $e = \{x,y\} \in E(G)$, we use instead the notation $e = xy$, that is equivalent to $e = yx$. Given a vertex $v \in V(G)$, we define the *neighborhood* of v as $N_G(v) = \{u \mid u \in V(G), uv \in E(G)\}$. If $X \subseteq V(G)$, then we write $N_G(X) = (\bigcup_{v\in X} N_G(v))\setminus X$. The *degree* of a vertex v in G is the quantity $|N_G(v)|$. Given two graphs G_1, G_2, we define the *union* of G_1, G_2 as the graph $G_1 \cup G_2 = (V(G_1) \cup V(G_2), E(G_1) \cup E(G_2))$.

A *subgraph* of a graph $G = (V,E)$ is every graph H where $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$. If $S \subseteq V(G)$, the subgraph of G *induced by* S, denoted by $G[S]$, is the graph $(S, E(G) \cap \binom{S}{2})$. We also define $G \setminus S$ to be the subgraph of G induced by $V(G) \setminus S$. If $S \subseteq E(G)$, we denote by $G \setminus S$ the graph $(V(G), E(G) \setminus S)$. Given a vertex $x \in V(G)$ we define $G \setminus x = G \setminus \{x\}$ and given an edge $e \in E(G)$ we define $G \setminus e = G \setminus \{e\}$.

An edge $e \in E(G)$ is a *bridge* of G if G has less connected components than $G \setminus e$. Given a set $S \subseteq V(G)$, we say that S is a *separator* of G if G has less connected components than $G \setminus S$. Let G be a graph and $S \subseteq V(G)$ and let $V_1, \dots, V_q$ be the vertex sets of the connected components of

$G \setminus S$. We define $\mathcal{C}(G, S) = \{G_1, \ldots, G_q\}$ where, for $i \in [q]$, G_i is the graph obtained from $G[V_i \cup S]$ if we add all edges between vertices in S. Given a vertex $x \in V(G)$ we define $\mathcal{C}(G, x) = \mathcal{C}(G, \{x\})$.

A vertex $v \in V(G)$ is a *cut-vertex* of G if $\{v\}$ is a separator of G. A *block* of a graph G is a maximal biconnected subgraph of G.

By K_r we denote the complete graph on r vertices, also known as r*-clique*. Similarly, by K_{r_1,r_2} we denote the complete bipartite graph of which one part has r_1 vertices and the other r_2. We denote by K_r^- the graph obtained by K_r after removing any edge. For an $r \geq 3$, we denote by C_r the cycle on r vertices. Given a graph G and an $r \geq 1$ we denote by rG the graph with r connected components, each isomorphic to G.

Given a graph class $\mathcal{G}$ and a graph G, a vertex $v \in V(G)$ is a $\mathcal{G}$*-apex of* G if $G \setminus v \in \mathcal{G}$.

Minors. We define G/e, the graph obtained from the graph G by *contracting* an edge $e = xy \in E(G)$, to be the graph obtained by replacing the edge e by a new vertex v_e which becomes adjacent to all neighbors of x, y (apart from y and x). Given two graphs H and G we say that H is a *minor* of G, denoted by $H \leq G$, if H can be obtained by some subgraph of G after contracting edges. We say that H is a *proper minor* of G if it is a minor of G but is not isomorphic to G. Given a set $\mathcal{H}$ of graphs, we write $\mathcal{H} \leq G$ to denote that $\exists H \in \mathcal{H} : H \leq G$.

Sub-unicyclic Graphs. We now resume some basic concepts that we already mentioned in the introduction. A *sub-unicyclic* graph is a graph that contains at most one cycle. A graph is a *pseudoforest* if all its connected components are sub-unicyclic. We denote by $\mathcal{S}$ (resp. $\mathcal{P}$) the set of all sub-unicyclic graphs (resp. pseudoforests). The study of the class $\mathcal{P}$ dates back in [6,24]. Clearly, $\mathcal{S} \subseteq \mathcal{P}$ and therefore $\mathcal{A}_k(\mathcal{S}) \subseteq \mathcal{A}_k(\mathcal{P})$, for every $k \in \mathbb{N}$. For simplicity, instead of saying that a graph is 1-apex sub-unicyclic/pseudoforest/acyclic we just say *apex sub-unicyclic/pseudoforest/acyclic*.

Given a graph G and a set $S \subseteq V(G)$ we say that S is an *apex sub-unicyclic set* (resp. *apex forest set*) of G if $G \setminus S$ is sub-unicyclic (resp. forest). If $|S| \leq k$, for some $k \in \mathbb{N}$, then we say that S a k*-apex sub-unicyclic set* (resp. k*-apex forest set*) of G if $G \setminus S$ is sub-unicyclic (resp. forest).

3 Minor-obstructions for apex sub-unicyclic graphs

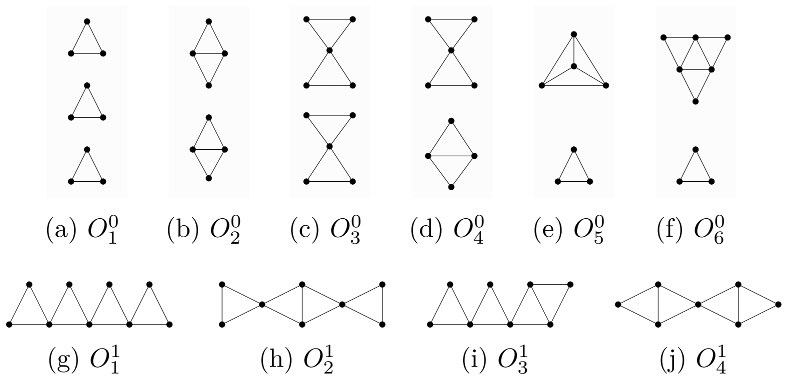
In this section we will identify the set $\mathbf{obs}(\mathcal{A}_1(\mathcal{S}))$. Part of it will be the set $\mathcal{L}_0$ containing the graphs depicted in Figure 1.

3.1 Structure for general obstructions

We need the following lemma on the general structure of the obstructions of $\mathcal{A}_k(\mathcal{S})$.

Lemma 3.1. *Let $G \in \mathbf{obs}(\mathcal{A}_k(\mathcal{S})), k \geq 0$. Then the following hold:*

1. *The minimum degree of a vertex in G is at least 2.*
2. *G has no bridges.*
3. *All of its vertices of degree 2 have adjacent neighbors.*



(a) O_1^0 (b) O_2^0 (c) O_3^0 (d) O_4^0 (e) O_5^0 (f) O_6^0

(g) O_1^1 (h) O_2^1 (i) O_3^1 (j) O_4^1

Figure 1: The set $\mathcal{L}_0$ of obstructions for $\mathcal{A}_1(\mathcal{S})$ that are not nearly-biconnected.

Proof. It is clear that every vertex and every edge of G participates in a cycle. Thus, we get (1) and (2). Regarding (3), suppose, to the contrary, that there exists a vertex $v \in V(G)$ of degree 2 whose neighbors are no adjacent, and let $e \in E(G)$ be an edge incident to v, i.e. $e = uv$ for some $u \in V(G)$. As $G \in \mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$ we have that $G' := G/e \in \mathcal{A}_k(\mathcal{S})$. Let S be a k-apex sub-unicyclic set of G' and v_e the vertex formed by contracting e. Observe that, every cycle in G that contains v also contains u and so if $v_e \in S$ then $(S \setminus \{v_e\}) \cup \{u\}$ is a k-apex sub-unicyclic set of G, a contradiction. Therefore, $v_e \notin S$ and so $S \subseteq V(G)$. Since the neighbors of v are not adjacent, the contraction of e can only shorten cycles and not destroy them. Hence, S is a k-apex sub-unicyclic set of G, a contradiction. □

3.2 The disconnected case

We set $\mathcal{O}^0 = \{O_1^0, \ldots, O_6^0\}$. We begin with an easy observation:

Observation 3.2. Let G be a connected graph such that $\mathbf{obs}(\mathcal{S}) \leq G$. Then, $\mathbf{obs}(\mathcal{S}) \setminus \{2K_3\} \leq G$.

Lemma 3.3. *If $G \in \mathbf{obs}(\mathcal{A}_1(\mathcal{S}))$ and G is not connected, then $G \in \mathcal{O}^0$.*

Proof. Notice first that $O^0 \subseteq \mathbf{obs}(\mathcal{A}_1(\mathcal{S}))$. Suppose, to the contrary, that there exists some disconnected graph $G \in \mathbf{obs}(\mathcal{A}_1(\mathcal{S})) \setminus \mathcal{O}^0$. Note that due to Lemma 3.1 each connected component of G contains at least one cycle and so if G has more than two connected components, it follows that $O_1^0 \leq G$, a contradiction. Therefore, G has exactly two connected components, namely G_1, G_2.

Claim 1: One of G_1, G_2 is isomorphic to K_3.
Proof of Claim 1: Suppose, towards a contradiction, that $G_1, G_2 \notin \mathcal{S}$. Then, since both G_1, G_2 are connected, Observation 3.2 implies that $\mathbf{obs}(\mathcal{S}) \setminus \{2K_3\} \leq G_1, G_2$ and therefore $\{O_2^0, O_3^0, O_4^0\} \leq G$, a contradiction. Hence, one of G_1, G_2 is sub-unicyclic and therefore, by Lemma 3.1, isomorphic to K_3. Claim 1 follows.

By Claim 1, we can assume, without loss of generality, that $G_2 \cong K_3$.

Claim 2: G_1 biconnected but not triconnected.
Proof of Claim 2: If G_1 is triconnected then $K_4 \leq G_1$, and therefore $O_5^0 \leq G$, a contradiction. Now, suppose that there exists a cut-vertex x of G_1. Note that, by Lemma 3.1, it follows that every

$H \in \mathcal{C}(G_1, x)$ contains at least one cycle. If x belongs to every cycle of G_1, then x is an $\mathcal{S}$-apex vertex of G, which is a contradiction. Therefore, there exists an $H \in \mathcal{C}(G_1, x)$ such that $H \setminus x$ contains a cycle C which together with a cycle in some $H' \in \mathcal{C}(G_1, x) \setminus \{H\}$ and G_2 form O_1^0 as a minor of G, a contradiction. Therefore, G is biconnected. Claim 2 follows.

Claim 2 implies that there exists a 2-separator $S = \{x, y\}$ of G_1 such that every $H \in \mathcal{C}(G_1, S)$ is a biconnected graph.

Observation: Every cycle in G_1 contains either x or y. Indeed, suppose to the contrary that there exists a cycle $C \subseteq G_1$ disjoint to both x, y and consider an $H \in \mathcal{C}(G_1, S)$ such that $C \not\subseteq H$. Then, due to Lemma 3.1, $G[V(H)]$ contains a cycle and together with C and G_2 form O_1^0 as a minor of G, a contradiction.

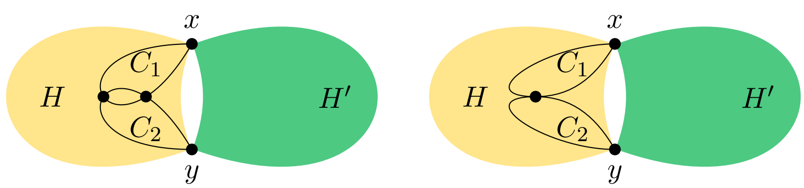


Figure 2: The cycles C_1, C_2 in the last part of the proof of Lemma 3.3

Since x, y are not $\mathcal{S}$-apex vertices of G, then, apart from G_2, there exist two cycles C_1, C_2 in G_1 such that $y \notin V(C_1)$ and $x \notin V(C_2)$. The above Observation implies that $x \in V(C_1)$ and $y \in V(C_2)$. Due to O_1^0-freeness of G, we have that $V(C_1) \cap V(C_2) \neq \emptyset$ and therefore there exists an $H \in \mathcal{C}(G_1, S)$ such that $C_1 \cup C_2 \subseteq H$. Consider, now, an $H' \in \mathcal{C}(G_1, S)$ different from H and observe that by Lemma 3.1, $G[V(H')]$ contains a cycle. Then, if C_1, C_2 share more than one vertex, $O_5^0 \leq G$, while if they share only one vertex, $O_6^0 \leq G$, a contradiction in both cases (see Figure 2). Lemma follows. $\square$

3.3 The connected cases

Lemma 3.4. *If G is a connected graph in $\mathbf{obs}(\mathcal{A}_1(\mathcal{S}))$, with at least three cut-vertices, then $G \cong O_1^1$.*

Proof. Consider a connected graph $G \in \mathbf{obs}(\mathcal{A}_1(\mathcal{S}))$ with at least three cut-vertices. We first exclude the case where there is a block B of G containing three cut-vertices x, y, z. Indeed, due to Lemma 3.1, each block of G contains a cycle and this holds for B and the blocks of G that share a cut-vertex with B. This implies the existence of O_1^0 as a proper minor of G, a contradiction as $O_1^0 \in \mathbf{obs}(\mathcal{A}_1(\mathcal{S}))$.

We just proved that G contains 4 blocks B_1, B_2, B_3, and B_4 such that $V(B_1) \cap V(B_2) = \{x\}$, $V(B_2) \cap V(B_3) = \{y\}$, $V(B_3) \cap V(B_4) = \{z\}$ are singletons each consisting of a cut-vertex. In this case, again by Lemma 3.1, each block in $\{B_1, B_2, B_3, B_4\}$ contains a cycle, which implies that $O_1^1 \leq G$. As $O_1^1 \in \mathbf{obs}(\mathcal{A}_1(\mathcal{S}))$, it follows that $G \cong O_1^1$. $\square$

Lemma 3.5. *If G is a connected graph in $\mathbf{obs}(\mathcal{A}_1(\mathcal{S}))$ with exactly two cut-vertices, then $G \in \{O_2^1, O_3^1\}$.*

Proof. Observe first that $\{O_2^1, O_3^1\} \subseteq \mathbf{obs}(\mathcal{A}_1(\mathcal{S}))$.Suppose, to the contrary, that there is a graph $G \in \mathbf{obs}(\mathcal{A}_1(\mathcal{S})) \setminus \{O_2^1, O_3^1\}$ that has exactly two cut-vertices, namely u_1 and u_2. Let B be the (unique) block containing the two cut-vertices u_1, u_2 and let

$$H_1 = \bigcup \{H \in \mathcal{C}(G, u_1) : u_2 \notin V(H)\} \text{ and } H_2 = \bigcup \{H \in \mathcal{C}(G, u_2) : u_1 \notin V(H)\}.$$

Keep in mind that G cannot contain any graph in $\mathcal{O}^0$ as a minor because, due to the connectivity of G, it would contain it as a proper minor, a contradiction to the fact that $\mathcal{O}^0 \subseteq \mathbf{obs}(\mathcal{A}_1(\mathcal{S}))$.

We prove a series of claims:

Claim 1: Every cycle in G contains either u_1 or u_2.
Proof of Claim 1: Suppose, to the contrary, that there exists a cycle C not containing any of the cut-vertices. We distinguish two cases:

Case 1: C is in B. Note that, due to Lemma 3.1, each block contains a cycle. Therefore the cycle C along with two more cycles, one from H_1 and one from H_2, form O_1^0 as a proper minor of G, a contradiction.

Case 2: C is either in H_1 or H_2. Suppose, without loss of generality, that C is in some block of H_1. Then, due to Menger's theorem, there exist two paths from C to u_1 that intersect only in u_1. Since each block of G contains at least one cycle, we have that C together with the aforementioned paths, the block B and any block in H_2, form O_3^1 as minor of G, a contradiction (See Figure 3). Claim 1 follows.

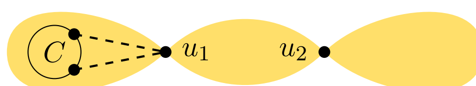


Figure 3: The cycle C in Case 2 of the proof of Claim 1.

Claim 2: Both H_1 and H_2 are isomorphic to K_3.
Proof of Claim 2: Suppose, towards a contradiction, that one of H_1, H_2, say H_1, is not sub-unicyclic (we will use Lemma 3.1). Since H_1 is connected, then, by Observation 3.2, we have that $\mathbf{obs}(\mathcal{S}) \backslash \{2K_3\} \leq H_1$. Also, since u_1 is not an $\mathcal{S}$-apex vertex of G and since, due to Claim 1, all cycles of H_1 contain u_1, then $G \setminus V(H_1) \notin \mathcal{S}$. Now, since $G \setminus V(H_1)$ is connected then Observation 3.2 implies that $\mathbf{obs}(\mathcal{S}) \setminus \{2K_3\} \leq G \setminus V(H_1)$. Hence, $\{O_2^0, O_3^0, O_4^0\} \leq G$, a contradiction. Therefore $H_1, H_2 \in \mathcal{S}$ and, by Lemma 3.1, Claim 2 follows.

Since u_1 is not a $\mathcal{S}$-apex of G, then Claim 2 implies that (apart from H_2) there exists a cycle C_2 in $B \setminus u_1$, which by Claim 1, contains u_2. The same holds for u_2, i.e. there exists a cycle C_1 in $B \setminus u_2$ that contains u_1. Then $O_3^0 \leq G$, if C_1, C_2 are disjoint, $O_1^1 \leq G$, if C_1 and C_2 share exactly one vertex, and $O_2^1 \leq G$, if C_1, C_2 share at least 2 vertices, a contradiction in all cases (see Figure 4). Lemma follows.

□

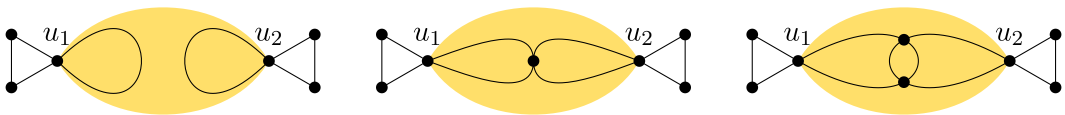


Figure 4: The ways the cycles C_1, C_2 may intersect in the last part of the proof of Lemma 3.5.

Nearly-biconnected graphs. We say that a graph G is *nearly-biconnected* if it is either biconnected or it contains exactly one cut-vertex x and $\mathcal{C}(G,x) = \{H, K_3\}$ where H is a biconnected graph.

Lemma 3.6. *Let $G \in \mathbf{obs}(\mathcal{A}_1(\mathcal{S}))$ be a connected graph that contains exactly one cut-vertex. Then either $G \cong O_4^1$ or G is nearly-biconnected.*

Proof. Notice that $O_4^1 \in \mathbf{obs}(\mathcal{A}_1(\mathcal{S}))$. Let G be a graph in $\mathbf{obs}(\mathcal{A}_1(\mathcal{S})) \setminus \{O_4^1\}$. As in the the proof of Lemma 3.5, keep in mind that G does not contain any graph in $\mathcal{O}^0$ as a minor.

We first prove the following claim.

Claim 1: There exists a unique component in $\mathcal{C}(G,x)$ which contains a cycle disjoint from x.

Proof of Claim 1: First, we easily observe that there exists such a component in $\mathcal{C}(G,x)$. Suppose that there exist two different components in $\mathcal{C}(G,x)$, each of which contains a cycle disjoint to x. Then, due to Menger's theorem, for each of said cycles there exist two paths from x to the cycle being considered, intersecting only in x. But then O_4^1 is formed as a minor of G, a contradiction (see Figure 5). Claim follows.

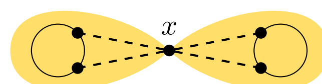


Figure 5: The configuration in the proof of Claim 1.

Let $H \in \mathcal{C}(G,x)$ be the unique, by Claim 1, component in $\mathcal{C}(G,x)$ which contains a cycle disjoint to x. Also, let $D = \bigcup\{H' \in \mathcal{C}(G,x) : H' \neq H\}$.

Claim 2: $D \cong K_3$

Proof of Claim 2: We argue that $D \in \mathcal{S}$, which, due to Lemma 3.1, implies that $D \cong K_3$. Suppose, to the contrary, that $D \notin \mathcal{S}$. Then, since D is connected, Observation 3.2 implies that $\mathbf{obs}(\mathcal{S}) \setminus \{2K_3\} \leq D$. By Claim 1, every cycle in D contains x and therefore, since x is not an $\mathcal{S}$-apex vertex of G, $H \setminus x$ contains at least two cycles. Then, taking into account the connectivity of $H \setminus x$, Observation 3.2 implies that $\mathbf{obs}(\mathcal{S}) \setminus \{2K_3\} \leq H \setminus x$. Hence, $\{O_2^0, O_3^0, O_4^0\} \leq G$, a contradiction. Claim 2 follows.

Claim 2 implies that G is nearly-biconnected, as required. $\square$

3.4 Borrowing obstructions from apex-presudoforests

We need the following fact:

Fact 3.7. The graphs in $\mathbf{obs}(\mathcal{A}_1(\mathcal{P}))$ that are nearly-biconnected and belong in $\mathbf{obs}(\mathcal{A}_1(\mathcal{S}))$ are the graphs in Figure 6.

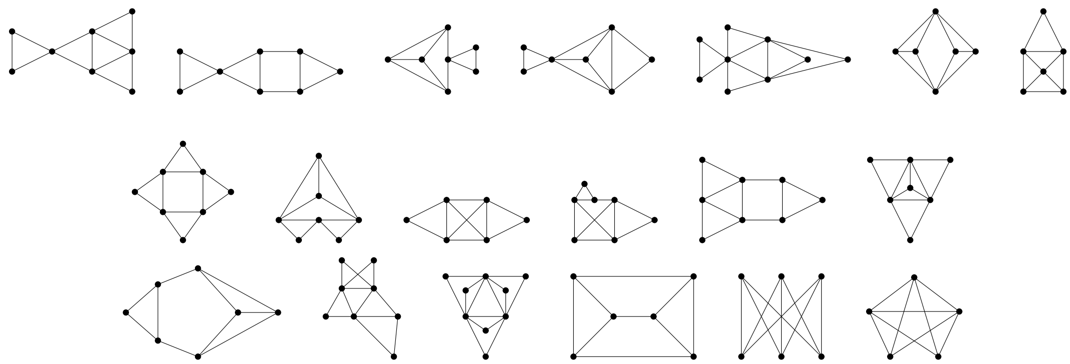


Figure 6: The set $\mathcal{L}_1$ of the 19 nearly-biconnected minor-obstructions for $\mathcal{A}_1(\mathcal{S})$ that are also obstructions for $\mathcal{A}_1(\mathcal{P})$.

The set $\mathbf{obs}(\mathcal{A}_1(\mathcal{P}))$ consists of 33 graphs and has been identified in [20]. The correctness of Fact 3.7 can be verified by exhaustive check, considering all nearly-biconnected graphs in $\mathbf{obs}(\mathcal{A}_1(\mathcal{P}))$ (they are 26) and then filter those that belong in $\mathbf{obs}(\mathcal{A}_1(\mathcal{S}))$. For this, one should pick those that become apex sub-unicyclic after the contraction or removal of each of their edges. Notice that the fact that these graphs are not apex-sub-unicyclic follows directly by the fact that they are not apex-pseudoforests (as members of $\mathbf{obs}(\mathcal{A}_1(\mathcal{P}))$) and the fact that $\mathcal{S} \subseteq \mathcal{P}$. The choice of $\mathcal{L}_1$ is justified by the next lemma.

Lemma 3.8. *If G is a nearly-biconnected graph in $\mathbf{obs}(\mathcal{A}_1(\mathcal{S}))$, then $G \in \mathbf{obs}(\mathcal{A}_1(\mathcal{P}))$.*

Proof. Let G be a graph satisfying the assumptions of the lemma. We need to show that $G \notin \mathcal{A}_1(\mathcal{P})$ and that for every proper minor H of G it holds that $H \in \mathcal{A}_1(\mathcal{P})$. Notice that the latter is trivial since $\mathcal{A}_1(\mathcal{S}) \subseteq \mathcal{A}_1(\mathcal{P})$ and therefore it remains to show that $G \notin \mathcal{A}_1(\mathcal{P})$. We begin with the following claim:

Claim: If $x \in V(G)$ is a $\mathcal{P}$-apex of G then, then x is a cut-vertex of G.
Proof of Claim: Consider a vertex $x \in V(G)$. Since $G \in \mathbf{obs}(\mathcal{A}_1(\mathcal{S}))$, x is not an $\mathcal{S}$-apex of G and so there exist two cycles C_1, C_2 in $G \setminus x$. If x is not a cut-vertex of G, then $G \setminus x$ is connected and therefore C_1, C_2 are in the same connected component of $G \setminus x$. Hence, $G \setminus x$ is not a pseudoforest and Claim follows.

Suppose, towards a contradiction, that $G \in \mathcal{A}_1(\mathcal{P})$. Then, there exists a vertex $x \in V(G)$ such that $G \setminus x$ is a pseudoforest. From the above Claim, x is a cut-vertex of G and since G is nearly biconnected, $\mathcal{C}(G, x) = \{H, K_3\}$ where H is a biconnected graph. Therefore, $H \setminus x$ is a connected component of $G \setminus x$ while the other connected component of $G \setminus x$ is a single edge. Therefore, $G \setminus x$ contains at most one cycle which implies that $G \setminus x \in \mathcal{S}$, a contradiction. $\square$

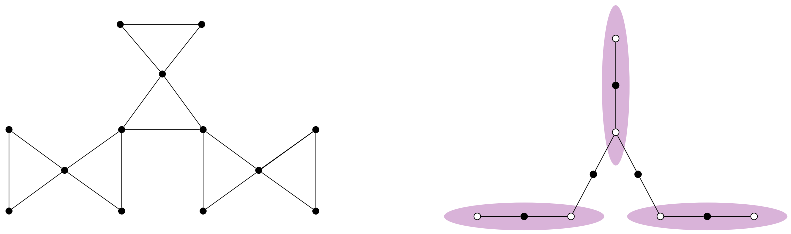


Figure 7: An example of a graph $G \in \mathcal{Z}_3$ and its block-cut-vertex tree T_G with the P_3-subgraphs corresponding to the butterflies composing G highlighted.

We are now ready to prove the main result of this section.

Theorem 3.9. $\mathbf{obs}(\mathcal{A}_1(\mathcal{S})) = \mathcal{L}_0 \cup \mathcal{L}_1$.

Proof. Recall that $\mathcal{L}_0 = \mathcal{O}^0 \cup \{O_1^1, O_2^1, O_3^1, O_4^1\}$. Notice that $\mathcal{L}_0 \cup \mathcal{L}_1 \subseteq \mathbf{obs}(\mathcal{A}_1(\mathcal{S}))$. Let $G \in \mathbf{obs}(\mathcal{A}_1(\mathcal{S}))$. If G is disconnected, then, from Lemma 3.3, $G \in \mathcal{O}^0$. If G is connected and has at least three cut-vertices, then from Lemma 3.4, $G \cong O_1^1$. If G is connected and has exactly two cut-vertices, then from Lemma 3.5, $G \in \{O_2^1, O_3^1\}$. If G is connected with exactly one a cut-vertex and is not nearly-biconnected then, from Lemma 3.6, $G \cong O_4^1$. We just proved that if G is not nearly-biconnected, then $G \in \mathcal{L}_0$. On the other side, if G is nearly-biconnected, then from Lemma 3.8, $G \in \mathbf{obs}(\mathcal{A}_1(\mathcal{P}))$, therefore, from Fact 3.7, $G \in \mathcal{L}_1$, as required. □

4 Structural Characterisation of Cactus Obstructions

Recall that a *cactus graph* is a graph where all its blocks are either edges or cycles. Equivalently, a graph is a cactus graph, if it does not contain K_4^- as a minor. We denote by $\mathcal{K}$ the set of all cactus graphs. In this section we provide a complete characterization of the class of $\mathbf{obs}(\mathcal{A}_k\mathcal{S}) \cap \mathcal{K}$, i.e., the obstructions for k-apex sub-unicyclic graphs that are cactus graphs.

Given a graph G and two vertices x and y of G, we call a pair $(x, y) \in (V(G))^2$ *anti-diametrical* if there is no other pair (x', y'), where the distance between x' and y' in G is bigger than the distance in G between x and y. Notice that if G is a tree, the two vertices in any anti-diametrical pair of G are both leaves.

Block-cut-vertex Tree. Let G be a connected graph. We denote by $\mathcal{B}(G)$ the set of its blocks and by $C(G)$, the set of its cut-vertices. We define the graph $T_G = (\mathcal{B}(G) \cup C(G), E)$ where $E = \{\{B, c\} \mid B \in \mathcal{B}(G), v \in C(G), v \in V(B)\}$. Notice that T_G is a tree, called the *block-cut-vertex tree* of G (or *bc-tree* in short). Furthermore, note that all its leafs are blocks of G. We call a block of G *leaf-block* if B is a leaf of T_G. We call a leaf-block B of G *peripheral* if there is some leaf-block B' of G such that the pair (B, B') is an anti-diametrical pair of T_G.

4.1 Characterization of connected cactus-obstructions

Butterflies and Butterfly-Cacti. We denote by Z the butterfly graph. We will frequently refer to graphs isomorphic to Z simply as *butterflies*. Given a butterfly Z we call all its four vertices that have degree two, *extremal vertices* of Z and the unique vertex of degree four, *central vertex* of Z.

Let k be a positive integer. We recursively define the graph class of the *k-butterfly-cacti*, denoted by $\mathcal{Z}_k$, as follows: We set $\mathcal{Z}_1 = \{Z\}$, where Z is the butterfly graph, and given a $k \geq 2$ we say that $G \in \mathcal{Z}_k$ if there is a graph $G' \in \mathcal{Z}_{k-1}$ such that G is obtained if we take a copy of the butterfly graph Z and then we identify one of its extremal vertices with a non-central vertex of G'. The *central vertices* of the obtained graph G are the central vertices of G' and the central vertex of Z. If $G \in \mathcal{Z}_k$, we denote by $K(G)$ the set of all central vertices of G.

We need the following observation.

Observation 4.1. For every $k \geq 1$ and for every $G \in \mathcal{Z}_k$, $K(G)$ is the unique k-apex forest set of G.

Proof. It is easy to observe that $K(G)$ is a k-apex forest set of G. To prove that $K(G)$ is unique, suppose to the contrary that k is the minimum number such that there is a $G \in \mathcal{Z}_k$ and a k-apex forest set $S \subseteq V(G)$ where $S \neq K(G)$. Recall that G is obtained by identifying a non-central vertex of some member G' of $\mathcal{Z}_{k-1}$ with an extremal vertex of some graph H isomorphic to the butterfly graph Z. Let now C be the cycle of H in G that contains no vertices of G'. By the minimality of k, $S \setminus V(C) = K(G')$ and therefore $S \cap V(C)$ must contain only one vertex, namely x, which must also belong to the cycle of H different from C. This implies that x is the central vertex of Z, thus $S = K(G)$, a contradiction. □

The objective of this section is to prove the following theorem.

Theorem 4.2. *For every non-negative integer k, the connected graphs in $\mathbf{obs}(\mathcal{A}_k\mathcal{S}) \cap \mathcal{K}$ are exactly the graphs in $\mathcal{Z}_{k+1}$.*

The following lemma proves one direction of Theorem 4.2.

Lemma 4.3. *If $G \in \mathcal{Z}_{k+1}, k \geq 0$, then $G \in \mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$.*

Proof. We proceed by induction on k. The lemma clearly holds for $k = 0$. Let $G \in \mathcal{Z}_{k+1}$ for some $k \geq 1$ and assume that the lemma holds for smaller values of k. We argue that G is not k-apex sub-unicyclic while all its proper minors are. By the construction of G, we know that G is the result of the identification of an extremal vertex of a new copy of the butterfly graph Z and a non-central vertex of some graph $G' \in \mathcal{Z}_k$. By the induction hypothesis, we have that $G' \in \mathbf{obs}(\mathcal{A}_{k-1}(\mathcal{S}))$. Let C (resp. C') be the cycle of the new copy of Z in G that is (resp. is not) a leaf-block of G.

Claim 1: G is not k-apex sub-unicyclic.

Proof of Claim 1: Suppose, towards a contradiction, that G is k-apex sub-unicyclic and therefore there exists some k-apex sub-unicyclic set S of G.

Case 1: $S \cap V(C) \neq \emptyset$. We set $S' = S \cap V(G')$. Then $|S'| \leq k - 1$ and we observe that $G' \setminus S'$ is sub-unicyclic contradicting the fact that $G' \in \mathbf{obs}(\mathcal{A}_{k-1}(\mathcal{S}))$.

Case 2: $S \cap V(C) = \emptyset$. Then S is a k-apex forest set of $G \setminus V(C)$ that should contain at least one vertex of C'. This means that G' contains a k-apex forest set that is different from $K(G')$, a contradiction to Observation 4.1.

Claim 2: Every proper minor of G is k-apex sub-unicyclic.

Proof of Claim 2: Consider a minor H of G created by the contraction (or removal) of some edge e of G. If e is an edge of the copy of Z in G, then observe that $K(G')$ is a k-apex sub-unicyclic set of H and so the claim is proven. Suppose now that e is an edge of G' in G and let H' be the minor of G' created after contracting (or removing) e in G'. Since $G' \in \mathbf{obs}(\mathcal{A}_{k-1}(\mathcal{S}))$, there exists a $(k-1)$-apex sub-unicyclic set S' of H'. But then S', together with the central vertex of Z, form a k-apex sub-unicyclic set of H, as required.

From the above two claims, we conclude that $G \in \mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$. □

The following is a direct consequence of the application of Lemma 3.1 on cacti.

Observation 4.4. Let $G \in \mathbf{obs}(\mathcal{A}_k(\mathcal{S})) \cap \mathcal{K}, k \geq 0$. Then all blocks of G are triangles.

Lemma 4.5. *Let $k \geq 1$, G be a connected cactus graph in $\mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$ and let B be some peripheral block of G. Then the (unique) neighbour c of B in T_G has degree 2.*

Proof. Notice that T_G has diameter at least 3 since otherwise G has a unique cut-vertex that is an 1-apex forest set, and therefore also an 1-apex sub-unicyclic set, of G, contradicting the fact that $G \notin \mathcal{A}_1(\mathcal{S})$. Suppose, towards a contradiction, that c has degree at least three in T_G. Since T_G has diameter at least 3 and B is a peripheral leaf, there is exactly one neighbour, say B', of c in T_G that is not a leaf-block of G. Let $e \in E(B')$ be some edge of said neighbour. Since $G \in \mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$, we have that $G' = G \setminus e$ contains a k-apex sub-unicyclic set S. If $c \notin S$, S must contain at least one vertex from a leaf-block of G that contains c. This follows from the assumption that c has at least two neighbours in T_G which are leaf-blocks of G. But then the set S' which is constructed by replacing these vertices with c is also a k-apex sub-unicyclic set of G'. Therefore, we can assume that $c \in S$. But then S is also an k-apex sub-unicyclic set for G, as $c \in V(B')$, a contradiction. □

Lemma 4.6. *Let $k \geq 1$ and G be a connected cactus graph in $\mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$. Let also B be a peripheral block of G. Then T_G contains a path of length 3 whose one endpoint is B and its internal vertices are of degree 2.*

Proof. Let c be the unique neighbour of B in T_G. By Lemma 4.5, there exists a unique block B' of G, different from B, that is a neighbour of c in T_G. Observe that it suffices to prove that B' has degree 2 in T_G.

Suppose, towards a contradiction, that the block B' has 3 neighbours c, c', c'' in T_G. Since B is a peripheral leaf, we have that at least one of c', c'', say c'', is such that all its neighbours in T_G, except for B', are leaf-blocks. Let B'' be a neighbour of c'' in T_G different than B'. Consider now some edge $e \in E(B')$. Since $G \in \mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$, we have that $G' = G \setminus e$ must contain a k-apex sub-unicyclic set S. We can assume that S contains one of c, c''. Indeed, we have that S contains a vertex $x \in V(B) \cup V(B'')$. If $x \in V(B)$ then the set $S' = (S \setminus \{x\}) \cup \{c\}$ is a k-apex sub-unicyclic set of G'. Respectively, if $x \in V(B'')$ then the set $S' = (S \setminus \{x\}) \cup \{c''\}$ is a k-apex sub-unicyclic set of G'. Assume then that S is a k-apex sub-unicyclic set of G' such that either c or c'' is in S. Then, S is also a k-apex sub-unicyclic set of G since both c and c'' are vertices of B', a contradiction. □

Given a graph G we say that a subgraph Q of G is a *leaf-butterfly of G* if

- Q is an induced subgraph of G,

- Q is isomorphic to a butterfly graph,
- all the vertices of Q, except from an extremal one, called the *attachment* of Q, have all their neighbours inside Q in G, and
- the block of Q that does not contain its attachment is a peripheral block of G.

A *butterfly bucket* of G is a maximal collection $\mathcal{Q} = \{Q_1, \ldots, Q_r\}$ of leaf-butterflies of G with the same attachment w in G. If $G = \bigcup \mathcal{Q}$ then we say that $\mathcal{Q}$ is a *trivial butterfly bucket*, otherwise we say that $\mathcal{Q}$ is a *non-trivial butterfly bucket*. We call w the *attachment* of $\mathcal{Q}$ in G.

By considering Lemma 4.6 and Observation 4.4 together, we have the following corollary:

Corollary 4.7. *Let $k \geq 1$, and let G be a connected cactus graph in $\mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$. Then G contains a butterfly bucket.*

Lemma 4.8. *Let $k \geq 1$ and let $\mathcal{Q}$ be a non-trivial butterfly bucket of a connected cactus graph G. If $G \in \mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$ then there is no leaf-block of G containing the attachment of $\mathcal{Q}$.*

Proof. Suppose to the contrary that there exists a leaf-block B of G containing the attachment w of $\mathcal{Q}$. Let $Q \in \mathcal{Q}$, let c be the central vertex of Q, and let A and C be the two cycles of Q such that w is a vertex of A. Let e be an edge of A and $G' = G \setminus e$. As $G \in \mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$, it follows that $G' = G \setminus e$ contains a k-apex sub-unicyclic set S. If $S \cap V(C) = \emptyset$ then there exists some $x \in S \cap V(B)$ and therefore $S' = (S \setminus \{x\}) \cup \{w\}$ is a k-apex sub-unicyclic set of G, a contradiction. If there exists some $y \in S \cap V(C)$ then $S' = (S \setminus \{y\}) \cup \{c\}$ is a k-apex sub-unicyclic set of G, again a contradiction. $\square$

Lemma 4.9. *Let $k \geq 1$, G be a connected cactus graph in $\mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$, and $\mathcal{Q}$ be a non-trivial butterfly bucket of G with attachment w. Then the graph $G' = G \setminus (V(\bigcup \mathcal{Q}) \setminus \{w\})$ is a connected cactus in $\mathbf{obs}(\mathcal{A}_{k-r}(\mathcal{S}))$ where $r = |\mathcal{Q}|$.*

Proof. Let $\mathcal{Q} = \{Q_1, \ldots, Q_r\}$. For $i \in [r]$, let A_i and B_i be the two cycles of Q_i such that w is a vertex of A_i. Recall that $V(A_i) \cap V(B_i)$ is a singleton consisting of the central vertex, say c_i, of Q_i. Observe that G' is a connected cactus and w is contained in exactly one, say B^*, of the blocks of G'. This follows from the non-triviality of the butterfly bucket $\mathcal{Q}$, Lemma 4.8, Lemma 4.6, and the definition of a butterfly bucket.

In what follows, we prove that G' is a member of $\mathbf{obs}(\mathcal{A}_{k-r}(\mathcal{S}))$.

Claim 1: G' is not $(k-r)$-apex sub-unicyclic.

Proof of Claim 1: Suppose, to the contrary, that S is a $(k-r)$-apex sub-unicyclic set of G'. Then $S \cup \{c_1, \ldots, c_r\}$ is a k-apex sub-unicyclic set of G, a contradiction as $G \in \mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$.

Claim 2: Every proper minor of G' is $(k-r)$-apex sub-unicyclic.

Proof of Claim 2: Consider a minor H' of G' created by the contraction (or removal) of some edge e of G'. Let H be the result of the contraction (or removal) of e in G. As $G \in \mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$, there is a k-apex sub-unicyclic set S in H.

We can assume that $\{c_1, \ldots, c_r\} \subseteq S$. Indeed, to see this is so, we can distinguish two cases:

Case 1: for every $i \in [r]$, $S \cap V(B_i) \neq \emptyset$. Then, for all $i \in [r]$ let $x_i \in S \cap V(B_i)$ and observe that the set $S' = (S \setminus \{x_1, \ldots, x_r\}) \cup \{c_1, \ldots c_r\}$ is a k-apex sub-unicyclic set of G.

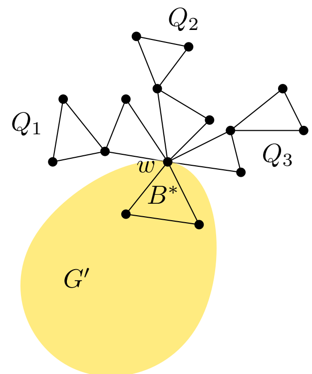


Figure 8: An example of a graph G and a butterfly bucket $\mathcal{Q} = \{Q_1, Q_2, Q_3\}$ of G with attachment w. The graph $G' = G \setminus (V(\bigcup \mathcal{Q}) \setminus \{w\})$ is depicted in yellow and B^* is the unique block of G' that contains w.

Case 2: there is some $i \in [r]$ such that $S \cap V(B_i) = \emptyset$. Without loss of generality, we can assume that $i = 1$. Then, the only cycle in $G \setminus S$ is B_1 and therefore for every $j \in [2, r]$, there exist some $x_j \in S \cap V(B_j)$. Observe that $S' = (S \setminus \{x_2, \ldots, x_r\}) \cup \{c_2, \ldots, c_r\}$ is a k-apex sub-unicyclic set of G (see Figure 9). As before, we have that there exists $x \in S \cap V(A_1)$. Set $S'' = (S' \setminus \{x\}) \cup \{c_1\}$. If $x \neq w$ then S'' is a k-apex sub-unicyclic set of G. If $x = w$ then since B_i is the only cycle in $G \setminus S'$ and B^* is the only cycle in G' that contains w, S'' is again a k-apex sub-unicycle set of G.

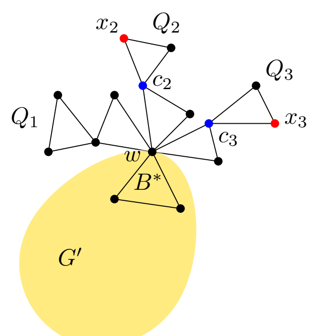


Figure 9: Following the example in Figure 8, for every $i \in [2]$, x_i is the vertex of S that is in $V(B_i)$ (depicted in red) and c_i is the center of Q_i (depicted in blue). The set S' is obtained by replacing in S the red vertices with the blue ones.

Now, since $\{c_1, \ldots, c_r\} \subseteq S$, we have that $S \setminus \{c_1, \ldots, c_r\}$ is a $(k - r)$-apex sub-unicyclic set of H' and so the claim follows.

Based on the above two claims, we conclude that $G' \in \mathbf{obs}(\mathcal{A}_{k-r}(\mathcal{S}))$. □

Observation 4.10. For every $k \in \mathbb{N}$, $(k + 2)K_3 \in \mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$.

Lemma 4.11. *Let $k \geq 0$ and G be a connected cactus graph in $\mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$. Then $G \in \mathcal{Z}_{k+1}$.*

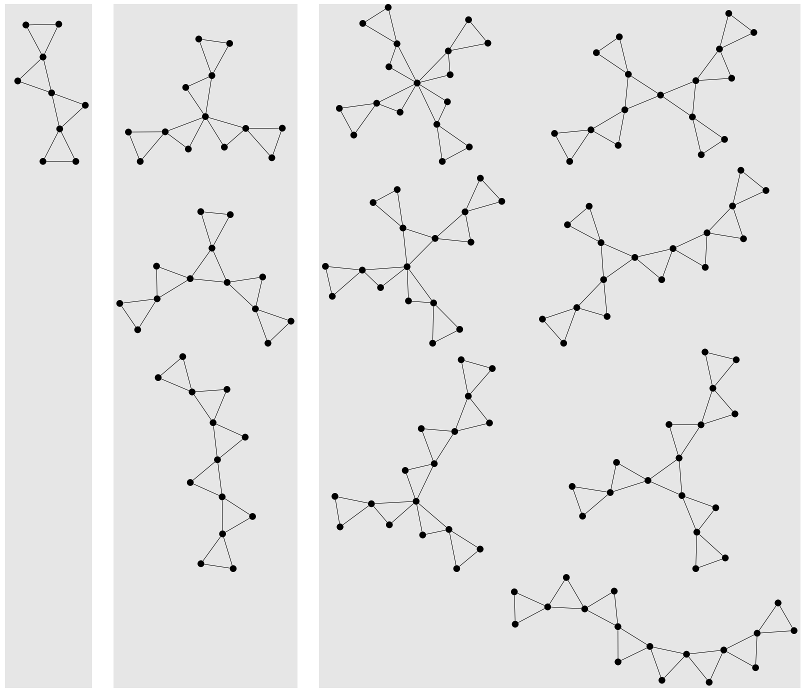


Figure 10: The connected graphs in $\mathbf{obs}(\mathcal{S}^k)$ for $n = 1, 2, 3$ respectively (presented left to right).

Proof. We proceed by induction on k. The base case where $k = 0$ is trivial. Let G be a connected cactus graph in $\mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$ for some $k \geq 1$ and assume that the statement of the lemma holds for smaller values of k.

Let $\mathcal{Q}$ be a butterfly bucket in G that exists because of Corollary 4.7. We first examine the case where $\mathcal{Q}$ is trivial. We claim that if $\mathcal{Q}$ is trivial, then $|\mathcal{Q}|= k + 1$. Indeed, if $|\mathcal{Q}| \leq k$, then the central vertices of the leaf buckets of $\mathcal{Q}$ form a k-apex sub-unicyclic set, contradicting the fact that $G \in \mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$. Also, if $|\mathcal{Q}| \geq k + 2$, then $(k + 2)K_3$ is a minor of G, a contradiction as $(k+2)K_3 \in \mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$. The triviality of $\mathcal{Q}$ and the fact that $|\mathcal{Q}|= k+1$ then imply that $G \in \mathcal{Z}_{k+1}$.

Suppose now that $\mathcal{Q}$ is not trivial. By Lemma 4.9, $G' = G \setminus (V(\bigcup \mathcal{Q}) \setminus \{w\})$ is a connected cactus in $\mathbf{obs}(\mathcal{A}_{k-r}(\mathcal{S}))$ where $r = |\mathcal{Q}|$. Since, due to the induction hypothesis, we have $G' \in \mathcal{Z}_{k-r+1}$, it follows that $G \in \mathcal{Z}_{k+1}$, as required. $\square$

Proof of Theorem 4.2. The proof is an immediate consequence of Lemma 4.3 and Lemma 4.11. $\square$

4.2 Characterization of disconnected cactus-obstructions

The objective of this section is to prove the following theorem.

Theorem 4.12. *Let $k \in \mathbb{N}$, let G be a disconnected cactus graph in $\mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$, and let $G_1, G_2, \ldots, G_r$ be the connected components of G. Then, one of the following holds:*

- $G \cong (k + 2)K_3$
- *there is a sequence $k_1, k_2, \ldots, k_r$ such that for every $i \in [r]$, G_i is a graph in $\mathcal{Z}_{k_i}$ and $\sum_{i \in [r]} k_i = k + 1$.*

We begin with the following Lemma which implies that every obstruction $G \in \mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$ not isomorphic to $(k+2)K_3$ is also a $(k+1)$-forest.

Lemma 4.13. *For every $k \in \mathbb{N}$ and for every cactus graph G it holds that if $(k+2)K_3 \not\leq G$ then G contains a $(k+1)$-apex forest set S.*

Proof. Suppose, towards a contradiction, that k is the minimum non-negative integer for which the contrary holds. Let G be a cactus graph with the minimum number of vertices such that $(k+2)K_3 \not\leq G$ and that for every apex-forest set S of G it holds that $|S| > k+1$. Observe that $k \geq 1$ and that there exists some connected component H of G that is not isomorphic to a cycle. As such, let B be a leaf-block of H and observe that, since G has the minimum number of vertices, every vertex of G has degree at least 2 and therefore B is isomorphic to a cycle. Since H is not isomorphic to a cycle, there exists a cut-vertex $c \in V(B)$, which is unique since B is a leaf-block of H. Now, consider the graph $G' = G \setminus c$ and observe that this too is a cactus. Observe, also, that $(k+1)K_3 \not\leq G'$, since otherwise $(k+2)K_3 \leq G$, a contradiction. Thus, by the minimality of k, we have that there exists a k-apex forest set S' of G'. But then, the set $S = S' \cup \{c\}$ is a $(k+1)$-apex forest set of G, a contradiction to our assumption for G. ☐

We now proceed with the main lemma of this section.

Lemma 4.14. *Let $k \geq 1$ and let G be a disconnected cactus graph in $\mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$ non-isomorphic to $(k+2)K_3$. Let also $\{\mathcal{C}_1, \mathcal{C}_2\}$ be a partition of the connected components of G and $G_i = \bigcup \mathcal{C}_i, i \in [2]$. Then $G_1 \in \mathbf{obs}(\mathcal{A}_{k_1-1}(\mathcal{S}))$ and $G_2 \in \mathbf{obs}(\mathcal{A}_{k_2-1}(\mathcal{S}))$ for some $k_1, k_2 \geq 1$ such that $k_1 + k_2 = k+1$.*

Proof. Clearly, since G is a cactus graph, then the same holds for G_1, G_2. By Lemma 4.13, there exists a $(k+1)$-apex forest set S of G. Notice that, since $G \notin \mathcal{A}_k(\mathcal{S})$, we have that $|S| = k+1$. Also observe that, by Lemma 3.1, neither of G_1, G_2 is a forest. Let $S_1 = S \cap V(G_1), S_2 = S \cap V(G_2)$ and let $k_1 = |S_1|, k_2 = |S_2|$. Note that, $k_1, k_2 \geq 1$ and, since $V(G_1) \cap V(G_2) = \emptyset$, $k_1 + k_2 = k+1$. We argue that the following holds:

Claim 1: For each $i \in [2]$, $G_i \notin \mathcal{A}_{k_i-1}(\mathcal{S})$.

Proof of Claim 1: Suppose, towards a contradiction, that $G_i \in \mathcal{A}_{k_i-1}(\mathcal{S})$ for some $i \in [2]$. Then, there exists a (k_i-1)-apex sub-unicyclic set X_i of G_i. But then, the set $X_i \cup S_j$, where $j \neq i$, is a k-apex sub-unicycle set of G, a contradiction to the fact that $G \in \mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$. Claim 1 follows.

Claim 2: For each $i \in [2]$, it holds that if H_i is a proper minor of G_i then $H_i \in \mathcal{A}_{k_i-1}(\mathcal{S})$.

Proof of Claim 2: Suppose, towards a contradiction, that for some $i \in [2]$ there exists a proper minor H_i of G_i such that $H_i \notin \mathcal{A}_{k_i-1}(\mathcal{S})$. Let $H = H_i \cup G_j$, where $j \neq i$. As $G \in \mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$, there exists a k-apex sub-unicyclic set X of H. Let $X_i = X \cap H_i$ and $X_j = X \cap G_j$. Then, as $H_i \notin \mathcal{A}_{k_i-1}\mathcal{S}$, we have that $|X_i| \geq k_i$ and therefore the fact that $|X| \leq k$ implies that $|X_j| = |X| - |X_i| \leq k - k_i = k_j - 1$. Hence, the set $X_j \cup S_i$ is a k-apex sub-unicyclic set of G, a contradiction to the fact that $G \in \mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$. Claim 2 follows.

Claim 1 and Claim 2 imply that $G_1 \in \mathbf{obs}(\mathcal{A}_{k_1-1}(\mathcal{S}))$ and $G_2 \in \mathbf{obs}(\mathcal{A}_{k_2-1}(\mathcal{S}))$, which concludes the proof of the Lemma. ☐

Proof of Theorem 4.12. The proof follows by Observation 4.10 and by repeated applications of Lemma 4.14, as required. ☐

Set Operation		GF operation
Disjoint sum	$\mathcal{A} = \mathcal{B} + \mathcal{C}$	A(z)=B(z)+C(z)
Cartesian Product	$\mathcal{A} = \mathcal{B}\mathcal{C}$	A(z)=B(z)C(z)
Multiset	$\mathcal{A} = MSET(\mathcal{B})$	$A(z) = \exp\left(\sum_{k\geq 1} \frac{B(z^k)}{k}\right)$
2-multiset	$\mathcal{A} = MSET_2(\mathcal{B})$	$A(z) = \frac{A(z)^2+A(z^2)}{2}$

Table 1: Operations between combinatorial classes and their counterparts in terms of generating functions.

5 Enumeration of cactus obstructions

Let $\mathcal{G} = \mathbf{obs}(\mathcal{A}_k(\mathcal{S})) \cap \mathcal{K}$. In this section, we determine the asymptotic growth of $g_k = |\mathbf{obs}(\mathcal{A}_k(\mathcal{S})) \cap \mathcal{K}|$ and $z_k = |\mathcal{Z}_k|$. To that end, we make use of the *Symbolic Method* framework and the corresponding analytic techniques, as developed in [15].

The Symbolic Method. A *combinatorial class* is a tuple $(\mathcal{A}, f)$, where $\mathcal{A}$ is a set and f is a *size* function $f : \mathcal{A} \to \mathbb{N}^*$. When the nature of f is clear, we refer to $(\mathcal{A}, f)$ as $\mathcal{A}$ for convenience. Let $a_k = |\{a \in \mathcal{A} : f(a) = k\}|$. The *generating function*, or simply *GF*, $A(z)$ is defined as the power series $A(z) = \sum_{n\geq 0} a_n z^n$.[1] We also employ the notation $[z^k]A(z) = a_k$ to refer to the k-th coefficient of some GF $A(z)$. Two combinatorial classes $\mathcal{A}, \mathcal{B}$ are *isomorphic*, written as $\mathcal{A} = \mathcal{B}$, if $a_k = b_k$ for all k. The simplest combinatorial class is the *atomic* one, denoted by $\mathcal{X}$, with GF $X(x) = x$.

The Symbolic Method allows us to translate operations between combinatorial classes into functional operations between their generating functions. In particular, we shall make use of the operations of *disjoint sum* $(+)$, *cartesian product*, *multiset* ($MSET$), *2-multiset* ($MSET_2$), i.e. multisets of two objects. Each of these operations defines a new set upon given ones, in the obvious way. The size function upon the new class is an additive function over the size of the objects that compose the new object. For instance, the size of a multiset $b \in MSET(\mathcal{A})$ equals the sum of the sizes of all objects in b. The functional relations corresponding to each of these operations can be seen in Table 1. We refer to [15, Chapter I] for details.

Rooted trees. A *tree* is a connected graph for which it holds that $|V(G)|-1 = |E(G)|$. Let $\mathcal{T}$ be a family of trees. We define the family of trees in $\mathcal{T}$ *rooted at a vertex*, denoted by $\mathcal{T}^\bullet$, to be all tuples (T, v), where $T \in \mathcal{T}$ and $v \in V(T)$. We define the family of trees in $\mathcal{T}$ *rooted at an edge*, denoted by $\mathcal{T}^{\bullet-\bullet}$, to be all tuples (T, e), where $T \in \mathcal{T}$, and $e \in E(G)$. Finally, we define the family of trees in $\mathcal{T}$ *rooted at an oriented edge*, denoted by $\mathcal{T}^{\bullet\to\bullet}$, to be all tuples $(T, \overrightarrow{e})$, where $T \in \mathcal{T}$, $\overrightarrow{e} = (a, b) \in V(T)^2$, and $ab \in E(G)$. We say that two rooted trees $(T_1, r_1), (T_2, r_2)$ are isomorphic when there exists a graph isomorphism between T_1, T_2 that maps r_1 to r_2. When no confusion can

[1] By convention, we denote combinatorial classes by calligraphic uppercase letters, their GFs by the same uppercase letters in plain form, and use subscripted lowercase letters to denote the coefficients of the GFs.

arise, we will refer to a rooted tree (T, r) simply as T. By the well-known *Dissymmetry Theorem for Trees* (see [3]), it holds that

$$\mathcal{T} + \mathcal{T}^{\bullet\to\bullet} = \mathcal{T}^{\bullet} + \mathcal{T}^{\bullet-\bullet}. \tag{1}$$

5.1 A bijection of $\mathcal{Z}$ with a family of trees.

We begin by giving a bijection between the combinatorial class $\mathcal{Z}$, i.e., connected graphs in $\mathbf{obs}(\mathcal{A}_k(\mathcal{S})) \cap \mathcal{K}$ with size equal to the number of butterfly-subgraphs, and the following family of trees. Let $\mathcal{T}$ be the family of trees having three different types of vertices, namely $\square$-, $\triangle$-, and $\circ$-vertices, and meeting the following conditions:

1. The neighbourhood of a $\square$-vertex consists of two $\triangle$-vertices.

2. The neighbourhood of a $\triangle$-vertex consists of a $\square$-vertex and two $\circ$-vertices.

3. The neighbourhood of a $\circ$-vertex consists of one or more $\triangle$-vertices.

Consider the combinatorial class $(\mathcal{T}, f)$ where f assigns to a tree size equal to the number of its $\square$-vertices. Then the following holds.

Lemma 5.1. *The combinatorial classes $\mathcal{Z}$ and $\mathcal{T}$ are isomorphic.*

Proof. We shall construct a bijection $\phi : \mathcal{Z} \to \mathcal{T}$ that preserves the size function. Given a graph $G \in \mathcal{Z}$ whose butterfly-subgraphs we denote as $\{Z_1, \ldots, Z_k\}$, let $\phi(G) = T \in \mathcal{T}$ be a tree constructed as such:

- To every central vertex c_i of Z_i we associate a $\square$-vertex s_i.

- To every vertex $v \in G$ which is not a central vertex of some Z_i, we associate a $\circ$-vertex o_v.

- To each K_3-subgraph T_{i_1}, T_{i_2} of Z_i, we associate a $\triangle$-vertex t_{i_1}, t_{i_2}, respectively. The neighbourhood of t_{i_j} consists of the $\square$-vertex c_i and the two $\circ$-vertices associated to the vertices of $T_{i_j} \setminus c_i$.

Observe that the described tree belongs in $\mathcal{T}$ and that ϕ is a bijection (see also Figure 11). Also, notice that ϕ is also size-preserving, since the number of butterfly-subgraphs of $Z \in \mathcal{Z}$ equals the number of $\square$-vertices in $\phi(Z)$. $\square$

By Lemma 5.1, enumerating $\mathcal{Z}$ is equivalent to enumerating $\mathcal{T}$. To that end, we will make use of the combinatorial classes $\mathcal{T}^{\square}, \mathcal{T}^{\triangle}, \mathcal{T}^{\circ}, \mathcal{T}^{\circ-\triangle}, \mathcal{T}^{\square-\triangle}, \mathcal{T}^{\square\to\triangle}, \mathcal{T}^{\triangle\to\square}, \mathcal{T}^{\triangle\to\circ}, \mathcal{T}^{\circ\to\triangle}$, which correspond to trees in $\mathcal{T}$ that are rooted in the indicated way.

Lemma 5.2. *The following functional relations hold for $T(z)$ and $G(z)$:*

$$T(x) = T^{\square}(x) + T^{\triangle}(x) + T^{\circ}(x) - T^{\square\to\triangle}(x) - T^{\triangle\to\circ}(x) \tag{2}$$

$$G(x) = \exp\Big(\sum_{k\geq 1} \frac{T(x^k)}{k}\Big).$$

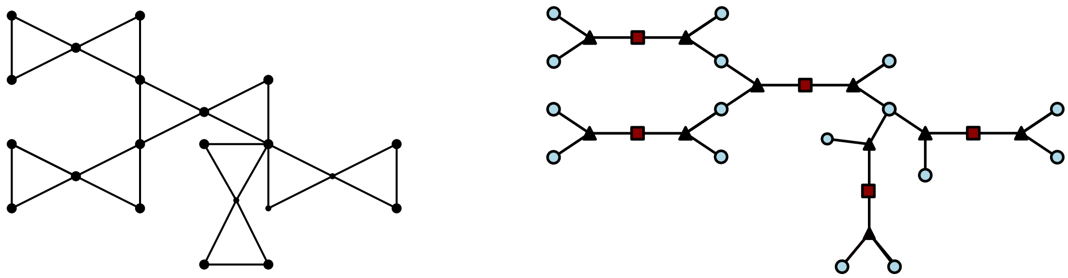


Figure 11: A graph in $\mathcal{Z}$ and its image in $\mathcal{T}$, under the bijection described in Lemma 5.1.

Proof. It is clear that

$$\begin{aligned}
\mathcal{T}^{\bullet} &= \mathcal{T}^{\square} + \mathcal{T}^{\triangle} + \mathcal{T}^{\circ} \\
\mathcal{T}^{\bullet\to\bullet} &= \mathcal{T}^{\square\to\triangle} + \mathcal{T}^{\triangle\to\square} + \mathcal{T}^{\triangle\to\circ} + \mathcal{T}^{\circ\to\triangle} \\
\mathcal{T}^{\bullet-\bullet} &= \mathcal{T}^{\circ-\triangle} + \mathcal{T}^{\square-\triangle} \\
\mathcal{T}^{\circ-\triangle} &= \mathcal{T}^{\circ\to\triangle} \\
\mathcal{T}^{\square-\triangle} &= \mathcal{T}^{\triangle\to\square}
\end{aligned}$$

Then, the first relation follows by substituting the above in Equation 1 and translating to GFs. The second relation follows by noticing that $\mathcal{G} = MSET(\mathcal{Z}) = MSET(\mathcal{T})$. $\square$

To obtain defining systems for $T^{\square}(x), T^{\triangle}(x), T^{\circ}(x), T^{\square\to\triangle}(x), T^{\triangle\to\circ}(x)$, we define the auxiliary combinatorial classes $\mathcal{T}_{\diamond}$ and $\mathcal{T}_{\star}$. $\mathcal{T}_{\diamond}$ contains trees in $\mathcal{T}$ rooted at a leaf and $\mathcal{T}_{\star}$ contains multisets of trees in $\mathcal{T}_{\diamond}$.

Lemma 5.3. *The generating functions $\mathcal{T}_{\star}, \mathcal{T}_{\diamond}, T^{\square}, T^{\triangle}, T^{\circ}, T^{\square\to\triangle}, T^{\triangle\to\circ}$ are defined through the following system of functional equations.*

$$\begin{aligned}
T_{\diamond}(x) &= \frac{x}{2} \exp\Big(\sum_{k\geq 1} \frac{T_{\diamond}(x^k)}{k}\Big)\Big(\exp\Big(\sum_{k\geq 1} \frac{2\,T_{\diamond}(x^k)}{k}\Big) + \exp\Big(\sum_{k\geq 1} \frac{T_{\diamond}(x^{2k})}{k}\Big)\Big) \\
T_{\star}(x) &= \exp\Big(\sum_{k\geq 1} \frac{T_{\diamond}(x^k)}{k}\Big) \\
T^{\circ}(x) &= \exp\Big(\sum_{k\geq 1} \frac{T_{\diamond}(x^k)}{k}\Big) - 1 \\
T^{\square}(x) &= \frac{x}{8}\, T_{\star}(x)^4 + \frac{x}{4} T_{\star}(x)^2 T_{\star}(x^2) + \frac{3x}{8}\, T_{\star}(x^2)^2 + \frac{x}{4}\, T_{\star}(x^4) \\
T^{\triangle}(x) &= \frac{x}{4}\, T_{\star}(x)^4 + \frac{x}{2}\, T_{\star}(x)^2 T_{\star}(x^2) + \frac{x}{4} T_{\star}(x^2)^2 \\
T^{\square\to\triangle}(x) &= \frac{x}{4}\, T_{\star}(x)^4 + \frac{x}{2}\, T_{\star}(x)^2 T_{\star}(x^2) + \frac{x}{4} T_{\star}(x^2)^2 \\
T^{\triangle\to\circ}(x) &= \frac{x}{2}\, T_{\star}(x)^4 + \frac{x}{2}\, T_{\star}(x)^2\, T_{\star}(x^2)
\end{aligned}$$

Proof. We obtain the indicated functional equations by establishing the following combinatorial bijections in the language of the Symbolic method. The result follows by applying their translation to GF relations.

$$\mathcal{T}^{\diamond} = \mathcal{X} MSET(\mathcal{T}_{\diamond}) MSET_2(MSET(\mathcal{T}_{\diamond})) \tag{3}$$
$$\mathcal{T}_{\star} = MSET(\mathcal{T}_{\diamond}) \tag{4}$$
$$\mathcal{T}^{\circ} = MSET(\mathcal{T}_{\diamond}) - 1 \tag{5}$$
$$\mathcal{T}^{\square} = \mathcal{X} MSET_2(MSET_2(\mathcal{T}_{\star})) \tag{6}$$
$$\mathcal{T}^{\triangle} = \mathcal{X} MSET_2(\mathcal{T}_{\star})^2 \tag{7}$$
$$\mathcal{T}^{\square \to \triangle} = \mathcal{X} MSET_2(\mathcal{T}_{\star})^2 \tag{8}$$
$$\mathcal{T}^{\triangle \to \circ} = \mathcal{X} (\mathcal{T}_{\star})^2 MSET_2(\mathcal{T}_{\star}). \tag{9}$$

We now justify each of the equations presented above.

Equation 4 immediately follows from the definition of $\mathcal{T}_{\star}$.

Let $T \in \mathcal{T}$ and let s be a $\square$-vertex. We define its *extended neighbourhood* to be the set $\{o_1, o_2, o_3, o_4, t_1, t_2\}$ where $\{t_1, t_2\}$ is the neighbourhood of s, o_1, o_2 are the $\circ$-neighbours of t_1, and o_3, o_4 are the $\circ$-neighbours of t_2. Given some s whose extended neighbourhood contains the $\circ$-vertices o_i, $i \in [4]$, we define $S_i = \{G \mid G \in \mathcal{C}(T, o_i) \wedge s \notin V(G)\}$, $i \in [4]$. Observe that each S_i is a multiset of graphs which, rooted at o_i, are elements of $\mathcal{T}_{\diamond}$. Hence, $S_i \in MSET(\mathcal{T}_{\diamond})$, which equals $S_i \in \mathcal{T}_{\star}$.

Equation 3: Let $T \in \mathcal{T}_{\diamond}$, o_1 be its root vertex, and s be the closest $\square$-vertex to o_1 in T. Consider the extended neighbourhood defined by s and the corresponding multisets S_i. Notice that if S_3 is exchanged with S_4, then the resulting tree remains the same However, this does not hold when S_2 is exchanged with S_3 or S_4. Hence, T defines uniquely (and is defined by) an object of $T_{\star}$ and a 2-set of objects in $T_{\star}$. The object $\mathcal{X}$ of the atomic class accounts for the vertex s, whose size equals 1.

Equation 5: Let o_1 be the root of $T \in \mathcal{T}^{\circ}$. Observe that $\mathcal{C}(T, o_1) \neq \emptyset$ (this fact corresponds to the term -1 in Equation 5) and all elements of $\mathcal{C}(T, o_1)$, rooted at o_1, belong in $T_{\diamond}$. Hence, T is uniquely defined by (and defines) a multiset of elements in $T_{\diamond}$.

Equation 6: Let $T \in \mathcal{T}^{\square}$ with root s. Consider the multisets S_i, $i \in [4]$, as defined using the extended neighbour of s. Observe that S_1, S_2 can be exchanged to give the same tree, and the same holds for S_3, S_4, so we can consider them as two 2-multisets. Moreover, one can exchange the pair S_1, S_2 with the pair S_3, S_4 to obtain the same tree. Therefore, the desired relation holds, where $\mathcal{X}$ accounts for s.

Equation 7: Let $T \in \mathcal{T}^{\triangle}$ and s the $\square$-vertex connected to the root. Consider the extended neighbourhood of s and the sets S_i, $i \in [4]$. S_1 and S_2 are exchangeable, as well as S_3 and S_4. However, as pairs, they cannot be exchanged to give the same graph. Hence, $\mathcal{T}^{\triangle}$ is equivalent to the cartesian product of two 2-multisets of objects in $\mathcal{T}_{\star}$. $\mathcal{X}$ accounts for the vertex s.

Equation 8: Holds by arguments similar to the ones used to prove Equation 7.

Equation 9: Let $T \in \mathcal{T}^{\triangle \to \circ}$, (t_1, o_1) be its root, and s be the $\square$-vertex closest to t_1. Consider the multisets S_i, $i \in [4]$, as defined using the extended neighborhood of s. Note that one may exchange S_3, S_4 to obtain the same tree T. Note, also, that one may not exchange S_1 with S_2, since then one obtains a different tree.The desired relation then follows, with the $\mathcal{X}$ factor accounting for s. $\square$

By the defining systems of $T(x)$ and $G(x)$, we can obtain the first terms of the series:

$$T(x) = x + x^2 + 3\,x^3 + 7\,x^4 + 25\,x^5 + 88\,x^6 + 366\,x^7 + 1583\,x^8 + 7336\,x^9 + 34982\,x^{10} + \cdots$$
$$G(x) = 1 + z + 2\,x^2 + 5\,x^3 + 13\,x^4 + 41\,x^5 + 143\,x^6 + 558\,x^7 + 2346\,x^8 + 10546\,x^9 + 49397\,x^{10} + \cdots$$

5.2 Asymptotic Analysis

Having set up a system of functional equations for the generating functions $Z(x)$ and $G(x)$, we can determine the asymptotic growth of z_k and g_k via the process of *Singularity Analysis*. We briefly mention the main tools we will use and refer to [15] for details.

We call *dented domain* at $x = \rho$ a set of the form $\{x \in \mathbb{C} \mid |x| < R, \arg(x - \rho) \notin [-\theta, \theta]\}$, for some $R > \rho$ and $0 < \theta < \pi/2$. Let $f(x) = \sum_{k \geq 0} f_k x^k$ a GF analytic in a dented domain at $x = \rho$ that satisfies an expansion of the form

$$f(x) = F_0 + F_1 X + F_2 X^2 + F_3 X^3 + \cdots + F_{2k} X^{2k} + F_{2k+1} X^{2k+1} + O\left(X^{2k+2}\right)$$

locally around ρ, where $X = \sqrt{1 - x/\rho}$. We call *singular exponent* the smallest odd exponent of X divided by two, and denote it by α. If $f_k > 0$ for all k big enough, then we can apply the so-called *Transfer Theorems* of singularity analysis [15, Corrollary VI.1, Theorem VI.4] and obtain

$$[x^n] f(x) \sim c \cdot n^{-\alpha - 1} \cdot \rho^{-n}, \tag{10}$$

where $c = \frac{F_{2\alpha}}{\Gamma(-\alpha)}$ and Γ is the standard Gamma function. To obtain such expansions, we will use the following Theorem.

Theorem 5.4 ([12, Proposition 1, Lemma 1])**.** *Suppose that $F(x, y)$ is an analytic function in x, y such that $F(0, y) \equiv 0$, $F(x, 0) \not\equiv 0$, and all Taylor coefficients of F around 0 are real and nonnegative. Then, the unique solution $y = y(x)$ of the functional equation $y = F(x, y)$ with $y(0) = 0$ is analytic around 0 and has nonnegative Taylor coefficients y_k around 0. Assume that the region of convergence of $F(x, y)$ is large enough such that there exist nonnegative solutions $x = x_0$ and $y = y_0$ of the system of equations*

$$y = F(x, y), \tag{11}$$
$$1 = F_y(x, y), \tag{12}$$

where $F_x(x_0, y_0) \neq 0$ and $F_{yy}(x_0, y_0) \neq 0$.[2] *Assume also that $y_k > 0$ for large enough k. Then, ρ is the unique singularity of f on its radius of convergence and there exist functions $q(x), h(x)$ which are analytic around $x = x_0$, such that $y(x)$ is analytically continuable in a dented domain at ρ and, locally around $x = \rho$, it has a representation of the form*

$$y(x) = q(x) + h(x)\sqrt{\left(1 - \frac{x}{\rho}\right)}. \tag{13}$$

[2]Here, and in the sequel, subscripts will denote partial differentiation with respect to the subscripted variable(s).

In the proof of the latter Theorem, an explicit way is given to compute the coefficients q_i, h_i. Using a computer algebra program like `Maple`, we can easily obtain:

$$h_0 = \sqrt{\frac{2\rho F_x(x_0,y_0)}{F_{yy}(x_0,y_0)}}, \quad h_1 = \frac{1}{6}\frac{-F_{yyy}(x_0,y_0)h_0^2 + 6F_{xy}(x_0,y_0)\rho}{2F_{yy}(x_0,y_0)}, \tag{14}$$

$$\begin{aligned} q_1 = & -\frac{1}{24}\frac{F_{yyyy}(x_0,y_0)h_0^4 - 12F_{xyyy}(x_0,y_0)h_0^2\rho + 12F_{yyy}(x_0,y_0)h_1h_0^2}{F_{yy}(x_0,y_0)h_0} + \\ & + \frac{12F_{xx}(x_0,y_0)\rho^2 - 24F_{xy}(x_0,y_0)h_1\rho + 12F_{xx}(x_0,y_0)h_1^2}{F_{yy}(x_0,y_0)h_0}. \end{aligned} \tag{15}$$

Lemma 5.5. *The generating functions $T_\diamond, T^\square, T^\triangle, T^\circ, T^{\square\to\triangle}, T^{\triangle\to\circ}$ have a unique singularity of smallest modulus, at the same positive number $\rho < 1$. Moreover, they are analytic in a dented domain at ρ and satisfy expansions of the form*

$$A_0 + \sum_{k\geq 1} A_k X^k, \quad \textit{where} \quad X = \sqrt{1 - x/\rho},$$

locally around ρ. The coefficients A_i and ρ are computable; in particular, $\rho \approx 0.15926$.

Proof. Let $\rho_\diamond < 1$ the positive radius of convergence of $T_\diamond$ (it is easy to see combinatorially that $0 < \rho_\diamond < 1$). All functions $T^\square, T^\triangle, T^\circ, T^{\square\to\triangle}, T^{\triangle\to\circ}$ can be defined with respect to $T_\diamond$, as indicated in Lemma 5.3. In particular, they depend on $T_\diamond$ in three different ways: by composing $T_\diamond(x)$ with either a polynomial having positive coefficients or the exponential function, by performing a change of variables from x to x^k, and by the operator $\exp\left(\frac{1}{k}\sum_{k\geq 2} T_\diamond(x^k)\right)$. We observe that all three of them preserve the number and nature of singularities, hence these are determined solely by the behaviour of $T_\diamond$. In the case of composition with polynomials or exponentials, it is trivial to see. In the case of variable change, observe that $T_\diamond(x^k)$ has radius of convergence $\sqrt[k]{\rho_\diamond} > \rho_\diamond$. In the case of $\exp\left(\frac{1}{k}\sum_{k\geq 2} T_\diamond(x^k)\right)$, it is enough to notice that in $|x| < \rho_\diamond$ it holds that

$$\sum_{k\geq 2} T_\diamond(x^k) \leq T_\diamond(x^2) + \sum_{k\geq 3} x^{k-2} T_\diamond(x^2) = \frac{T_\diamond(x^2)}{1-x}.$$

Therefore, it is enough to prove the claimed properties for $T_\diamond(z)$.

To analyse $T_\diamond(z)$, we will use Theorem 5.4. Let

$$F(x,y) = \frac{x}{2}\exp\left(y + \sum_{k\geq 2}\frac{T_\diamond(x^k)}{k}\right)\left(\exp\left(2y + \sum_{k\geq 2}\frac{2T_\diamond(x^k)}{k}\right) + \exp\left(\sum_{k\geq 1}\frac{T_\diamond(x^{2k})}{k}\right)\right). \tag{16}$$

The system $\{y = F(x,y), 1 = F_y(x,y)\}$ can be solved numerically, using truncations of the functions $T_\diamond(z^k)$. We find a solution (x_0, y_0), where $x_0 \approx 0.15926$ and $y_0 \approx 0.41738$. Clearly, the rest of the requirements of Theorem 5.4 are met and the coefficients of the desired expansion can be computed by Equations 14, 16. The coefficients for the expansions of $T^\square(x)$, $T^\triangle(x)$, $T^\circ(x)$, $T^{\square\to\triangle}(x)$, $T^{\triangle\to\circ}(x)$ can be computed straightforwardly by the coefficients of $T_\diamond(z)$. Notice that Theorem 5.4 guarantees $A_1 \neq 0$ in all cases. $\square$

Lemma 5.6. *The generating functions $Z(x), G(x)$ have a unique singularity of smallest modulus at the same positive number $\rho < 1$. Moreover, they are analytic in a dented domain at ρ and satisfy expansions*

$$Z(x) = Z_0 + \sum_{k\geq 2} Z_k X^k, \quad G(x) = G_0 + \sum_{k\geq 2} G_k X^k, \quad \textit{where} \quad X = \sqrt{1 - x/\rho},$$

locally around ρ. The coefficients Z_i, G_i, and ρ are computable; in particular, $\rho \approx 0.15926$ (the same as in Lemma 5.5).

Proof. By Equation 2, the singular behaviour of $Z(x)$ depends entirely on the functions $T_i(x)$ that were studied in Lemma 5.5 (recall that $Z(x) = T(x)$). In particular, $Z(x)$ has a unique positive singularity of minimum modulus at the same point ρ and the same holds for $G(x)$.

The coefficients of the expansions are directly computable by the coefficients of $T_i(x)$. In particular, we can show that the coefficient Z_1 vanishes identically and $Z_3 \neq 0$. Let $A_0 + A_1 X + \ldots$ be the expansion given by Lemma 5.5 for $T_\star(x)$ and notice that $A_0 = T_\star(\rho)$. Then, Z_1 is equal to the following expression, which can be easily obtained on computational software such as `Maple`:

$$Z_1 = A_1 \left(\frac{3\rho A_0^3}{2} + \frac{\rho A_0 C_0}{2} - 1 \right),$$

where $C_0 = T_\star(\rho^2)$. Recall the function F in Equation 16 and the system $\{y = F(x,y), 1 = F_y(x,y)\}$. The latter has solution (ρ, y_0) and thus it holds that:

$$\begin{aligned} 0 &= F_y(\rho, y_0) - 1 \\ &= \frac{3\rho}{2} \exp\left(y_0 + \sum_{i\geq 2} \frac{T_\diamond(\rho^i)}{i} \right)^3 + \frac{\rho}{2} \exp\left(y_0 + \sum_{k\geq 2} \frac{T_\diamond(x^k)}{k} \right) \exp\left(\sum_{k\geq 1} \frac{T_\diamond(\rho^{2k})}{k} \right) - 1. \end{aligned}$$

This is equal to $\frac{1}{A_1} Z_1$, since $T_\star(\rho) = \exp\left(y_0 + \sum_{i\geq 2} \frac{T_\diamond(\rho^i)}{i} \right)$ and $T_\star(\rho^2) = \exp\left(\sum_{k\geq 1} \frac{T_\diamond(\rho^{2k})}{k} \right)$. Thus, $Z_1 = 0$. This is a typical behaviour after applying the Dissymmetry Theorem (see [4], [27]).

To see that Z_3 does not vanish, it is enough to argue combinatorially. First, observe that $t_n^\bullet \sim \frac{c\rho^{-n}}{n^{3/2}}$ by Lemma 5.5 and the Transfer Theorem (see Equation 10 and the related account). If Z_3 vanished, then the singular exponent would be bigger than $3/2$. Consequently, by the Transfer Theorem we would obtain $n \cdot z_k = n \cdot t_k = o(\frac{c\rho^{-n}}{n^{3/2}})$ for large n, a contradiction to the asymptotic growth of $t_n^\bullet$. □

Corollary 5.7. *The coefficients of $Z(x), G(x)$ satisfy an asymptotic growth of the form*

$$c n^{-\frac{5}{2}} \rho^{-n},$$

where c is equal to $\frac{Z_3}{\Gamma(-3/2)} \approx 0.27160$ and $\frac{G_3}{\Gamma(-3/2)} \approx 0.33995$, respectively, and $\rho^{-1} \approx 6.27888$.

Proof. It follows by Lemma 5.6 and the Transfer Theorem. The computations are straightforward and can be easily confirmed on computational software such as `Maple` (see

http://www.cs.upc.edu/~sedthilk/osmc/apexmo.mw

for the detailed calculations). □

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