Structure and Enumeration of Cactus Minor-Obstructions for k-Apex Sub-unicyclic Graphs

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ABSTRACT

A graph is *sub-unicyclic* if it contains at most one cycle, while it is *k-apex sub-unicyclic* if it can be made sub-unicyclic by removing k of its vertices. The purpose of this thesis is to structurally characterise and enumerate subsets of minor-obstructions for the families of k-apex sub-unicyclic graphs. Specifically, we are interested in minor-obstructions which are cacti. To achieve this, we employ results and techniques from structural graph theory, enumerative and analytic combinatorics, and the theory of combinatorial species.

ΣΥΝΟΨΗ

Ένα γράφημα είναι υπομονοκυκλικό εάν περιέχει το πολύ έναν κύκλο. Ένα γράφημα είναι k-απόγειο υπομονοκυκλικό εάν μπορεί να γίνει υπομονοκυκλικό μέσω διαγραφής k κορυφών του. Σκοπός της διπλωματικής εργασίας είναι ο δομικός χαρακτηρισμός και η απαρίθμηση του υποσυνόλου των ελασσόνων παρεμποδίσεων των k-απόγειων υπομονοκυκλικών γραφημάτων που είναι κάκτοι για κάθε k. Για την επίλυση αυτού του προβλήματος, έγινε χρήση αποτελεσμάτων και τεχνικών από την δομική γραφοθεωρία, την απαριθμητική και αναλυτική συνδυαστική, καθώς και τη θεωρία των συνδυαστικών φυλών.

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CONTENTS

CHAPTER 1

INTRODUCTION

A family of graphs $\mathcal{G}$ is minor-closed if for all $G \in \mathcal{G}$ we have that every minor of G, that is every graph obtained from G via vertex and edge deletions as well as edge contractions, is also in $\mathcal{G}$. A major result of graph theory is the theorem of Robertson–Seymour stating that undirected graphs form a well-quasi-ordering under the minor relation. A consequence of that is that every minor-closed family (a *minor ideal*) $\mathcal{G}$ can be characterised by a finite set $\mathbf{obs}(\mathcal{G})$ of *forbidden-minors*, which is referred to as the *obstruction set* of that family. Therefore such a family $\mathcal{G}$ can be equivalently be identified with the set of graphs having no minor which belongs to $\mathbf{obs}(\mathcal{G})$.

Identifying $\mathbf{obs}(\mathcal{G})$ for various minor-closed families $\mathcal{G}$ is an important topic in structural graph theory and one which has attracted much attention. For a list of some open problems in this area, see [1].

Among the several ways to construct a new minor-closed family from some given one, a particularly popular one is to consider the families of graphs "within k vertices of $\mathcal{G}$". That is, given some minor ideal $\mathcal{G}$, we can define the families $\mathcal{A}_k(\mathcal{G})$, k being a non-negative integer, containing all graphs where we can delete k of their vertices to obtain a graph in $\mathcal{G}$. We graphs in such a family $\mathcal{A}_k(\mathcal{G})$ *k-apex $\mathcal{G}$-graphs*.

A lot of research has been carried to (partially) identify obstruction sets for classes of the form $\mathcal{A}_k(\mathcal{G})$ For example, the set $\mathbf{obs}(\mathcal{A}_k(\mathcal{G}))$, when $\mathcal{G}$ is the family of edgeless graphs, has been identified for values of k up to 7 ([2],[3],[4]). Similarly, the set $\mathbf{obs}(\mathcal{A}_k(\mathcal{G}))$, when $\mathcal{G}$ is the family of acyclic graphs, has been identified for $k \in \{1, 2\}$ [5]. The case when $\mathcal{G}$ is the class of planar graphs has attracted much attention (for example, see [6], [7]). A recent development on this question is presented in [8] wherein the authors identify all biconnected minor-obstructions for 1-apex planar graphs.

Ideally, there would be an effective way to characterise and enumerate all obstructions for a given minor closed family. Unfortunately, this is known to not be the case.

Theorem 1.0.1 ([9])**.** *There is no algorithm which, given a finite description of a minor-closed family F of graphs in the form of a Turing machine which accepts precisely the graphs in F, computes the set of obstructions for F.*

For an extension of this theorem in the context of monadic second-order logic, see [10].

While such an algorithm for the general problem of identifying all obstructions of a minor-closed family does not exist, a major result in this area is that a restricted version of it is, in fact, computable ([11]): given a finite set O, one can compute the obstruction set of the family of graphs having k vertices, called *apex vertices*, whose removal results in a $excl(O)$ graph.

Another direction in the study of minor-obstructions for families $\mathcal{A}_k(\mathcal{G})$ is proving upper-bounds in the size of $\mathbf{obs}(\mathcal{A}_k(\mathcal{G}))$. In [12] it was shown 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 $\mathbf{obs}(\mathcal{G})$ contains a planar graph (see also [13]). Alternatively, one can try to prove lower bounds for the size of $\mathbf{obs}\mathcal{A}_k(\mathcal{G})$ instead. For example, it was shown in[14] that if all graphs in $\mathbf{obs}(\mathcal{G})$ are connected, then $|\mathbf{obs}\mathcal{A}_k(\mathcal{G})|$ is exponentially big. To this end, the author shows in [14] that, assuming all graphs in $\mathbf{obs}(\mathcal{G})$ are connected, every connected component of a graph in $\mathbf{obs}\mathcal{A}_k(\mathcal{G})$ belongs to $\mathbf{obs}\mathcal{A}_{k'}(\mathcal{G})$ for some $k' < k$. Another approach to lower bounds is to completely characterise, for every k, the set $\mathbf{obs}\mathcal{A}_k(\mathcal{G}) \cap \mathcal{H}$, for some family $\mathcal{H}$. Equipped with this characterisation, one can then derive lower bounds for $|\mathbf{obs}\mathcal{A}_k(\mathcal{G})|$ by counting all graphs in $\mathbf{obs}\mathcal{A}_k(\mathcal{G})$. This is the approach followed by the authors in [13] where $\mathcal{G}$ is taken to be the family of acyclic graphs and $\mathcal{H}$ the family of outerplanar graphs.

Consider now the minor-closed families of graphs having the following property: there exists some k-sized subset of their vertices whose removal leaves the graph with at most one cycle. For the family corresponding to $k = 1$ the set of obstructions was determined in [15]. Our interest lies in understanding the obstructions for k-apex sub-unicyclicity which are cactus graphs; let us call such obstructions *cactus-obstructions*. Cacti are a class of graphs which are complex enough to be of interest but are also restricted enough in structure so that our undertaking of characterising and enumerating them can succeed. In particular, their tree-like structure (cacti have treewidth 2) means that combinatorial and enumerative methods developed for trees can be brought to bear on the problems of enumeration and characterisation of cacti. The purpose of this work is to structurally characterise and enumerate, both exactly and asymptotically, these cactus-obstructions. For this purpose, we employ tools from graph theory, the theory of combinatorial species, and analytic combinatorics.

The structure of this work is as follows. We begin with preliminaries in graph theory, where we define the notions of graph minors, k-apex sub-unicyclic graphs, cactus graphs, and obstructions for minor-closed families. We follow this up with an introduction to the species-theoretic notions, defining the notion of species, their related generating series, and various operations on them, as well as the notions of species isomorphism and of virtual species. Finally, concluding the preliminary section of our work, we present some basic notions of analytic combinatorics.

We then present the first main part of this work, the characterisation of cactus-obstructions for the family of k-apex sub-unicyclic graphs. Intuitively, this characterisation takes the following form for the connected case: the connected cactus-obstructions for k-apex sub-unicyclicity are exactly those that can be constructed by gluing together butterfly graphs while avoiding gluing on their central vertices. We also characterise the disconnected cactus-obstructions in a manner similar to the aforementioned results obtained in [14]. These are essentially either disjoint unions of $k + 2$ copies of the triangle graph or disjoint unions of obstructions for families of "lower levels" of apex sub-unicyclicity (in the sense that they are obstructions for k'-apex sub-unicyclicity with $k' < k$).

The third and final part of our work makes use of this characterisation to enumerate cactus-obstructions and analyse their asymptotic growth, answering, both exactly and asymptotically, the question of how many cactus-obstructions exist for k-apex sub-unicyclicity for given k. To achieve this, we present a bijection between cactus-obstructions and *4-cacti*, that is cacti whose blocks are all isomorphic to the 4-cycle. Then, using this correspondence, we describe a species-theoretic way to enumerate a slight variant of 4-cacti which yields an exact enumeration of our cactus-obstructions. From this species-theoretic description we then derive relations for the generating series of cactus-obstructions which we analyse, employing tools from analytic combinatorics, so as to obtain a characterisation of the asymptotic growth of cactus-obstructions. A topic in graphical enumeration which is closely related to our work is the enumeration of *k-cacti*, that is cacti whose blocks are all isomorphic to the k-cycle, and their variants. For example, in [16] the authors enumerate *plane* k-cacti, while in [17] the authors enumerate general k-cacti using a decomposition-based technique. Another example of enumeration of general/free k-cacti is given in [18] where the authors propose a method for enumerating unlabeled k-cacti and derive functional equations for 3- and 4-cacti. Our approach will be quite different from both [18] (although we do derive the same functional relation for 4-cacti) and especially [17]. Instead we will more closely follow the approach seen in [19]. The benefit of our approach is that it allows us to quickly derive the required functional equations and establish the required asymptotic estimates for both rooted and unrooted 4-cacti.

We note that throughout this work we made use of the SageMath 8.4 and Maple 2015.1 software systems as aids in both symbolic and numerical computation. In the sequel, all references to either SageMath or Maple should be understood to refer to the aforementioned versions of the respective software system.

CHAPTER 2

PRELIMINARIES

2.1 Notation, Sets, and Functions

We begin with some useful notation for the sets of natural and complex numbers, intervals, and set operations.

Notation 2.1.1. We denote by $\mathbb{N}$ the set of all non-negative integers and by $\mathbb{N}^+$ the set $\mathbb{N} \setminus \{0\}$ of positive integers. We denote by $\mathbb{C}$ the set of complex numbers.

Given two integers p and q we let $[p, q] = \{p, \ldots, q\}$ and given some $k \in \mathbb{N}^+$ we denote by $[k]$ the set $[1, k]$. 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 set of objects for which the operation $\cup$ is defined, we denote by $\bigcup \mathcal{S}$ the set $\bigcup_{X \in \mathcal{S}} X$.

If $k \in \mathbb{N}^+$ we let $\mathcal{P}(k)$ be the set $P = \{\{p_1, \ldots, p_k\} | k \in \mathbb{N}^+ \wedge p_i \in \mathbb{N}^+ \wedge \sum\limits_{i \in k} p_i = k\}$ of *partitions* of k.

The following complex-valued function, called the *Gamma* function, is an extension of the factorial function to non-integral arguments.

Definition 2.1.2 (Gamma Function)**.** Euler's gamma function is

$$\Gamma(s) = \int_0^\infty e^{-t} t^{s-1} dt, \tag{2.1}$$

where the integral converges when $\Re(s) > 0$. Observe that, via integration by parts, we have that

$$\Gamma(s+1) = s\Gamma(s) \tag{2.2}$$

Two specific values of the Gamma function which will be useful in our work are $\Gamma(-\frac{1}{2}) = -2\sqrt{\pi}$ and $\Gamma(-\frac{3}{2}) = \frac{4\sqrt{\pi}}{3}$.

Following the notation introduced in [20] we write $a \doteq d$ to represent a numerical approximation of the real number a by the decimal d.

The following will prove useful in comparing exact and approximate values.

Definition 2.1.3 (Relative Error)**.** Let $x, y \in \mathbb{R}$. We define the *relative error* to be

$$\left| \frac{x - y}{x} \right|$$

We will be using relative errors to evaluate the accuracy of our approximations compared to the exact values. Therefore, in what follows, we will implicitly assume x to be the corresponding exact value and y to be its approximation, when computing relative errors.

Let $G(x_1, x_2, \ldots, x_n)$ be a multivariate function. We will write $G_{x_i}(x_1, x_2, \ldots)$ (or just G_{x_i}) to denote the partial derivative of G with respect to x_i. We will also write $G_{x_i x_j \ldots x_k}(x_1, x_2, \ldots, x_n)$ (or just $G_{x_i x_j \ldots x_k}$) to denote $\frac{\partial}{\partial x_k} \ldots \frac{\partial}{\partial x_j} \frac{\partial}{\partial x_i} G(x_1, x_2, \ldots, x_n)$.

2.2 Graph Theory

We begin with an introduction to some basic notions of graph theory required for this work. We will largely follow [21] and [22], where the interested reader will find the notions we discuss below presented in much more detail.

We will assume that all graphs in this work 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 *vertex count* of G. Given a vertex $v \in V(G)$, we define the *neighbourhood* of v to be the set $N_G(v) = \{u \mid u \in V(G), \{u, v\} \in E(G)\}$. The *degree* of a vertex v in G is the quantity $|N_G(v)|$. We write K_r to denote the *r-clique*, that is, the complete graph on r vertices. Finally, if G is some graph, we write kG for $k \in \mathbb{N}^+$ to denote the union of k disjoint graphs, all isomorphic to G.

Definition 2.2.1 (Union of graphs)**.** Given two graphs G_1, G_2, we define the *union* of G_1, G_2 as the graph $G_1 \cup G_2 = (V(G_1) \cup V(G_2), E(G_1) \cup E(G_2))$.

Definition 2.2.2 (Trivial Graph)**.** We say that a graph G is trivial if $V(G)$ is a singleton and $E(G)$ is the empty set.

The following three operations allow us to produce new graphs from given ones.

Definition 2.2.3 (Vertex Deletion)**.** Let $G = (V, E)$ be a graph and $S \subseteq V$. We denoted by $G \setminus S$ the graph obtained from G by *deleting* the vertices of S from V and removing all their incident edges. Formally, we have that $G \setminus S = (V', E')$ where $V' = V \setminus S$ and $E' = \{uv | \{u, v\} \cap S = \emptyset\}$.

Definition 2.2.4 (Edge Deletion)**.** Let $G = (V, E)$ be a graph and $e = uv$ be one of its edges. We denoted by $G \setminus e$ the graph obtained from G by *deleting* the edge. Formally, we have that $G \setminus S = (V, E')$ where $E' = E \setminus \{u, v\}$.

Definition 2.2.5 (Edge Contraction)**.** Let $G = (V, E)$ be a graph and $e = uv$ be one of its edges. We denoted by G/e the graph obtained from G by *contracting* e, that is replacing it with a new vertex v_e such that $N(v_e) = N(u) \cup N(v)$. More formally, $G/e = (V', E')$ where $V' = (V \setminus \{x, y\}) \cup \{v_e\}$ and $E' = \{xy | \{x, y\} \cap \{u, v\} = \emptyset\} \cup \{v_e w | uw \in E \setminus uv \vee vw \in E \setminus uv\}$.

Using the above operations we can define the notions of a *subgraph* and a *graph minor*.

Definition 2.2.6 (Subgraph)**.** Let $G = (V, E)$ be a graph and let H be a graph obtained from G after repeated application of the edge and vertex deletion operations. We then say that H is a *subgraph* of G and that G contains H as a subgraph. If H can be obtained from G via vertex deletions alone we say that H is an *induced* subgraph of G.

Definition 2.2.7 (Graph Minor)**.** Let $G = (V, E)$ be a graph and let H be a graph obtained from G after repeated application of the edge and vertex deletion and edge contration operations. We say that H is a *minor* of G and that G *contains* H *as a minor*. We write $H \leq_m G$ if G contains (a graph isomorphic to) H as a minor.

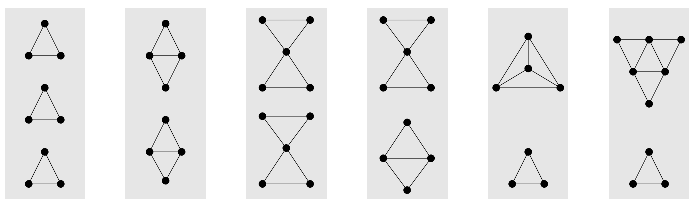
Observe that the minor relation $\leq_m$ is transitive. Observe also that the deletion of some non-isolated vertex v can be "simulated" by first deleting all but one of the edges incident to v and then contracting along it. As such, when it is clear that no isolated vertices are at play, we will frequently assume that a minor H of some G can be obtained from G using edge deletions and contractions only.

We say that a graph family $\mathcal{G}$ is *closed under minors* if for every $G \in \mathcal{G}$ it holds that every minor of G also belongs to $\mathcal{G}$. Observe that such a class can be characterised by listing all minor-minimal graphs not in $\mathcal{G}$ (i.e graphs not in $\mathcal{G}$ whose minors all belong to G). Then a graph H belongs to $\mathcal{G}$ if and only if it contains none of these graphs as a minor, hence the use of the term *obstructions* when referring for these graphs. A major result in graph minor theory is the resolution of Hadwinger's conjecture by Robertson and Seymour, from which it follows that for every minor-closed family, the set of minor-minimal graphs is always finite.

Theorem 2.2.8 (Robertson - Seymour)**.** *Finite graphs form a well-quasi-order under the minor relation* $\leq_m$.

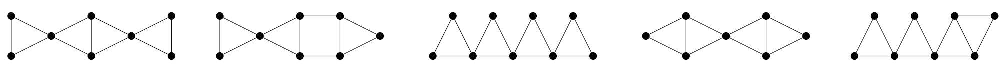
As a corollary, we have that for every minor-closed family $\mathcal{G}$ the set of minor-minimal graphs not in $\mathcal{G}$ is finite and therefore every minor-closed property can be characterised by a finite set of excluded minors.

A graph is *sub-unicyclic* if it contains at most one cycle and is *k-apex sub-unicyclic* if there exists a subset $S \subseteq V(G)$ of size k such that $G \setminus S$ is sub-unicyclic. One easily verifies that the class of $\mathcal{A}_k(\mathcal{S})$ of k-apex sub-unicyclic graphs is closed under minors. The obstruction set for 1-apex sub-unicyclicity, as determined in [15] is show in Figure 2.1, Figure 2.2, Figure 2.3, and Figure 2.4.

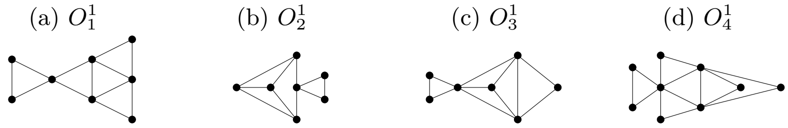


(a) O_1^0 (b) O_2^0 (c) O_3^0 (d) O_4^0 (e) O_5^0 (f) O_6^0

Figure 2.1: The set $\mathcal{O}^0$ of obstructions for $\mathcal{A}_1(\mathcal{S})$ with vertex connectivity 0.

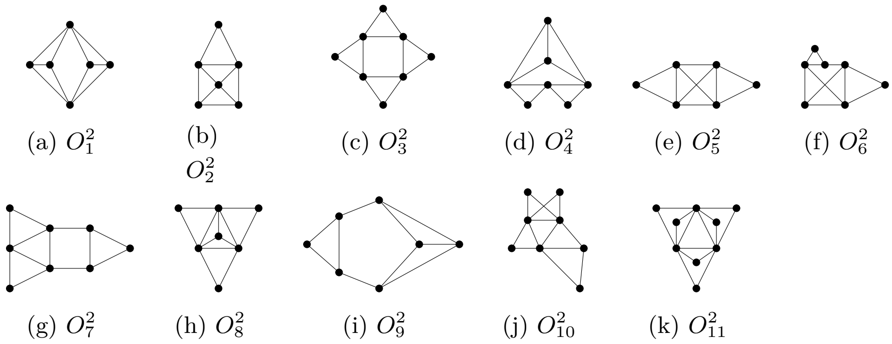


(a) O_1^1 (b) O_2^1 (c) O_3^1 (d) O_4^1 (e) O_5^1



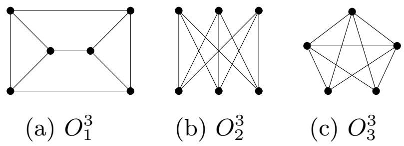
(f) O_6^1 (g) O_7^1 (h) O_8^1 (i) O_9^1

Figure 2.2: The set $\mathcal{O}^1$ of obstructions for $\mathcal{A}_1(\mathcal{S})$ of vertex connectivity 1.



(a) O_1^2 (b) O_2^2 (c) O_3^2 (d) O_4^2 (e) O_5^2 (f) O_6^2 (g) O_7^2 (h) O_8^2 (i) O_9^2 (j) O_{10}^2 (k) O_{11}^2

Figure 2.3: The set $\mathcal{O}^2$ of obstructions for $\mathcal{A}_1(\mathcal{S})$ with vertex connectivity 2.



(a) O_1^3 (b) O_2^3 (c) O_3^3

Figure 2.4: The set $\mathcal{O}^3$ obstructions for $\mathcal{A}_1(\mathcal{S})$ with vertex connectivity 3.

Definition 2.2.9 (Cactus graphs)**.** A *cactus* graph is a graph in which any two cycles have at most one cycle in common. or equivalently one in which every edge belongs to at most one cycle. Yet another equivalent definition is that a graph is a cactus if it does not contain K_4^- as a minor. Therefore all blocks of a cactus are isomorphic either to some n-cycle or an edge. We say that a cactus is a n*-cactus* if all of its blocks are isomorphic to the n-cycle graph. We are particularly interested in the case of 4-cacti, whose blocks are all isomorphic to the 4-cycle *square graph*, which we denote by C_4. A particularly simple case of a cactus graph is the *butterfly* graph, denoted as Z, which is obtained by identifying the vertices of two 3-cycle graphs (*triangles*). As mentioned in the introductory section, these two graphs, Z and C_4, will play a central role in our work.

We will denoted the family of cactus graphs (or just *cacti*) by $\mathcal{K}$. If $\mathcal{F}$ is some minor-closed family of graphs, then we will refer to elements of $\mathbf{obs}(\mathcal{F}) \cap \mathcal{K}$ as cactus-obstructions.

Another useful notion is that of *augmented connected components*, defined in relation to some set S of G.

Definition 2.2.10 (Augmented connected components)**.** Let G be a graph and $S \subseteq V(G)$ and let $V_1, \ldots, V_q$ 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. We call the members of the set $\mathcal{C}(G,S)$ *augmented connected components*. Given a vertex $x \in V(G)$ we define $\mathcal{C}(G,x) = \mathcal{C}(G,\{x\})$.

2.3 Combinatorial Species Theory

We now present some basic notions of the theory of *combinatorial species*. This theory has its origins in the work of André Joyal (see [23]) and is very closely related to the *symbolic method* of Flajolet and Sedgewick (for a detailed comparison see [24]). Our exposition largely follows [19]. We will omit some technical proofs in favour of clarity of exposition; please refer to [19] for some of these ommited proofs.

We begin with a definition of the central notion of species theory, that of *species of structures*, which serves to encapsulate the notion of combinatorial constructions such as graphs, trees, permutations, and linear orders.

Definition 2.3.1 (Species of Structures)**.** A *species of structures* is a rule F which for each finite set U produces a finite set $F[U]$ and for each bijection $\sigma : U \to V$ produces a bijection $F[\sigma] : F[U] \to F[Vv]$, such that $F[\tau \circ \sigma] = F[\tau] \circ F[\sigma]$ and $F[Id_U] = Id_{F[u]}$. An element $s \in F[U]$ is called an *F-structure on U* , while a function $F[\sigma]$ is called the *transport of F-structures along σ.*

Remark 1. For the reader acquainted with category theory, the above definition of species can be succinctly be recast as such: a species F is an endofunctor on the category $\mathbf{B}$ of finite sets and bijections.

For ease of notation we write $[n]$ for the set $\{1, 2, 3, \ldots, n\}$ and $F[n]$, rather than $F[[n]]$, for $F[\{1, 2, 3, \ldots, n\}]$.

Example 2.3.2. The following species are particularly useful and can easily be defined explicitely (we omit writing the corresponding transports since they are obvious).

- The species E of sets, defined by $E[U] = \{U\}$ which on each finite set U puts a unique E-stucture, namely the set itself.
- The species X of singletons defined as

$$X[U] = \begin{cases} \{U\}, & \text{if } |U|= 1 \\ \emptyset, & otherwise. \end{cases} \tag{2.3}$$

- The species E_2 of sets of cardinality 2 defined as

$$E_2[U] = \begin{cases} \{U\}, & \text{if } |U|= 2 \\ \emptyset, & otherwise. \end{cases} \tag{2.4}$$

- The species 1 of the empty set, defined as

$$1[U] = \begin{cases} \{U\}, & \text{if } U = \emptyset \\ \emptyset, & otherwise. \end{cases} \tag{2.5}$$

Two more examples of species are given by $\mathcal{S}$, the species of permutations, and L the species of linear orders.

These species will be used to construct the species of graphs which we are interested in enumerating. To do this, we will make use of operations between species, as defined later in this section.

It is important to note that we consider F-structures to be *labeled.* Since we are interested in the enumeration of graphs up to isomorphism, we must first define a notion of "unlabeled" F-structures, which is done via the following the notion of isomorphism between two F-structures.

Definition 2.3.3 (Isomorphism of F-structures)**.** Let F be some species and consider two F-structures $s_1 \in F[U]$ and $s_2 \in F[V]$. A bijection $\sigma : U \to V$ is called an isomorphism of s_1 to s_2 if $s_2 = F[\sigma](s_1)$. One says that such structures have the same isomorphism type (or just *type*) and writes $s_1 \sim s_2$. When such an isomorphism is from some F-structure s to itself, we say it is an *automorphism* of s. Equivalence classes modulo the isomorphism relation are referred to as isomorphism types of F-structures or *unlabeled* F-structures.

To every species we can associate three kinds of formal power series which aid in the enumeration of both labeled and unlabeled F-structures. We begin by defining the exponential generating series associated to a species of structures F, which is frequently used when one deals with labeled enumeration problems.

Definition 2.3.4 (Exponential Generating Series)**.** The exponential generating series of a species of structures F is the following formal power series:

$$F(x) = \sum_{n=0}^{\infty} f_n \frac{x^n}{n!}, \tag{2.6}$$

where $f_n = |F[n]|$, that is, the number of F-structures on a set of cardinality n.

The "exponential" designation comes from the fact that $n!$ appears in the denominator of a term of degree n.

The following notation is useful when referring to coefficients of formal power series. If $G(x)$ is some ordinary formal power series

$$G(x) = \sum_{n \geq 0} g_n x^n, \tag{2.7}$$

we define

$$[x^n]G(x) = g_n. \tag{2.8}$$

Therefore, for a power series of exponential type (as in Definition 2.3.4),

$$n![x^n]F(x) = f_n, \tag{2.9}$$

Example 2.3.5. We now list the exponential generating series associated with each of the species defined in Example 2.3.2, which are well known and can easily be verified by straight-forward enumeration:

- $E(x) = e^x$,
- $X(x) = x$,
- $E_2(x) = \frac{x^2}{2}$,
- $1(x) = 1$,
- $L(x) = \frac{1}{1-x}$,
- $\mathcal{S}(x) = \frac{1}{1-x}$.

Next, we define the notion of an *(isomorphism) type generating series*, which is useful when enumerating structures up to isomorphism. This is an ordinary formal power series (i.e having no factorials in the denominators) in one variable x. We denote by $T(F_n)$ the quotient $F[n]/\sim$ of types of F-tructures on [n] (called *F-structures of order n*).

Definition 2.3.6 (Type Generating Series)**.** The type generating series of a species of structures F is the formal power series

$$\widetilde{F}(x) = \sum_{n \geq 0} \widetilde{f}_n x^n, \tag{2.10}$$

where $\widetilde{f}_n = |T(F_n)|$ is the number of unlabeled F-structures of order n.

Example 2.3.7. The following type generating series associated with the species of Example 2.3.2 are well-known and can be obtained in a straight-forward way:

- $\widetilde{E}(x) = \frac{1}{1-x}$,
- $\widetilde{X}(x) = x$,
- $\widetilde{E_2}(x) = x^2$,
- $\widetilde{1}(x) = 1$,
- $\widetilde{L}(x) = \frac{1}{1-x}$,
- $\widetilde{\mathcal{S}}(x) = \prod_{k=1}^{\infty} \frac{1}{1-x^k}$.

Notice that while the exponential generating series of the species L and S are the same, this is not the case for their type generating series. This hints to the fact that L and $\mathcal{S}$ are somehow different from a combinatorial point of view, a result we will show formally once we have defined the notion of *species isomorphism*.

The final kind of formal power series associated with a species F is that of the cycle index series, denoted by Z_F. The cycle index series is perhaps the most useful of the three formal power series associated to some species F, bearing more information that both of $F(x)$ and $\widetilde{F}(x)$. In fact, knowledge of Z_F is enough to fully, and mechanically, determine both $F(x)$ and $\widetilde{F}(x)$.

Before defining Z_F, we must first define the notion of *cycle type* of a permutation.

Definition 2.3.8. Let U be a finite set and σ be a permutation of U. Recall that any permutation σ of a finite set admits a unique decomposition in terms of disjoint cycles. Then the cycle type of σ is defined to be the sequence $(\sigma_1, \sigma_2, \dots)$ where σ_k is the number of cycles of σ having length k in said decomposition.

Observe that for finite sets U with $|U|= n$ we have that $\forall i > n\ \sigma_i = 0$ and so the cycle type of σ can be written as an n-component vector $(\sigma_1, \sigma_2, \dots, \sigma_n)$. We denoted by $Fix\sigma$ the set $\{u \in U | \sigma(u) = u\}$ of fixed points of σ and by $fix\sigma = |Fix\sigma|= \sigma_1$ the number thereof.

Given the above definitions we can now define the notion of the cycle index series.

Definition 2.3.9. The *cycle index series* of a species of structures F is the following formal power series on countably infinite variables $x_1, x_2, x_3, \dots$:

$$Z_F(x_1, x_2, \dots) = \sum_{n\geq 0} \frac{1}{n!} \left(\sum_{\sigma \in \mathcal{S}_n} fixF[\sigma] x_1^{\sigma_1} x_2^{\sigma_2} x_3^{\sigma_3}, \dots \right), \tag{2.11}$$

where $\mathcal{S}_n$ is the symmetric group of order n and $fixF[\sigma]$ is the number of F-structures on $[n]$ fixed by $F[\sigma]$, that is, the number of F-structures on $[n]$ having σ as an automorphism.

Example 2.3.10. We now present the cycle index series associated with the species given in Example 2.3.2:

- $Z_E(x_1, x_2, x_3, \dots) = exp\left(x_1 + \frac{x_2}{2} + \frac{x_3}{3} + \dots\right)$,
- $Z_X(x_1, x_2, x_3, \dots) = x$,
- $Z_{E_2}(x_1, x_2, x_3, \dots) = \frac{x_1^2}{2} + \frac{x_2}{2}$,
- $Z_1(x_1, x_2, x_3, \dots) = 1$,
- $Z_L(x_1, x_2, x_3, \dots) = \frac{1}{1-x_1}$,
- $Z_{\mathcal{S}}(x_1, x_2, x_3, \dots) = \frac{1}{(1-x_1)(1-x_2)(1-x_3)\dots}$.

As mentioned before, the series $F(x)$ and $\widetilde{F}(x)$ can be determined from Z_F, as shown in the following theorem.

Theorem 2.3.11. *Let F be a species of structures. Then the following hold:*

- $F(x) = Z_F(x, 0, 0, \dots)$,
- $\widetilde{F}(x) = Z_F(x, x^2, x^3, \dots)$.

Proof. For the first case, observe that setting $x_1 = x, x_i = 0$ for all $i \geq 2$ in Z_F's definition gives us:

$$Z_F(x, 0, 0, \dots) = \sum_{n\geq 0} \frac{1}{n!} \left(\sum_{\sigma \in \mathcal{S}_n} fixF[\sigma] x^{\sigma_1} 0^{\sigma_1} 0^{\sigma_3} \dots \right). \tag{2.12}$$

But then for all $n \geq 0$ we have that $x^{\sigma_1} 0^{\sigma_1} 0^{\sigma_2} \dots = 0$ unless $\sigma_1 = n$ (and of course $\sigma_i = 0$ for all other i). Therefore the only permutations contributing to the sum are the identity permutations on $[n]$ and since all F-structures are fixed by $F[Id_n]$ we have that

$$\begin{aligned} Z_F(x, 0, 0, \dots) &= \sum_{n\geq 0} \frac{1}{n!} fixF[Id_n] x^n \\ &= \sum_{n\geq 0} \frac{1}{n!} f_n x^n \\ &= F(x). \end{aligned}$$

For the second case we have that, via Burnside's lemma (see, for example, [19, Proposition 7, Appendix 1]) and the observation that for any $\sigma \in \mathcal{S}_n$ with cycle type $(\sigma_1, \sigma_2, \sigma_3, \dots)$, $\sigma_1 + 2\sigma_2 + 3\sigma 3 + \dots = n$:

$$\begin{aligned} Z_F(x, x^2, x^3, \dots) &= \sum_{n\geq 0} \frac{1}{n!} \sum_{\sigma \in \mathcal{S}_n} fixF[\sigma] x^{\sigma_1} x^{2\sigma_2} x^{3\sigma 3} \dots \\ &= \sum_{n\geq 0} \frac{1}{n!} \sum_{\sigma \in \mathcal{S}_n} fixF[\sigma] x^n \\ &= \sum_{n\geq 0} |F[n]/\sim| x^n \\ &= \widetilde{F}(x). \end{aligned}$$

□

We now define the following notion of a *species isomorphism*.

Definition 2.3.12 (Isomorphism of Species)**.** Let F, G be two species. An isomorphism α from F to G is a family of bijections $a_U : F[U] \to G[U]$ for every finite set U, such that for every bijection $\sigma : U \to V$ and every $s \in F[U]$ we have $G[\sigma](\alpha_U(s)) = \alpha_V F([\sigma](s))$.

Remark 2. For the categorically-minded. A species isomorphism α is a natural isomorphism between the corresponding functors, such that the following diagram commutes.

$$\begin{array}{ccc} F[U] & \xrightarrow{\alpha_u} & G[U] \\ {\scriptstyle F[\sigma]}\downarrow & & \downarrow{\scriptstyle G[\sigma]} \\ F[V] & \xrightarrow{\alpha_v} & G[V] \end{array}$$

We say that two species F, G are *combinatorially equal* (denoted as $F = G$) if they are isomorphic. Observe that the notion of species isomorphism doesn't necessarily mean that the structures of each species are exactly identical but only that the two species possess essentially the "same" combinatorial properties, including having equal associated series:

$$F = G \Rightarrow \begin{cases} F(x) = G(x), \\ \widetilde{F}(x) = \widetilde{G}(x), \\ Z_F(x_1, x_2, x_3, \dots) = Z_G(x_1, x_2, x_3, \dots). \end{cases} \tag{2.13}$$

Equipped with an appropriate notion of equality we now return to our discussion of how L and S seem to behave differently as combinatorial objects, even though there are as many L-structures as there are S ones on any given set U. This example shows that knowledge of the exponential generating series is not enough to uniquely identify a species of structures.

Example 2.3.13. The species L of linear orders and $\mathcal{S}$ of permutations are non-isomorphic even though both have the same number of structures at any given set, namely $n!$ where n is the cardinality of said set. Consider for example the case where the underlying set is [2]. Then $L[2] = \{12, 21\}$ and $S[2] = \{(1)(2), (12)\}$, but one can easily check that there exists no natural bijection between the two sets (one which doesn't dependent on an ordering on the underlying set). Observe also that the permutation of [2] which exchanges 1 and 2 leaves both elements of $S[2]$ fixed but exchanges the elements of $L[2]$.

As hinted to before, much of the power of species theory comes from the ability to produce new species from old ones via the *combinatorial algebra* of sum, product, substitution, and differentiation operations on species. To each of these operations correspond operations on the exponential, type, and cycle index series of species operated on, which let us construct the associated series of the resulting species.

Definition 2.3.14 (Sum of Species)**.** Let F, G be two species. Then $F + G$, the *sum* of F and G, is defined as follows: an $(F + G)$-structure on U is either (exclusively) a F-structure on U or a G-structure on U. That is, we have that:

$$(F + G)[U] = F[U] + G[U] \tag{2.14}$$

where, on the right-hand side of the equation, $+$ denotes the operation of disjoint union.

Transports along some bijection $\sigma : U \to V$ are as follows,

$$(F + G)[\sigma](s) = \begin{cases} F[\sigma](s), & \text{if } s \in F[u] \\ G[\sigma](s), & \text{if } s \in G[u] \end{cases} \tag{2.15}$$

The following proposition allows us to easily compute the series associated to a sum $F + G$ given the series associated to each of the constituent species F, G.

Proposition 2.3.15. *Let F and G be two species. Then the following hold, with regards to their sum's associated series:*

- $(F + G)(x) = F(x) + G(x)$,
- $\widetilde{(F + G)}(x) = \widetilde{F}(x) + \widetilde{G}(x)$,
- $Z_{F+G} = Z_F + Z_G$.

This notion of addition is associative and commutative (up to species isomorphism).

Definition 2.3.16 (Product of Species)**.** Let F, G be two species. Then $F \cdot G$, their *product*, is the species defined as such:

$$(F \cdot G)[U] = \sum_{\substack{(U_1,U_2) \\ U=U_1+U_2}} F[U_1] \times G[U_2] \tag{2.16}$$

That is, an $(F \cdot G)$-structure on U is an ordered pair $s = (f, g)$ where f is an F-structure on some subset $U_1 \subseteq U$ and g is a G-structure on $U_2 \subseteq U$, where U_1, U_2 form a partition of U, i.e $U = U_1 \cup U_2$ and $U_1 \cap U_2 = \emptyset$.

Transports of an $(F \cdot G)$-structure $s = (f, g)$ on U along some bijection $\sigma : U \to V$ are defined as such:

$$(F \cdot G)[\sigma](s) = (F[\sigma_1](f), G[\sigma_2](g)), \tag{2.17}$$

where σ_i is the restriction of σ to U_i.

This notion of multiplication is associative, commutative (up to species isomorphims) and furthermore distributes over addition.

As with sums of species there exists a proposition, similar to Proposition 2.3.15, that allows us to compute the series associated to some product $(F \cdot G)$, given knowledge of F and G's generating series.

Proposition 2.3.17. *Let F, G be two species. Then the following hold with regards to the series associated with the product $F \cdot G$:*

- $(F \cdot G)(x) = F(x)G(x)$,
- $(\widetilde{F \cdot G})(x) = \widetilde{F}(x)\widetilde{G}(x)$,
- $Z_{F \cdot G}(x_1, x_2, x_3, \ldots) = Z_F(x_1, x_2, x_3, \ldots) \cdot Z_G(x_1, x_2, x_3, \ldots)$,

The following operation allows us to "compose species".

Definition 2.3.18 (Substitution of Species)**.** Let F, G be two species such that $G[\emptyset] = \emptyset$. Then, the species $F \circ G$, also written as $F(G)$, is defined as such: an $(F \circ G)$-structure on U is a triplet $s = (\pi, \phi, \gamma)$, where π is a partition of U, ϕ is an F-structure on the set of parts (or classes) of π, and γ is a set (γ_p) of G-structures, one on each part $p \in \pi$. That is, for a given finite set U, the composite is:

$$(F \circ G)[U] = \sum_{\pi \text{ partition of } U} F[\pi] \times \prod_{p \in \pi} G[p], \tag{2.18}$$

where the disjoint sum is taken over the partitions π of U. The transport along some $\sigma : U \to V$ of an $(F \circ G)$-structure $s = (\pi, \phi, \gamma)$ on U is as follows:

$$(F \circ G)[\sigma](s) = (\pi', \phi', \gamma'), \tag{2.19}$$

where π' is the partition of V obtained by transport of π along σ, for each $\pi' = \sigma(p) \in \pi'$, the structure $\gamma'_{p'}$ is obtained from γ_p by G-transport along $\sigma|_p$, and the structure ϕ' is obtained from ϕ by F-transport along the σ' bijection induced on σ on π.

Substitution of species is associative, right-distributive over sums and products, and has X as a neutral element.

Example 2.3.19. Some species can naturally be characterised recursively by a functional equation employing these combinatorial operations. Some examples are:

- The species $\mathcal{A}$ of *rooted trees* is $\mathcal{A} = X \cdot E(\mathcal{A})$.
- The species L of *linear orders* is $L = 1 + X \cdot L$.

The use of such functional equations is especially common when one works with trees and tree-like structures, as will become evident in the sequel.

Unlike Proposition 2.3.15 and Proposition 2.3.17, where passing from a product or sum species to its associated series amounted to performing sums and products of formal power series respecitvely, passing from a species $F \circ G$ to its generating series is not as straightforward. In fact, we must make use of the associated cycle index series to facilitate this passage, as is shown in the following proposition.

Proposition 2.3.20. *Let F, G be two species such that $G[\emptyset] = \emptyset$. Then the series associated to $F \circ G$ satisfy the following equalities:*

- $(F \circ G)(x) = F(G(x))$,
- $\widetilde{(F \circ G)}(x) = Z_F(\widetilde{G}(x), \widetilde{G}(x^2), \widetilde{G}(x^3), \dots)$,
- $Z_{F \circ G} = Z_F(Z_G(x_1, x_2, \dots), Z_G(x_2, x_4, \dots), \dots)$.

The last series is refered to as the *plethystic substitution of Z_G in Z_f* and is also written as $Z_F \circ Z_G$ or even $Z_F(Z_G)$.

The final operation we present in this section is that of differentiation, which most notably finds use in the definition of the notion of a *pointed* or *rooted* species.

Definition 2.3.21 (Derivative of a Species)**.** Let F be a species of structures. Then the *derivative* F' of F is defined as follows: an F'-structure on U is an F-structure on $U \cup \{*\}$, where $* \notin U$. That is $F'[U] = F[U \cup \{*\}]$. The transport along some bijection $\sigma : U \to V$ is defined as $F'[\sigma](s) = F[\sigma']$ where $\sigma' : U + \{*\} \to V + \{*\}$ is the extention of σ such that $\sigma'(*) = *$ and $\sigma'(u) = \sigma(u)$ for $u \in U$.

Note that the element $*$ is *distinguished* from those of U and this results in the following fact: the automorphisms of F' must all fix $*$.

The series associatied to the derivative of some species F can be computed, given knowledge of F's series, as follows.

Proposition 2.3.22. *Let F be some species. Then the following equalities concerning the series associated to F' hold:*

- $F'(x) = \frac{d}{dx}F(x)$,
- $\widetilde{F'}(x) = (\frac{\partial}{\partial x_1} Z_F)(x, x^2, x^3, \dots)$,
- $Z_{F'}(x_1, x_2, x_3, \dots) = (\frac{\partial}{\partial x_1} Z_F)(x_1, x_2, x_3, \dots)$.

Another very useful fact about differentiation of species is that it also follows some rules analogous to the well-known chain and product rules of differential calculus.

Proposition 2.3.23. *Let F, G be two species. Then the following combinatorial equalities hold:*

- $(F + G)' = F' + G'$,
- $(F \cdot G)' = F' \cdot G + F \cdot G'$,
- $(F \circ G)' = (F' \circ G) \cdot G'$.

As mentioned above, differention is related to the notion of a *pointed* or *rooted* structure as in the following definition.

Definition 2.3.24 (Pointed Species)**.** Let F be a species. Then $F^\bullet$ is defined as follows: an $F^\bullet$ structure on U is a pair $s = (f, u)$ where f is an F-structure on U and $u \in U$ is a distinguished elementl. Such structures are called *pointed* or *rooted* F-structures. Equivalently, we have that

$$F^\bullet[U] = F[U] \times U. \tag{2.20}$$

Transports along a bijection $\sigma : U \to V$ of an $F^\bullet$ structure $s = (f, u)$ are defined as follows:

$$F^\bullet[\sigma](s) = (F[\sigma](f), \sigma(u)). \tag{2.21}$$

This notion of pointing or rooting is related to the operation of derivation as follows:

$$F^\bullet = X \cdot F', \tag{2.22}$$

where X is the species of singletons. This amounts to saying that an $F^\bullet[U]$ structure is an $F'[U]$ structure with a distinguised element taken from U itself.

Example 2.3.25*.* Given the above operations, we can define and enumerate various species of rooted trees, either plane or not.

For example, consider the species B of binary trees. We can make use of the following recursive definition of a binary tree: a binary tree is either a leaf, or root to which sub-trees are attached. This readily translates to the following recursive specification of B in terms of species: $B = X + (X \cdot E_2(B))$. Similarly, for plane binary trees we have $PB = X + (X \cdot L_2(PB))$, since specifying an order on the children of each root is equivalent to a unique embedding of a tree in the plane. Yet another example is given by general rooted trees (with no degree restrictions), whose species satisfies $A = X \cdot E(A)$, since a rooted tree t can be identified with its root and the set of subtrees attached to it, each rooted at some corresponding neighbour of t's root.

Given these recursive specifications, one can easily generate the first terms of the corresponding exponential or type generating series using a computer algebra tool such as SageMath or Maple. For the above examples we obtain:

$$\begin{aligned}
\widetilde{B}(x) &= x + x^3 + x^5 + 2x^7 + 3x^9 + 6x^{11} + 11x^{13} + 23x^{15} + 46x^{17} + 98x^{19} + \dots \\
\widetilde{PB}(x) &= x + x^3 + 2x^5 + 5x^7 + 14x^9 + 42x^{11} + 132x^{13} + 429x^{15} + 1430x^{17} + 4862x^{19} + \dots \\
\widetilde{A}(x) &= x + x^2 + 2x^3 + 4x^4 + 9x^5 + 20x^6 + 48x^7 + 115x^8 + 286x^9 + 719x^{10} \dots
\end{aligned}$$

Note the absence of even terms in the cases of the binary trees. For completeness, we note that the coefficients of $\widetilde{B}$ are the Wedderburn-Etherington numbers (see [25, Sequence A001190]), those of $\widetilde{PB}$ are the Catalan numbers (see [25, Sequence A000108]), while those of $\widetilde{A}$ are listed in [25, Sequence A000081].

In fact, not only can we compute the first few terms of the above generating series, but we can actually solve some of these equations algebraicaly. For example for PB, which can equivalently be defined as $PB = X + (X \cdot B^2)$ since $L_k = X^k$ and substitution right-distributes over products, we have:

$$\widetilde{PB}(x) = x + x\widetilde{PB}(x)^2,$$

therefore,

$$x\widetilde{PB}(x)^2 - \widetilde{PB}(x) + x = 0,$$

and by employing the quadratic formula we have:

$$\widetilde{PB} = \frac{1 \pm \sqrt{1-4x^2}}{2x}.$$

Expanding both solutions as Maclaurin series reveals that the one having minus as a sign before the root is the correct one and that its expansion's coefficients match the Catalan numbers.

Having defined both addition and multiplication on species, it is natural to wonder if some suitable notion of their inverses also exists. To this end, we define the notion of *virtual* species, which serve to give a species-theoretic notion of combinatorial subtraction. This is done in a manner similar to the way one construct the ring $\mathbb{Z}$ of integers from the semi-ring $\mathbb{N}$ of the natural numbers.

Definition 2.3.26 (Virtual Species)**.** A virtual species is an element of the quotient set $Virt = (Spe \times Spe)/\sim$ where $\sim$ is the following equivalence relation

$$(F, G) \sim (H, K) \iff F + K = G + H.$$

Then a virtual species $F - G$ is the class of (F, G) according to $\sim$.

The appropriate generalisations of the exponential, type, and cycle index series for virtual species are as follows.

Definition 2.3.27 (Series for virtual species)**.** Let F, G be two species and let $\Phi = F - G$. Then the following hold

$$\begin{aligned} \Phi &= F(x) - G(x), \\ \widetilde{\Phi} &= \widetilde{F}(x) - \widetilde{G}(x), \\ Z_\Phi(x_1, x_2, x_3, \dots) &= Z_F(x_1, x_2, x_3, \dots) - Z_G(x_1, x_2, x_3, \dots) \end{aligned}$$

Example 2.3.28. As a final (and particularly relevant to our work) example, we will perform an enumeration of general trees. To do this, in addition to the tools defined in this section, we employ the following *dissymmetry theorem.*

Theorem 2.3.29 (Dissymmetry theorem for trees [19, Section 4.1, Theorem 1])*. The species of structures a of trees, and A, of rooted trees, are related via the following isomorphism*

$$A + E_2(A) = a + A^2$$

The above equation can be rewritten, with the help of virtual species, as:

$$a = A + E_2(A) - A^2,$$

from which useful equalities between the series associated to each species can be derived.

For example, using the above equation, we will now compute the first few terms of the enumeration of all trees up to isomorphism. First, note that one can easily compute the cycle index series of E_2 to be

$$Z_{E_2}(x_1, x_2, x_3, \dots) = \frac{x_1^2}{2} + \frac{x_2}{2}.$$

Therefore we have that

$$\widetilde{a}(x) = \widetilde{A}(x) + \left(\frac{\widetilde{A}(x)^2}{2} + \frac{\widetilde{A}(x^2)}{2} \right) - \widetilde{A}(x)^2$$

Given this formula and a suitable truncation of $\widetilde{A}(x)$, we compute the first terms of $\widetilde{a}(x)$ to be:

$$\widetilde{a}(x) = 1x+1x^2+1x^3+2x^4+3x^5+6x^6+11x^7+23x^8+47x^9+106x^{10}+235x^{11}+551x^{12}+1301^{13}+\dots$$

as expected (see [25, Sequence A000055]).

A generalisation of Theorem 2.3.29 exists for connected graphs.

Theorem 2.3.30 (Dissymmetry theorem for graphs [19, Section 4.2, Theorem 3])**.** *Let B be a species of biconnected graphs and C_B be the species of connected graphs all of whose blocks are in B. Then*

$$C_B = C_B^\bullet + B(C_B^\bullet) - C_B^\bullet \cdot B'(C_B^\bullet).$$

2.4 Analytic Combinatorics

So far we have viewed generating functions arising from various species-theoretic constructions as formal objects, without regard to their convergence and analytic properties. A central theme of analytic combinatorics is that, by viewing these generating functions not as mere formal objects but as analytic ones, one can derive much information about the asymptotic behaviour of their coefficients.

In this section we will present some very basic material relevant to our work. This exposition is by no means complete and largely follows [20] which is the definitive textbook on the subject. We will, as in the previous section, omit many proofs in favour of clarity of exposition; for the proofs and details omitted, we refer to [20]. We should also note that analytic combinatorics comes with its own theory and techniques, the so called *symbolic method*, for constructing and manipulating generating series for families of combinatorial objects. This theory, as previously mentioned, is closely related to the theory of combinatorial species. We also note that we have chosen to employ, in this work, the framework of species instead of the symbolic method due the former's flexibility in handling objects with symmetries.

We briefly recall the notion of analytic functions.

Definition 2.4.1 (Analytic functions)**.** A function $f : \Omega \to \mathbb{C}$, defined over an open and connected subset Ω of $\mathbb{C}$, is *analytic* at some point $x_0 \in \Omega$ if it is expressible as a convergent power series

$$f(x) = \sum_{n\geq 0} c_n (x - x_0)^n, \tag{2.23}$$

for x in an open disc contained in Ω and centered at x_0. We say f is analytic in Ω if f is analytic at all $x_0 \in \Omega$.

A standard theorem of complex analysis is that a function is analytic if and only if it is (infinitely) differentiable.

A *singularity* of a function f is a point x_0 at which f is not analytic. Among the singularities of a function, the ones with the with smallest modulus are referred to as *dominant*. The following two theorems are very useful in locating such singularities, especially for generating functions arising in the context of combinatorics.

Theorem 2.4.2. *If a function $f : \Omega \to \mathbb{C}$ is analytic at $x_0 = 0$ and its power series has a finite radius of convergence R, then there exists at least one singularity on the circle $|x|= R$.*

Theorem 2.4.3 (Pringsheim)**.** *If a function $f : \Omega \to \mathbb{C}$ is analytic at $x = 0$ and an expansion*

$$f(x) = \sum_{n\geq 0} f_n x^n \tag{2.24}$$

with $f_n \geq 0$ for all n, then $x = R$, where R is f's radius of convergence, is a singularity of $f(x)$.

Power series such as $f(x) = \sum_n f_n x^n$, when they are convergent, define a function on some disc around 0 in $\mathbb{C}$ and furthermore the following holds.

Theorem 2.4.4 (Cauchy-Hadamard)**.** *For a series $f(x) = \sum_n f_n x^n$, its radius of convergence R is*

$$R = \frac{1}{\limsup_{n\to\infty} |f_n|^{1/n}} \tag{2.25}$$

The coefficients of the series we are interested in follow an *asymptotic scheme* of the form

$$a_n \sim A^n \theta(n). \tag{2.26}$$

The factor A^n is the so-called *exponential growth* and is modulated by the *subexponential factor* $\theta(n)$. We write $a_n \bowtie A^n$ to denote that a_n grows as A^n.

The study of the asymptotic behaviour of coefficients of some power series is largely guided by two principles, the first of which is the following.

First Principle of Coefficient Asymptotics: The location of a function's singularities dictates the exponential growth of its coefficients (A^n).

In light of the above theorems, we have the following justification for this principle.

Theorem 2.4.5. *If $f(x)$ is analytic at $x_0 = 0$ and its power series has radius of convergence R, then $f_n = [x^n]f(x) \bowtie \frac{1}{R^n}$.*

Proof. By Theorem 2.4.4 we have that $\limsup_{n\to\infty} |f_n|^{1/n} = \frac{1}{R}$. Therefore, for all $\epsilon > 0$ we have

$$|f_n| \geq \frac{1}{(R+\epsilon)^n}, \tag{2.27}$$

infinitely often. On the other hand we also have:

$$|f_n| = o\left(\frac{1}{(R-\epsilon)^n}\right) \tag{2.28}$$

since f's series is convergent for $|z| < R$. □

The second principle of coefficient asymptotics concerns the finer-grained behaviour of a function's coefficient asymptotics.

Second Principle of Coefficient Asymptotics: The nature of a function's singularities determines the subexponential factor ($\theta(n)$).

The specifics regarding the second principle largely depend on the nature of the function we want to study. In our case, results will be presented later on, which explicitly give a formula for $\theta(n)$.

The *stundard function scale* is the following set of functions.

$$S = \left\{ (1-z)^{-\alpha} \left(\frac{1}{z} log \frac{1}{1-z} \right)^{\beta} \right\}.$$

The following two theorems provide an asymptotic expansion of functions in the standard scale.

Theorem 2.4.6 (Standard function scale [20, Theorem VI.1])**.** *Let $\alpha \in \mathbb{C} \setminus \mathbb{Z}_{\leq 0}$. Then the coefficient of z^n in*

$$f(z) = (1-z)^{-\alpha}$$

admits, for large n, a complete asymptotic expansion in descending powers of n,

$$[z^n]f(z) \sim \frac{n^{\alpha-1}}{\Gamma(\alpha)} \left(1 + \sum_{k=1}^{\infty} \frac{e_k}{n^k} \right),$$

where e_k is a polynomial in α of degree $2k$.

Theorem 2.4.7 (Standard function scale with logarithmic factors [20, Theorem VI.2])**.** *Let $\alpha, \beta \in \mathbb{C} \setminus \mathbb{Z}_{\leq 0}$. The coefficient of z^n in the function*

$$f(z) = (1-z)^{-\alpha} \left(\frac{1}{z} log \frac{1}{1-z} \right)^{\beta}$$

admits, for large n, the following full asymptotic expansion in descending powers of $logn$,

$$f_n \equiv [z^n]f(z) \sim \frac{n^{\alpha-1}}{\Gamma(\alpha)} (logn)^{\beta} \left[1 + \frac{C_1}{logn} + \frac{C_2}{log^2 n} + \dots \right],$$

where $C_k = \binom{\beta}{k} \Gamma(\alpha) \frac{d^k}{ds^k} \left. \frac{1}{\Gamma(s)} \right|_{s=a}$.

The following kind of open domain is frequently used in analytic combinatorics.

Definition 2.4.8 (Δ-domains, Δ-analyticity)**.** Given two numbers ϕ, R with $R > 1$ and $0 < \phi < \frac{\pi}{2}$, the open Δ-domain at 1, denoted by $\Delta(\phi, R)$, is defined as follows

$$\Delta(\phi, R) = \{ z \mid |z| < R \wedge |arg(z-1)| > \phi \}.$$

For a non-zero $\zeta \in \mathbb{C}$, a Δ-domain at ζ is the image under the mapping $z \mapsto \zeta z$ of a Δ-domain at 1. A function is Δ-*analytic* if it is analytic in some Δ-domain.

We now state a theorem which allows us to translate an approximation of a function near a singularity to an asymptotic approximation of its coefficients.

Theorem 2.4.9 (Transfer [20, Theorem VI.3])**.** *Let $\alpha, \beta \in \mathbb{R}$ and $f(z)$ be a Δ-analytic function. Then the following hold.*

Assuming that $f(z)$ satisfies in the intersection of a neighbourhood of 1 with its Δ-domain the condition

$$f(z) = O\left((1-z)^{-\alpha} \left(log \frac{1}{1-z} \right)^{\beta} \right).$$

we have $[z^n]f(z) = O(n^{\alpha-1}(logn)^{\beta})$.

Similarly, assuming that $f(z)$ satisfies in the intersection of a neighbourhood of 1 with its Δ-domain the condition

$$f(z) = o\left((1-z)^{-\alpha} (log \frac{1}{1-z}^{\beta} \right).$$

we have $[z^n]f(z) = o(n^{\alpha-1}(logn)^{\beta})$.

Let $f(x)$ be a function analytic at 0 which we assume is not entire and has a single singularity located on its circle of convergence. Then the singularity analysis process for $f(x)$ can be summarised as follows [20].

1. The first task is to locate the dominant singularity ζ of $f(x)$ and establish that $f(x)$ is analytic in some domain of the form $\zeta\Delta_0$.

2. The second task is to study the behaviour of $f(x)$ as $x \to \zeta$ in the aforementioned domain and determine (in that domain) an expansion of the form

$$f(x) \underset{x\to 1}{=} \sigma(x/\zeta) + O(\tau(x/\zeta)) \text{ with } \tau(x) = o(\sigma(\zeta))$$

   where σ and τ belong to the standard scale of functions.

3. Finally we make use of Theorem 2.4.6 and Theorem 2.4.7 to obtain asymptotics for the coefficients of $\sigma(z)$ and of Theorem 2.4.9 to transfer the error term. As such we obtain

$$[x^n]f(x) \underset{n\to+\infty}{=} \zeta^{-n}\sigma_n + O(\zeta^{-n}\tau_m^*)$$

   where σ_n and τ_n^* are the coefficients of σ and τ's expansions, assuming $a \notin \mathbb{Z}_{\leq 0}$.

In our case, the specific singular expansions will follow from established results regarding generating series of tree(-like) structures which we expand upon later in this chapter.

Since the generating series arising from our enumeration have multiple dominant singularities (which is related to their periodicity), we make use of the following definitions and theorems.

Definition 2.4.10 (Support, span, periodicity)**.** Let (f_n) be a sequence with generating function $f(z)$. Then the *support* of f, denoted as $Supp(f)$, is the set of all n such that $f_n \neq 0$. We say that the sequence (f_n) and its generating function $f(z)$ admits a *span* d if for some r it holds that

$$Supp(f) \subseteq r + d\mathbb{Z}_{\geq 0} \equiv \{r, r+d, r+2d, \dots\}.$$

The largest span, say p, is called the period of (f_n) and $f(z)$, while all other spans are divisors of p. If the period is equal to 1 we say that the sequence and its generating function is aperiodic.

The following lemma relates the behaviour of $|f(z)|$, as z varies along circles centered at the origin, to its span.

Lemma 2.4.11 ("Daffodil" [20, Lemma IV.1])**.** *Let $f(z)$ be analytic in $|z| \leq \rho$ with non-negative coefficients at* 0. *Assuming f does not reduce to a monomial and that for some non-zero non-positive z, satisfying $|z| < \rho$, one has,*

$$|f(z)| = f(|z|),$$

the following hold

1. *The argument of z must be commensurate to 2π, that is, $z = Re^{i\theta}$ with $\theta/(2\pi) = \frac{r}{p} \in \mathbb{Q}$ (i.e an irreducible fraction) and $0 < r < p$.*

2. *f admits p as a span.*

The following theorem extends the previously presented process of singularity analysis allowing it to be carried out seamlessly in the case of functions with multiple dominant singularities.

Theorem 2.4.12 (Singularity analysis for multiple singularities [20]). *Let $f(x)$ be analytic in $|x| < \rho$ and have a funite number of singularities on the circle $|x| = \rho$, at points $\zeta_j = \rho e^{i\theta_j}$ for $j = 1 \dots r$. Assume that there exists a Δ-domain Δ_0 such that $f(x)$ is analytic in the indented disc*

$$D = \bigcap_{j=1}^{r} (\zeta_j \cdot \Delta_0)$$

with $\zeta \cdot \Delta_0$ the image of Δ_0 under the mapping $x \mapsto \zeta x$. Assume that there exist r functions $\sigma_1, \dots, \sigma_r$, each a liniear combination of standard functions, and a standard function τ such that

$$f(x) = \sigma_j(x/\zeta_j) + O(\tau(x/\zeta_j))$$

as $x \to \zeta_j$ in D. Then the coefficients of $f(x)$ satisfy the following asymptotic estimate

$$f_n = \sum_{j=1}^{r} \zeta_j^{-n} \sigma_{j,n} + O(\rho^{-n} \tau_n^*)$$

where the coefficients of $\sigma_{j,n}$ follow from standard theorems and $\tau_n^* = n^{a-1}(logn)^b$ if $\tau(x) = (1-x)^{-a}\lambda(x)^b$.

As seen in the last chapter, recursive functional equations naturally occur in the context of combinatorial problems related to trees and tree-like structures. Informally, this reflects the recursive nature of rooted trees and tree-like structures, which can frequently be described as a root to which other (smaller) instances of the structure in question are attached. In the context of analytic combinatorics, these recursive functional equations frequently take the form $y = F(x, y)$ and their behaviour is characterised by the following theorem (see also [20, Theorem VII.3, pg. 468]) which shows that these generally have singularities of *square-root type*.

Theorem 2.4.13 ([26, Theorem 2.19]). *Let $F(x, y)$ be a function analytic in x, y around $x = y = 0$ such that $F(0, y) = 0$ and that all Taylor coefficients of F around 0 are real and non-negative. Then there exists a unique analytic solution $y = y(x)$ of the following equation*

$$y = F(x, y)$$

with $y(0) = 0$ that has non-negative Taylor coefficients around 0.

Furthermore, subject to the condition that the radius of convergence of $F(x, y)$ is large enough so that there exist positive solutions $x = x_0$, $y = y_0$ for the following system

$$F(x, y) = y,$$
$$F_y(x, y) = 1.$$

with $F(x_0, y_0) \neq 0$ and $F_{yy}(x_0, y_0) \neq 0$, then $y(x)$ is analytic for $|x| \leq x_0$ and there exist functions $g(x), h(x)$ analytic around $x = x_0$ such that $y(x)$ has a representation of the form

$$y(x) = g(x) - h(x)\sqrt{1 - \frac{x}{x_0}} \tag{2.29}$$

locally around $x = x_0$. Furthermore, $g(x_0) = y(x_0)$ and

$$h(x_0) = \sqrt{\frac{2x_0 F_x(x_0, y_0)}{F_{yy}(x_0, y_0}}.$$

If in addition $[x^n]y(x) \geq 0$ *for* $n \geq n_0$*, then* $x = x_0$ *is the only singularity of* $y(x)$ *on the circle* $|x|= x_0$ *and the following is an asymptotic expansion for* $[x^n]y(x)$*:*

$$[x^n]y(x) = \frac{h(x_0)}{2\sqrt{pin^3}} x_0^{-n}(1 + O(n^{-1})). \tag{2.30}$$

In summary, the process of singularity analysis is the following. Let $f(z)$ be a generating function analytic in a Δ-domain at ρ. Then there exists a singular expansion for f of the form

$$f(z) = f_0 + f_1X + f_2X^2 + f_3X^3 + f_xX^4 + \cdots + f_{2k}X^{2k} + f_{2k+1}X^{2k+1} + O\left(X^{2k+2}\right),$$

where $X = \sqrt{1 - z/\rho}$ and $k = 0$ or 1. Note that the even powers of Z are analytic functions and therefore do not contribute to the asymptotics of $[z^n]f(z)$. In the above, let $2k + 1$ be the smallest odd integer such that $f_{2k+1} \neq 0$ and let $\alpha = (2k + 1)/2$ (this value is referred to as the *singular exponent*). Provided no other complex value, of the same modulus as ρ , exists on which such an expansion holds, we can obtain, via Theorem 2.4.9, estimates of the form

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

where $c = f_{2k+1}/\Gamma(-\alpha)$. In cases, such as ours, where a finite number of such values exist, we can apply Theorem 2.4.12 to obtain estimates by adding up the contributions of each value.

CHAPTER 3

STRUCTURAL CHARACTERISATION OF CACTUS-OBSTRUCTIONS

In this section we provide a structural characterisation of the class of $\mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$ of cactus-obstructions for k-apex sub-unicyclic graphs.

We begin with some useful definitions, observations, and lemmas.

3.1 Preliminaries

Lemma 3.1.1. *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 neighbours.*

Proof. Observe 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 neighbours 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 neighbours of v are not adjacent, the contraction of e can only shorten cycles and not completely remove/destroy them. Hence, S is a k-apex sub-unicyclic set of G, a contradiction. □

Definition 3.1.2 (Block-cut vertex tree, leaf block, peripheral block)**.** 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.

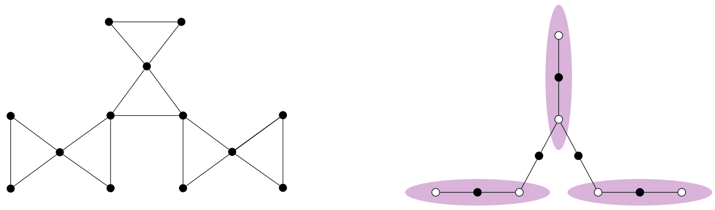


Figure 3.1: An example of a graph $G \in \mathcal{Z}_3$ and its block-cut-vertex tree T_G with the P_3-subgraphs corresponding to the butterflies composing G highlighted.

3.2 Characterisation of Connected Cactus-Obstructions

In what follows, we provide a structural characterisation of connected cactus-obstructions for k-apex sub-unicyclic graphs. Intuitively this characterisation takes the following form: the connected obstructions for k-apex sub-unicyclicity are exactly the graphs constructed by any possible "gluing along non-central vertices" of $k + 1$ butterflies.

Let us first formalise the aforementioned construction.

Definition 3.2.1 (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 family 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 observe the following useful property butterfly-cacti.

Lemma 3.2.2. *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 H isomorphic to the butterfly graph Z. Let now C be the cycle of H in G that contains no vertices of G'. By 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 3.2.3. *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 $\mathcal{Z}_{k+1}$.*

We begin our characterisation by proving that all graphs in $\mathcal{Z}_{k+1}$ are indeed obstructions for k-apex sub-unicyclicity.

Lemma 3.2.4. *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 induction hypothesis, we have that $G' \in \mathbf{obs}(\mathcal{A}_{k-1}(\mathcal{S}))$. Let C (resp. C') be the triangle 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 Lemma 3.2.2.

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 3.1.1 on cacti and will prove useful in the sequel.

Observation 3.2.5. Let $G \in \mathbf{obs}(\mathcal{A}_k(\mathcal{S})) \cap \mathcal{K}, k \geq 0$. Then all blocks of G are triangles.

We now need only show that all connected cacti $G \in \mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$ are of the desired form. We begin with the following two lemmas, which prove that a connected graph $G \in \mathbf{obs}(\mathcal{A}_k(\mathcal{S})) \cap \mathcal{K}$ contains a collection of butterflies which all correspond to leafs of the bc-tree of G and are all attached to the same vertex of the graph.

Lemma 3.2.6. *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 3.2.7. *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 3.2.6, 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, if neither of c', c'' are in S 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 in G'. Respectively, if $x \in V(B'')$ then the set $S' = (S \setminus \{x\}) \cup \{c''\}$ is a k-apex sub-unicyclic set in G'. Assume then that S is a k-apex sub-unicycle 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. □

We now introduce the notion of a leaf butterfly and of butterfly buckets.

Definition 3.2.8 (Leaf butterfly)**.** 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.

Definition 3.2.9 (Butterfly bucket)**.** A *butterfly bucket* of G is a maximal collection $\mathcal{Q} = \{Q_1, \dots, Q_r\}$ 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 3.2.7 and Observation 3.2.5 together we have the following corollary:

Corollary 3.2.10. *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 3.2.11. *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 triangles 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. □

Lemma 3.2.12. *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 $\mathcal{Q} = \{Q_1, \dots, Q_r\}$. For $i \in [r]$, let A_i and B_i be the two triangles 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 3.2.11, Lemma 3.2.7, and the definition of a butterfly bucket.

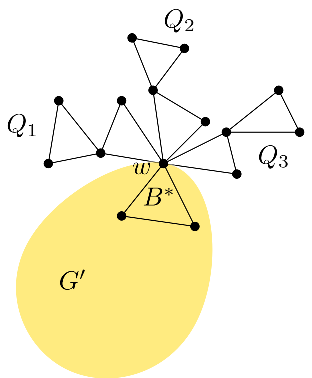


Figure 3.2: An example of a graph G and a butterfly bucket $\mathcal{Q} = \{Q_1, Q_2, Q_3\}$ of G with attachment w. The graph $G' = G \setminus (V(\bigcup \mathcal{Q}) \setminus \{w\})$ is depicted in yellow and B^* is the unique block of G' that contains w.

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 $S \cup \{c_1, \dots, c_r\}$ 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 $\{c_1, \dots, c_r\} \subseteq S$. 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 $S' = (S \setminus \{x_1, \dots, x_r\}) \cup \{c_1, \dots c_r\}$ is a k-apex sub-unicyclic set of G.

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 $S' = (S \setminus \{x_2, \dots, x_r\}) \cup \{c_2, \dots, c_r\}$ is a k-apex sub-unicyclic set of G (see Figure 3.3). 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.

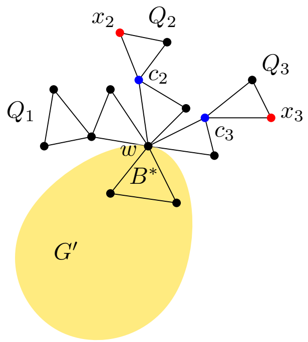


Figure 3.3: Following the example in Figure 3.2, for every $i \in [2]$, x_i is the vertex of S that is in $V(B_i)$ (depicted in red) and c_i is the center of Q_i (depicted in blue). The set S' is obtained by replacing in S the red vertices with the blue ones.

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 $G' \in \mathbf{obs}(\mathcal{A}_{k-r}(\mathcal{S}))$. □

We now proceed with the main lemma of this section.

Lemma 3.2.13. *Let $k \geq 0$ and G be a connected cactus graph in $\mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$. Then $G \in \mathcal{Z}_{k+1}$.*

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 3.2.10. 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 $(k+2)K_3 \in \mathbf{obs}(\mathcal{A}_{k+1}(\mathcal{S}))$. 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 3.2.12, $G' = G \setminus (V(\bigcup \mathcal{Q}) \setminus \{w\})$ 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. □

We are now equiped to prove the desired structural characterisation.

Proof of Theorem 3.2.3. The proof is an immediate consequence of Lemma 3.2.4 and Lemma 3.2.13. □

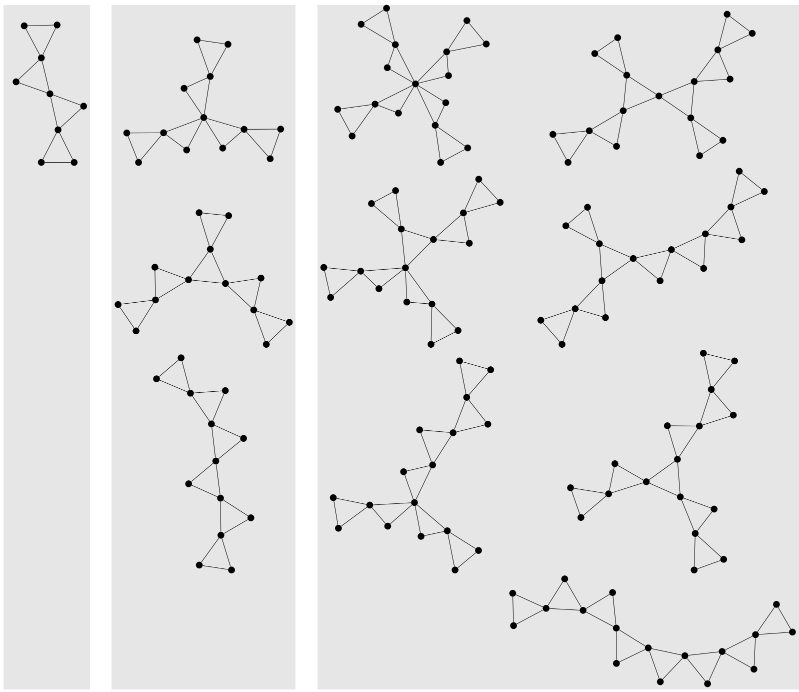


Figure 3.4: The connected graphs in $\mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$ for $k = 1, 2, 3$ respectively (presented left to right).

Therefore we have that the subset of $\mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$ consisting of connected graphs is exactly the set of all possible ways to "glue together" $k+1$ copies of $\mathcal{B}$ at non-central vertices. As an example, consider the sets of connected obstructions in $\mathbf{obs}(\mathcal{A}_1(\mathcal{S})), \mathbf{obs}(\mathcal{A}_2(\mathcal{S}))$, and $\mathbf{obs}(\mathcal{A}_3(\mathcal{S}))$ as shown in Figure 3.4.

3.3 Characterisation of Disconnected Cactus-Obstructions

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

Theorem 3.3.1. *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 a proof that every obstruction $G \in \mathbf{obs}(\mathcal{A}_k(\mathcal{S})))$ is also an $(k+1)$-forest.

Lemma 3.3.2. *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 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 3.3.3. *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 3.3.2, 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 3.1.1, 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 $H_i \notin \mathcal{S}^{(k_i-1)}$. 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 3.3.1. The proof follows by repeated applications of Lemma 3.3.3, as required. □

CHAPTER 4

ENUMERATION OF CACTUS-OBSTRUCTIONS

In general, we denote by $\mathcal{C}$ the set of all connected graphs. We now proceed with an enumeration of all connected cactus-obstructions. This is done in three steps: firstly we establish that the set $\mathcal{Z}_{k+1} = \mathbf{obs}(\mathcal{A}_k(\mathcal{S})) \cap \mathcal{K} \cap \mathcal{C}$ is equinumerous with the set of 4-cacti (cacti where all blocks are squares) with $k+1$ blocks. Then, using this bijection, we describe an enumeration of $\mathcal{Z}_{k+1}$ for all $k \geq 0$, based on species theory. Finally we use analytic combinatorics to obtain asymptotic estimates for the number of cactus-obstructions $\mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$ for each $k \geq 0$.

4.1 Exact Enumeration of $\mathbf{obs}(\mathcal{A}_k(\mathcal{S})) \cap \mathcal{K}$

In general, we denote by $\mathcal{C}$ the set of all connected graphs. We now proceed with an enumeration of all connected cactus-obstructions, from which, via Theorem 3.3.1, an enumeration of disconnected cactus-obstruction also follows. This is done in three steps: firstly we establish that the set $\mathcal{Z}_{k+1}$, which via Theorem 3.2.3 is exactly $\mathbf{obs}(\mathcal{A}_k(\mathcal{S})) \cap \mathcal{K} \cap \mathcal{C}$, is equinumerous with the set of 4-cacti with $k+1$ blocks. Then, using this bijection, we describe an enumeration of $\mathcal{Z}_{k+1}$ for all $k \geq 0$, based on species theory. Finally we use analytic combinatorics to obtain asymptotic estimates for the number of obstructions $\mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$ for each $k \geq 0$.

4.1.1 A Bijection between $\mathbf{obs}(\mathcal{A}_k(\mathcal{S})) \cap \mathcal{K} \cap \mathcal{C}$ and 4-cacti

Observe that the automorphism groups of the butterfly graph Z and C_4 are isomorphic. In particular, $\mathrm{Aut}(Z) \cong \mathrm{Aut}(C_4) \cong \mathbb{D}_4$, where $\mathbb{D}_4$ is the dihedral group of order 8. Observe, also, that every automorphism of Z fixes its central vertex. This group isomorphism implies a bijection between the extremal vertices of Z and the vertices of C_4 as in Figure 4.1.

Notice that each graph in $G \in \mathcal{Z}_k$ contains k subgraphs $\{Z_1, \ldots, Z_k\}$, each isomorphic to Z and whose edge sets are pairwise disjoint. We refer to these subgraphs as the *Z-subgraphs* of G. We define the family $\overline{\mathcal{Z}}_k$ of *rooted* graphs in $\mathcal{Z}$ to be the class containing the pairs (Z, v) where $Z \in \mathcal{Z}_k$ and v is an non-central vertex of Z.

We now list the definition of 4-cacti and their rooted counterparts.

Definition 4.1.1 (4-cacti, rooted 4-cacti)**.** Let $\mathcal{K}^{(4)}$ be the class of all 4-cacti, that is cacti whose blocks are all isomorphic to the square graph C_4. Let also $\mathcal{K}^{(4)}_k$ be the set of all 4-cacti having exactly k blocks.

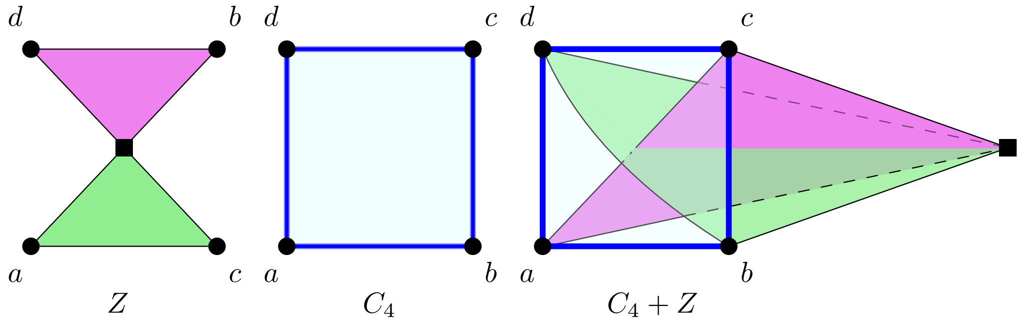


Figure 4.1: The correspondence between the extremal vertices of Z and the vertices of C_4 and a superposition of Z and C_4 that illustrates the isomorphism between $\text{Aut}(Z)$ and $\text{Aut}(C_4)$.

We denote by $\overline{\mathcal{K}}_k^{(4)}$ the class of all *rooted* 4*-cacti*,that is pairs (G, v) where $G \in \mathcal{K}^{(4)}$ and $v \in V(G)$.

The following two functions will be used to establish our result for this section.

Definition 4.1.2 (Functions ψ and $\overline{\psi}$)**.** We define the function $\psi_k : \mathcal{Z}_k \to \mathcal{K}_k^{(4)}$ such that for every $G \in \mathcal{Z}_k$ the graph $\psi(G)$ is obtained if we replace each Z-subgraph of G with a copy of C_4, as indicated in Figure 4.1. Accordingly, we define $\overline{\psi}_k : \overline{\mathcal{Z}}_k \to \overline{\mathcal{K}}_k^{(4)}$ such that $\overline{\psi}_k(G, v) = (\psi_k(G), v)$.

Observation 4.1.3. Let G be a graph in $\overline{\mathcal{Z}}_k$. Then $\overline{\psi}_k$ maps the non-central cut-vertices of G to the cut-vertices of $\overline{\psi}_k(G)$.

Finally, we define a notion of isomorphism between rooted graphs.

Definition 4.1.4 (Isomorphism of rooted graphs)**.** Two rooted graphs (G_1, v_1) and (G_2, v_2) are *isomorphic* if there exists an isomorphism between G_1 and G_2 that maps v_1 to v_2.

Lemma 4.1.5. *Let k be a positive integer. The function $\overline{\psi}_k$ is an injection.*

Proof. We proceed by induction on k. For $k = 1$ we have that $\overline{\psi}_1$ maps the unique graph in $\overline{\mathcal{Z}}_1$ to the unique graph in $\overline{\mathcal{K}}_1^{(4)}$ and so the result holds.

Suppose now that $k \geq 2$ and that the lemma holds for all smaller values of k. Let $(G_1, a_1), (G_2, a_2) \in \overline{\mathcal{Z}}_k$ be two graphs having the same image $(G_3, a_3) \in \overline{\mathcal{K}}_k^{(4)}$ under $\overline{\psi}_k$. We will show that $(G_1, a_1) = (G_2, a_2)$. Observe that, by definition of $\overline{\psi}_k$, $a_3 = a_1 = a_2$.

Let S be a block of G_3 containing a_3. Since $G_3 \in \mathcal{K}_k^{(4)}$, $S \cong C_4$. We fix a cyclic ordering of the vertices of S, such that $V(S) = (a_3, b_3, c_3, d_3)$. That is, we have that b, d are the neighbours of a in S, and c is the remaining vertex other than a, b, d. We use the notation Z_{G_1}, Z_{G_2} for the Z-subgraphs of (G_1, a_1) and (G_2, a_2), respectively, corresponding to S. We also make use of the notation b_i, c_i, d_i for the vertices of Z_{G_i}, $i \in [2]$, which are the images of b_3, c_3, d_3 under the bijection defined in Figure 4.1.

We distinguish the following two cases, based on whether the root a_3 of G_3 is a cut vertex or not.

Case 1: a_3 is not a cut vertex of G_3. Consider the (unrooted) graph G_3' obtained from G_3 by deleting all edges of S. Similarly, we define G_1' and G_2' by deleting the central vertex and all edges of Z_{G_1} and Z_{G_2}, respectively.

Observe that, since a_3 is not a cut-vertex, then for every $i \in [3]$, the connected component of G_i' that contains a_i is the singleton $\{a_i\}$. Let (B_i, b_i), (C_i, c_i), (D_i, d_i), $i \in [3]$, be the connected components of G_i' containing b_i, c_i, and d_i respectively, considered as graphs rooted at b_i, c_i, and d_i. Notice that these connected components are unique, since every G_i is a cactus graph.

From the inductive hypothesis we have that $\overline{\psi}_l$ is injective for all values of l smaller than k and therefore there exist left inverses ϕ_l of ψ_l for every $l \leq k-1$.

Observe, now that since $B_3 \in \mathcal{K}^{(4)}$ and has l blocks, where $l < k$, then the function $\overline{\psi}_l$ is injective and the fact that $(B_3, b_3) = \overline{\psi}_l(B_2, b_2) = \overline{\psi}_l(B_1, b_1)$ implies that $(B_1, b_1) = (B_2, b_2)$ - and the same holds for (C_i, c_i) and (D_i, d_i).

But then it must be the case that (G_1, a_1) and (G_2, a_2) are isomorphic since both are obtained from a copy of Z (labeled as in Figure 4.1 and rooted at a) by identifying b with the root of $\phi_l((B_3, b_3))$, c with the root of $\phi_l((C_3, c_3))$, and d with the root of $\phi_l((D_3, d_3))$, for appropriate values of l. This concludes Case 1.

Case 2: a_3 is a cut vertex of G_3. Observe that, by Observation 4.1.3, a_1, a_2 are also cut-vertices of G_1, G_2 respectively. Consider the graphs in $\mathcal{C}(G_3, a_3)$ each rooted at a_3 and observe that each belongs to some $\overline{\mathcal{K}}_i^{(4)}$ for appropriate values of $i < k$. Similarly the graphs in $\mathcal{C}(G_1, a_1)$ and $\mathcal{C}(G_2, a_2)$, rooted at a_1, a_2 respectively, all belong to some $\overline{\mathcal{Z}}_i$ for appropriate values of $i < k$.

As mentioned in the previous case, by inductive hypothesis, there exists a left-inverse ϕ_l of every ψ_l, $l \leq k-1$. But then, by the construction of ψ, we have that for every graph $G \in \mathcal{C}(G_3, a_3)$ considered rooted at a_3, there exists some $G' \in \mathcal{C}(G_2, a_2)$ considered rooted at a_2, and some $G'' \in \mathcal{C}(G_1, a_1)$ considered rooted at a_1, such that $\phi_l(G) \cong G' \cong G''$ for an appropriate value of l. Therefore we have that $(G_1, a_1) \cong (G_2, a_2)$ since both are obtained from identifying the roots of all graphs in the set $\{\phi_l((G_3, a_3)) \mid G \in \mathcal{C}(G_3, a_3) \wedge G \in \overline{\mathcal{K}}_l^{(4)}\}$. □

Corollary 4.1.6. *For all $k \in \mathbb{N}^+$, $|\mathcal{Z}_k| = |\mathcal{K}_k^{(4)}|$.*

Proof. We first prove that $|\mathcal{Z}_k| \leq |\mathcal{K}_k^{(4)}|$. To do this, it suffices to show that ψ_k is injective for all k. Suppose, towards a contradiction, that there exist $G_1 \not\cong G_2$ such that $\psi_k(G_1) \cong \psi_k(G_2) \cong H$ for some $H \in \mathcal{K}_k^{(4)}$. Consider now the graph H rooted at some arbitrary vertex v belonging to some block B and the graphs G_1, G_2 also rooted at the vertex v of Z-subgraphs corresponding to B in G_1, G_2 respectively. By Lemma 4.1.5 we have that $\overline{\psi}_k$ is injective and so we have that since $\overline{\psi}(G, v) \cong \overline{\psi}(G, v) \cong (H, v)$, $G_1 \cong G_2$ since two rooted graphs are isomorphic only if there exists an isomorphism between their underlying graphs that also maps one root to the other, a contradiction. Therefore ψ_k is injective.

The reverse inequality, that is $|\mathcal{Z}_k| \geq |\mathcal{K}_k^{(4)}|$, follows from arguments identical to the above, as well as the to those in Lemma 4.1.5, applied to some $\overline{\psi}_k' : \overline{\mathcal{K}}_k^{(4)} \to \overline{\mathcal{Z}}_k$, again defined as in Figure 4.1, by replacing the notions of $\mathcal{Z}_k$ with the respective notions of $\mathcal{K}_k^{(4)}$ where required, and vice versa.

□

Intuitively, the motivation behind this bijection is the observation that information about how the blocks of a 4-cactus are arranged (i.e. which blocks share vertices) and how their remaining non-shared vertices behave under the "local" automorphisms of each block is enough to fully determine the graph up to isomorphism and that the same holds if one considers connected obstructions and Z-subgraphs in place of 4-cacti and blocks. For an example of the constructions detailed in the above proofs, see Figure 4.2.

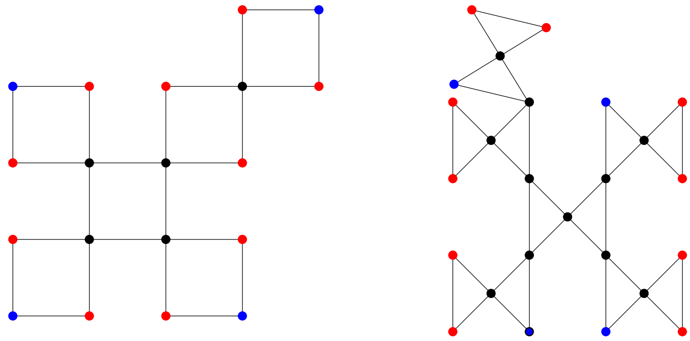


Figure 4.2: A pure 4-cactus and its corresponding image under ψ, with cut vertices in black and the remaining ones coloured the same if they belong to the same cycle of the automorphism which fixes each respective block/$\mathcal{Z}$-subgraph's cut vertices.

Therefore enumeration of graphs in the sets $\mathcal{Z}_k$ can be achieved via enumeration of graphs in the respective sets $\mathcal{K}_k^{(4)}$. The following is then an immediate corollary of Corollary 4.1.6 and the fact that $\forall G \in \mathcal{Z}_k\ |V(G)| = 4k+1$ and that $\forall H \in \mathcal{K}_k^{(4)}\ |V(H)| = 3k+1$. Both of these facts follow immediately from the definitions of $\mathcal{Z}_k$ and $\mathcal{K}_k^{(4)}$ respectively.

Corollary 4.1.7. *For every $n \in \mathbb{N}$, the bijection of Corollary 4.1.6 maps 4-cacti having k blocks to graphs in $\mathbf{obs}(\mathcal{A}_k(\mathcal{S})) \cap \mathcal{K} \cap \mathcal{C}$ having k Z-subgraphs. Moreover, in terms of vertex counts, this bijection maps a 4-cacti with n vertices to obstructions with $n + \frac{n-1}{3}$ vertices.*

4.1.2 Enumeration of $\mathbf{obs}(\mathcal{A}_k(\mathcal{S})) \cap \mathcal{K}$ and Augmented 4-cacti

The purpose of this section is to derive the ordinary generating series for the families $\overline{\mathcal{Z}}_k$ and $\mathcal{Z}_k$ of rooted and unrooted connected cactus-obstructions for k-apex sub-unicyclicity, respectively. We also derive the ordinary generating series for all graphs in $\bigcup_{k\in\mathbb{N}^+} \mathbf{obs}(\mathcal{A}_k(\mathcal{S})) \cap \mathcal{S}$. We prove the following.

Theorem 4.1.8. *The type generating series $\widetilde{\Pi^+}(x)$ of rooted augmented 4-cacti, and therefore also of graphs in $\overline{\mathcal{Z}}_k$, is*

$$\widetilde{\Pi^+}(x) = x \cdot exp\left(\sum_{i=1}^{\infty} \frac{1}{i}\left(\left(\frac{\widetilde{\Pi^+}(x^i)^3}{2} + \frac{\widetilde{\Pi^+}(x^i)\widetilde{\Pi^+}(x^{2i})}{2}\right) \cdot x\right)\right), \tag{4.1}$$

while the type generating series $\widetilde{\pi^+}(x)$ of unrooted augmented 4-cacti, and therefore also of graphs in $\mathcal{Z}_k$, is

$$\begin{aligned}\widetilde{\pi^+}(x) = \widetilde{\Pi^+}(x) + &\left(\left(\frac{\widetilde{\Pi^+}(x)^4}{8} + \frac{\widetilde{\Pi^+}(x)^2\widetilde{\Pi^+}(x^2)}{4} + \frac{3\widetilde{\Pi^+}(x^2)^2}{8} + \frac{\widetilde{\Pi^+}(x^4)}{4}\right) x\right) \\ - \widetilde{\Pi^+}(x) &\left(\left(\frac{\widetilde{\Pi^+}(x)^3}{2} + \frac{\widetilde{\Pi^+}(x)\widetilde{\Pi^+}(x^2)}{2}\right) x\right).\end{aligned} \tag{4.2}$$

Theorem 4.1.9. *The type generating series $\widetilde{C}(x)$ of graphs belonging in $\bigcup_{k\in\mathbb{N}^+} \mathbf{obs}(\mathcal{A}_k(\mathcal{S})) \cap \mathcal{K}$ is*

$$\widetilde{C}(x) = exp\left(\sum_{i=1}^{\infty} \frac{\widetilde{\pi^+}(x^i) - x}{i}\right) \tag{4.3}$$

We have seen in the last section that, by Corollary 4.1.6, enumerating $\mathcal{Z}_k$ amounts to enumerating sets of 4-cacti having k blocks. We also know, by Corollary 4.1.7, that the set of 4-cacti having n vertices is in bijection with the set of connected cactus-obstructions having $n + \frac{n-1}{3}$ vertices. Therefore, given a specification for the species of 4-cacti, we need only modify it so it accounts for some $\frac{n-1}{3}$ extra vertices. This can be done by including, for each block of a 4-cactus, a single vertex with no neighbours which we refer to as *isolated*. We will call a 4-cactus with an isolated vertex assigned to each of its blocks an *augmented* 4-cactus.

In the following, let X be the species of singletons, E be the species of sets, and E_2 be the species of sets having cardinality exactly 2.

First, we give a specification of the species of squares, that is graphs isomorphic to C_4.

Lemma 4.1.10. *The species of squares is $C_4 = E_2(E_2)$.*

Proof. We can see that the species of squares C_4 is (isomorphic to) the species $E_2(E_2)$ by passing to the latter's complementary graph. This can be verified by observing that the associated cycle index series of both species coincide. □

We continue by providing a specification of the species π of 4-cacti. Our plan is to closely follow the species-theoretic definition of unrooted trees as presented in Example 2.3.28: starting from the species of rooted 4-cacti we apply a dissymmetry theorem which yields the desired species of unrooted 4-cacti. The specification of augmented 4-cacti swiftly follows.

We define the species of *rooted 4-cacti* recursively: a rooted 4-cactus consists of a root r and a set of 4-cacti rooted at the other vertices of the blocks containing r, which we refer to as *sub-cacti*.

Lemma 4.1.11. *The species of rooted 4-cacti is $\Pi = X \cdot E(C_4'(\Pi))$.*

Proof. In translating the recursive definition of rooted 4-cacti to a species-theoretic defining equation, we'll use the singleton species X to represent the root of the cactus.

As for the set of sub-cacti, we know that these must be arranged in a way such that their roots form a block, isomorphic to C_4, containing the root vertex. In species-theoretic terms, this is a substitution of the species of rooted 4-cacti Π to the derivative of the species of squares (intuitively, the last one is species of squares having a "hole" where the root goes). It follows, via the product rule, that the derivative species of C_4 is $C_4' = E_2 \cdot X$.

Therefore we have that the species of rooted 4-cacti, Π equals that of pairs consisting of a root X and a (possibly empty) set of sub-cacti, which in terms of species translates to $X \cdot E(C_4'(\Pi))$. □

We can now describe the species of unrooted 4-cacti using the dissymmetry theorem, as follows.

Lemma 4.1.12. *The species of 4-cacti is $\pi = \Pi + C_4(\Pi) - \Pi \cdot C_4'(\Pi)$.*

Proof. This follows immediately from Theorem 2.3.30. □

Given the above specifications of π and Π one easily passes to their augmented versions by modifying the equations to include singletons standing for the isolated vertex assigned to each block, as follows.

Corollary 4.1.13. *The species Π^+ of rooted augmented 4-cact is (isomorphic to) $X \cdot E(C_4'(\Pi^+) \cdot X)$, while that of urooted augmented 4-cacti is given by $\pi^+ = \Pi^+ + (C_4(\Pi^+) \cdot X) - \Pi \cdot (C_4'(\Pi^+) \cdot X)$.*

Proof. This follows from a slightly altered form of Theorem 2.3.30. Consider the following equation:

$$\Pi^+ + (C_4(\Pi^+) \cdot X) = \pi^+ + \Pi \cdot (C_4'(\Pi^+) \cdot X). \tag{4.4}$$

The left-hand side represents graphs which are rooted at either a vertex or an augmented block (a block plus its isolated vertex). The right-hand side term π^+ represents those graphs which have been rooted in what we consider the canonical way: at the center of their block-cut-vertex-tree (which is always a vertex which corresponds to either a vertex of the graph or a block thereof). The remaining term $\Pi \cdot (C_4'(\Pi^+) \cdot X)$ corresponds to the bijection given in the proof of Theorem 2.3.30 presented in [19, Section 4.2, Theorem 3, page 302] with the addition of the isolated vertex which corresponds to each augmented block. □

Given the above, we can now prove our main results for this section.

Proof of Theorem 4.1.8. From Corollary 4.1.13, by straightforward computations using the corresponding cycle-index series, we obtain the following implicit equation for the type generating series $\widetilde{\Pi^+}(x)$ of rooted augmented 4-cacti.

$$\widetilde{\Pi^+}(x) = x \cdot exp\left(\sum_{i=1}^{\infty} \frac{1}{i}\left(\left(\frac{\widetilde{\Pi^+}(x^i)^3}{2} + \frac{\widetilde{\Pi^+}(x^i)\widetilde{\Pi^+}(x^{2i})}{2}\right)\cdot x\right)\right) \tag{4.5}$$

As for augmented 4-cacti, we have that the equation given in Corollary 4.1.13, via use of the corresponding cycle-index series, translates to the following equation between the corresponding isotype generating series.

$$\begin{aligned}\widetilde{\pi^+}(x) = \widetilde{\Pi^+}(x) &+ \left(\left(\frac{\widetilde{\Pi^+}(x)^4}{8} + \frac{\widetilde{\Pi^+}(x)^2\widetilde{\Pi^+}(x^2)}{4} + \frac{3\widetilde{\Pi^+}(x^2)^2}{8} + \frac{\widetilde{\Pi^+}(x^4)}{4}\right)x\right) \\ &- \widetilde{\Pi^+}(x)\left(\left(\frac{\widetilde{\Pi^+}(x)^3}{2} + \frac{\widetilde{\Pi^+}(x)\widetilde{\Pi^+}(x^2)}{2}\right)x\right)\end{aligned} \tag{4.6}$$

□

We can readily compute arbitrary truncations Π_k^+ of Π^+ by an iterative scheme starting with $\Pi_0^+ = x$ and defining Π_k^+ as the result of substituting Π_{k-1}^+'s Taylor expansion (at 0) in place of Π^+ in Equation 4.1.

Using such a truncation for Π^+, the first few terms $\widetilde{\Pi^+}(x)$ can be computed to be

$$\widetilde{\Pi^+}(x) = x + x^5 + 3x^9 + 11x^{13} + 46x^{17} + 208x^{21} + 1002x^{25} + 5012x^{29} + 25863x^{33} + O(x^{37}).$$

By substituting a suitable truncation Π_k^+ for Π^+ in Equation 4.2, we can compute the first terms of $\widetilde{\pi^+}(x)$, which are as follows

$$\widetilde{\pi^+}(x) = x + x^5 + x^9 + 3x^{13} + 7x^{17} + 25x^{21} + 88x^{25} + 366x^{29} + 1583x^{33} + 7336x^{37} + O(x^{41}).$$

Note 4.1.14. Notice that the species of the graph Z is isomorphic to $C_4 \cdot X$. To see this, consider the bijection between vertices of C_4 and extremal ones of Z given in Figure 4.1. This shows that Z, under action of $\mathbb{D}_4$, behaves as a C_4 graph plus a vertex, its central one, which is always fixed by all its automorphisms. Therefore the species of rooted augmented 4-cacti is isomorphic to the species of graphs in $\overline{\mathcal{Z}}_k$. The same relationship holds for the species of augmented 4-cacti and the species of graphs in $\mathcal{Z}_k$.

As a corollary of the above, in conjunction with Theorem 3.3.1, we obtain the following.

Corollary 4.1.15. *The number of disconnected graphs in* $\mathbf{obs}(\mathcal{A}_k(\mathcal{S})) \cap \mathcal{K}$ *having* k Z*-subgraphs is*

$$1 + \sum_{p \in \mathcal{P}(k+1) \wedge |p| \geq 2} \prod_{p_i \in P} [x^{4p_i+1}]\widetilde{\pi^+}, \tag{4.7}$$

Proof. From Theorem 3.3.1 we have that a disconnected graph $G \in \mathbf{obs}(\mathcal{A}_k(\mathcal{S})) \cap \mathcal{K}$ is either isomorphic to $(k+2)K_3$ (which in the expression above is accounted by the factor 1) or is the disjoint union of graphs $G_1, \ldots, G_r$ each of which is a connected cactus in $\mathbf{obs}(\mathcal{A}_{k_i-1}(\mathcal{S}))$ for appropriate values $k_1, \ldots, k_r$, respectively, of k. Furthermore we have that $\sum_{i \in [r]} k_i = k+1$ and therefore $k_1, \ldots, k_3$ form a partition of $k+1$. Therefore to account for the second case, where $G \ncong (k+2)K_3$, we need only sum over all possible partitions of $k+1$ (with at least 2 parts since G is disconnected) the number of possible ways to choose a graph in k_1, a graph in k_2, and so on. The number of ways to choose a graph in $\mathcal{Z}_{k_i}$ is given by the coefficient of x^{4k_i+1} in $\widetilde{\pi^+}$ and so the corollary follows. □

Given the above, we can now prove Theorem 4.1.9.

Proof of Theorem 4.1.9. Consider a graph G in $\mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$ for some k. If G is connected then $G \in \mathcal{Z}_k$. If G is not connected we have that, due to Theorem 3.3.1, G is the disjoint union of graphs in $\mathcal{Z}_{k'}$ for appropriate values of $k' < k$. Therefore a general graph belonging to $\mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$ for some k can be with the set of its connected components, that is, a set of one or more graphs in $\mathcal{Z}'_k$ for appropriate values of $k' < k$. Therefore the species C of graphs in $\bigcup_{k \in \mathbb{N}^+} \mathbf{obs}(\mathcal{A}_k(\mathcal{S}))$ is $C = E(\Pi^+ - X)$. Observe that we must consider the species $\Pi^+ X$ since Π alone has a structure on the singleton, which we do not wish to include in C. The result then follows from straightforward computations employing the cycle index series of each respective species. □

Using a suitable truncation of π_k^+ , we can compute the first terms of $\widetilde{C}(x)$, which are as follows

$$\widetilde{C}(x) = 1 + x + x^9 + x^{10} + 3x^{13} + x^{14} + x^{15} + 7x^{17} + 4x^{18} + x^{19} + x^{20} + 25x^{21} + 10x^{22} + 4x^{23} + O(x^{24}).$$

Observe that all power of x^i, for $i \geq 20$, will have positive coefficients and therefore, unlike $\widetilde{\pi^+}(x)$ and $\widetilde{\Pi^+}(x)$, $C(x)$ is eventually aperiodic. This can be explained as follows. We already know that the coefficients of x^i such that $i \geq 5$ and $i \cong 0(mod4)$ are positive, since $C(x)$ counts all connected graphs too. We also have that there exists a disconnected cactus-obstruction with 10 vertices, which is $G = 2Z$ and so by attaching copies of Z to either of the two disjoint copies of Z in G, we can generate graphs G' whose vertices satisfy $|V(G)| \cong 2(mod4)$. Similarly, by attaching copies of Z to the connected components of the graphs $G_1 = 3Z$ and $G_2 = 4Z$, having 15 and 20 vertices respectively, one can generate graphs with vertex counts equal to 3 and 0 modulo 4, respectively. Therefore, past $i = 20$, all coefficients of x^i will have positive coefficients.

4.2 Asymptotic Analysis

The purpose of this section is to derive asymptotic estimates for the number of connected and general (i.e both connected and disconnected) graphs in $\mathbf{obs}(\mathcal{A}_k(\mathcal{S})) \cap \mathcal{K}$. For connected graphs we provide asymptotic estimates in terms of both the number of Z-subgraphs and the number of vertices. For general graphs we provide an asymptotic estimate in terms of number of vertices. We prove the following.

Theorem 4.2.1. *The number of connected graphs in* $\mathbf{obs}(\mathcal{A}_k(\mathcal{S})) \cap \mathcal{K}$ *having* k Z*-subgraphs satisfies:*

$$|\mathcal{Z}_k| \sim 3.677727670\ (1+4k)^{-\frac{5}{2}}\ 6.278889833^k, \tag{4.8}$$

Let $\widetilde{C}(x)$ be the generating function for general obstructions derived in Theorem 4.1.9. Then we have the following.

Theorem 4.2.2. *The number of graphs in* $\bigcup_{k\in\mathbb{N}^+} \mathbf{obs}(\mathcal{A}_k(\mathcal{S})) \cap \mathcal{K}$ *having* n *vertices satisfies:*

$$[x^n]\widetilde{C}(x) \sim \frac{3c}{4\sqrt{\pi n^5}} \cdot r^{-n}(\widetilde{C}(r) - \widetilde{C}(-r)(-1)^{-n} - i\widetilde{C}(-ir)(-i)^{-n} + \widetilde{C}(ir)i^{1-n}), \tag{4.9}$$

where $r \doteq 0.6317267748$*,* $c = 1.372658593$*,* $\widetilde{C}(r) \doteq 1.148168784$*,* $\widetilde{C}(-ir) \doteq 0.986150197 - 0.131194851i$*,* $\widetilde{C}(ir) \doteq 0.986150197 + 0.131194851i$*, and* $\widetilde{C}(-r) \doteq 0.880102665$*.*

k	1	5	10	15
$\lvert\mathcal{Z}_k\rvert$	1	25	34982	122462546
Approximation	0.4130830923	17.76010979	32542.32340	$1.176245371 \cdot 10^8$
Relative Error	0.58691	0.28959	0.06974	0.03950

Table 4.1: Exact and estimated values for $|\mathcal{Z}_k|$ together with the relative error of approximation. Values computed using Maple with a precision setting of 10 digits. Error values truncated to their 5 first digits.

Note 4.2.3. The values of constants presented in this chapter have being numerically computed using Maple with a default precision of 10 digits for software floating-point numbers. As such, all values presented in this chapter, unless otherwise stated, are presented in this default precision.

We begin with an asymptotic analysis of the isotype generating series of the species Π^+ of rooted augmented 4-cacti.

Lemma 4.2.4. *The number of rooted augmented 4-cacti having* n *vertices satisfies*

$$[x^n]\widetilde{\Pi^+} = \frac{\gamma}{2\sqrt{\pi n^3}} r^{-n}\left(2sin\left(\frac{n\pi}{2}\right) - e^{in\pi} + 1\right) \cdot (1 + O(n^{-1})),$$

where $\gamma \doteq 1.123966302$ *and* $r \doteq 0.6317267748$*. We also have, approximately,* $[x^n]\widetilde{\Pi^+} \bowtie 1.58296^n$*.*

Proof. Let G be

$$G(x,y) = x \cdot exp\left(\left(\frac{y^3}{2} + \frac{y\,\widetilde{\Pi^+}(x^2)}{2}\right) \cdot x + \sum_{i=2}^{\infty} \frac{1}{i}\left(\left(\frac{\widetilde{\Pi^+}(x^i)^3}{2} + \frac{\widetilde{\Pi^+}(x^i)\widetilde{\Pi^+}(x^{2i})}{2}\right) \cdot x\right)\right).$$

Then the following holds (compare with Equation 4.2)

$$\widetilde{\Pi^+}(x) = G(x, \widetilde{\Pi^+}(x)).$$

In what follows, we treat the terms of the form $\widetilde{\Pi^+}(x^n)$ for $n \geq 2$, sometimes referred to as *Pólya terms*, as known. Since, as we'll see, $\widetilde{\Pi^+}(x)$ has some radius of convergence R less than 1, these Pólya terms are analytic on R and can be approximated via truncations of $\widetilde{\Pi^+}(x)$'s Taylor expansion.

Note that the radius of convergence of $\widetilde{\Pi^+}$ cannot be zero, since its coefficients are bound above by, say, the number of plane trees (whose ordinary generating function has radius 1/4).

Moreover G satisfies the required conditions set by Theorem 2.4.13. By taking appropriate truncations where needed, we can computationally approximate the positive solutions r, s of the following *characteristic system*:

$$G(r, s) = s,$$
$$G_y(r, s) = 1,$$

where G_y is the partial derivative of G with respect to y.

Using Maple, these have been computed to be:

$$r \doteq 0.6317267748,$$
$$s \doteq 0.9733854104.$$

Therefore, by Theorem 2.4.13, we have that $\widetilde{\Pi^+}$ has a square-root type singularity at r, where it admits a singular expansion valid in a Δ-domain centered at r, of the form:

$$\widetilde{\Pi^+}(z) \overset{z \to r}{=} s - \gamma\sqrt{1 - \frac{z}{r}} + O\left(1 - \frac{z}{r}\right),$$

where

$$\gamma = \frac{\sqrt{2rG_x(r, s)}}{G_{yy}(r, s)}. \tag{4.10}$$

Since we know via combinatorial means that

$$[x^n]\widetilde{\Pi^+}(x) \neq 0 \iff n \equiv 1 \mod 4,$$

it follows that $\widetilde{\Pi^+}(x)/x$ is periodic and

$$[x^n]\widetilde{\Pi^+}(x)/x \neq 0 \iff n \equiv 0 \mod 4.$$

Now, since $\widetilde{\Pi^+}(x)/x$ is periodic with period 4, there must exist four dominant singularities of $\widetilde{\Pi^+}(x)$ (all of square-root type), one of which is at r, while the rest are at $-r, ir, -ir$. By Lemma 2.4.11, there cannot be any more, and therefore these are exactly the four dominant singularities of $\widetilde{\Pi^+}(x)$. Then, by employing the identity $i = -\frac{1}{i}$, we have the following singular expansions at these four singularities:

$$\frac{\widetilde{\Pi^+}(x)}{x} \overset{x \to r}{=} \frac{1}{r}\left(s - \gamma\sqrt{1 - \frac{x}{r}}\right) + O\left(1 - \frac{x}{r}\right)$$
$$\frac{\widetilde{\Pi^+}(x)}{x} \overset{x \to ir}{=} \frac{1}{r}\left(s - \gamma\sqrt{1 - \frac{x}{-ir}}\right) + O\left(1 - \frac{x}{-ir}\right)$$
$$\frac{\widetilde{\Pi^+}(x)}{x} \overset{x \to -ir}{=} \frac{1}{r}\left(s - \gamma\sqrt{1 - \frac{x}{ir}}\right) + O\left(1 - \frac{x}{ir}\right)$$
$$\frac{\widetilde{\Pi^+}(x)}{x} \overset{x \to -r}{=} \frac{1}{r}\left(s - \gamma\sqrt{1 - \frac{x}{-r}}\right) + O\left(1 - \frac{x}{-r}\right).$$

Finally, by applying Theorem 2.4.12 and performing the appropriate transfers we have that the coefficients of $\frac{\widetilde{\Pi^+}(x)}{x}$ are asymptotically:

$$[x^n]\frac{\widetilde{\Pi^+}(x)}{x} = \frac{1}{r}\left(\frac{\gamma}{2\sqrt{\pi n^3}}r^{-n}\right) + \frac{1}{r}\left(\frac{\gamma}{2\sqrt{\pi n^3}}(-ir)^{-n}\right) + \frac{1}{r}\left(\frac{\gamma}{2\sqrt{\pi n^3}}(ir)^{-n}\right) + \frac{1}{r}\left(\frac{\gamma}{2\sqrt{\pi n^3}}(-r)^{-n}\right) \cdot (1+O(n^{-1})).$$

From this, we can recover an asymptotic estimate of $\widetilde{\Pi^+}(x)$'s coefficients by multiplying each factor by the appropriate corresponding singularity, to obtain:

$$\begin{aligned}[x^n]\widetilde{\Pi^+} &= \frac{\gamma}{2\sqrt{\pi n^3}}\left(r^{-n} - (-r)^{-n} - i(-ir)^{-n} + i(ir)^{-n}\right)\cdot(1+O(n^{-1})) \\ &= \frac{\gamma}{2\sqrt{\pi n^3}}\, r^{-n}\, \left(2sin\left(\frac{n\pi}{2}\right) - e^{in\pi} + 1\right)\cdot(1+O(n^{-1})).\end{aligned}$$

□

By expressing the asymptotic estimates of Lemma 4.2.4 in terms of number of Z-subgraphs instead of vertex counts, we have the following.

Corollary 4.2.5. *The number of rooted connected cactus-obstructions in $\overline{\mathcal{Z}}_k$ is asymptotically:*

$$|\overline{\mathcal{Z}}_k| \sim \frac{2\gamma}{\sqrt{\pi(1+4k)^3}} r^{-1-4k}, \tag{4.11}$$

where $\gamma \doteq 1.123966303$ and $r \doteq 0.6317267748$.

Proof. Immediately follows from Corollary 4.1.13, Lemma 4.2.4, and the fact that a graph in $\overline{\mathcal{Z}}_k$ with k Z-subgraphs has $4k+1$ vertices. □

k	1	5	10	15
$\lvert\overline{\mathcal{Z}}_k\rvert$	1	208	733902	3933700703
Approximation	1.12747	203.59374	$7.283362277 \cdot 10^5$	$3.916762707 \cdot 10^9$
Relative Error	0.12747	0.021183	0.00758	0.00430

Table 4.2: Exact and estimated values for $|\overline{\mathcal{Z}}_k|$ together with the relative error of approximation. Values computed using Maple with a precision setting of 10 digits. Error values truncated to their 5 first digits.

Before continuing with an asymptotic analysis of $\widetilde{\pi^+}$ we present the following lemma and its proof as adapted from [27, Theorem 4.3] and [28, Theorem 3.5]. Note that the proof follows the exact same steps as the cited theorems and is presented here, in its adapted form, for the sake of completeness.

Lemma 4.2.6. *The function $\widetilde{\pi}(x)$, at each singularity $p \in \{\rho, -\frac{1}{2}+i\frac{\sqrt{3}}{2}\rho, -\frac{1}{2}-i\frac{\sqrt{3}}{2}\rho\}$, has asymptotic expansions of the form*

$$\widetilde{\pi}(x) = \widetilde{\pi}(p) + \sum_{k\geq 2}\widetilde{\pi}_k X^k,$$

where $X = \sqrt{1-\frac{x}{r}}$. That is, the singular exponent of each of the singular expansions of $\widetilde{\pi}$ is $3/2$.

Proof. Let $D = C_4$ and $V = X \cdot C_4'$. The equation given for the species π in *Lemma* 4.1.12 readily translates, by employing the respective cycle index series,

$$Z_D(x_1, x_2, x_4) = \frac{x_1^4}{8} + \frac{x_1^2 x_2}{4} + \frac{3x_2^2}{8} + \frac{x_4}{4}$$
$$Z_V(x_1, x_2) = x\left(\frac{x_1^3}{2} + \frac{x_1 x_2}{2}\right)$$

to the following equation,

$$\widetilde{\pi}(x) = \widetilde{\Pi}(x) + Z_D(\widetilde{\Pi}(x), \widetilde{\Pi}(x^2)...) - Z_V(\widetilde{\Pi}(x), \widetilde{\Pi}(x^2), ...). \tag{4.12}$$

Observe that by translating the equation of Lemma 4.1.12, using the appropriate cycle index series of each species, into an equation in terms of their isotype generating function, we obtain an exact analogue of Equation 4.2 (with the only difference being that the second and third summands are missing the multiplicative factor x). From this we have that the dominant singularities of $\widetilde{\pi}(x)$ are the same as those of $\widetilde{\Pi}(x)$, since the terms $\widetilde{\Pi}(x^i)$ for $i \geq 2$ are all analytic at $\widetilde{\Pi}(x)$'s singularities. Also observe that, for reasons entirely analogous to those given for $\widetilde{\Pi^+}$, $\widetilde{\Pi}$ has three dominant singularities. Indeed, one of these dominant singularities, denoted as ρ, lies on the positive real axis (this is due to Theorem 2.4.3), while the other two are $-\frac{1}{2} + i\frac{\sqrt{3}}{2}\rho, -\frac{1}{2} - i\frac{\sqrt{3}}{2}\rho$. Also observe that the singularity ρ, as well as $\widetilde{\Pi}(x)$'s singular expansion at it, can be found using Theorem 2.4.13 in a way identical to the one we followed for $\widetilde{\Pi}$. That is, we define

$$F(x, y) = x \cdot exp\left(\left(\frac{y^3}{2} + \frac{y\,\widetilde{\Pi^+}(x^2)}{2}\right) + \sum_{i=2}^{\infty} \frac{1}{i}\left(\frac{\widetilde{\Pi^+}(x^i)^3}{2} + \frac{\widetilde{\Pi^+}(x^i)\widetilde{\Pi^+}(x^{2i})}{2}\right)\right). \tag{4.13}$$

and observe that $F(x, \widetilde{\Pi}(x)) = \widetilde{\Pi}(x)$. Therefore, by solving the related characteristic system we obtain ρ and $\sigma = \widetilde{\Pi}(\rho)$.

We will now proceed prove the desired result for the positive dominant singularity ρ of $\widetilde{\pi}(x)$; the case for the other two dominant singularities is largely identical.

We can obtain an asymptotic expansion of $\widetilde{\pi}(x)$ around its singularity ρ by substituting, in Equation 4.12, the singular expansion of $\widetilde{\Pi}(x)$ for $\widetilde{\Pi}(x)$, and the analytic expansion of $\widetilde{\Pi}$ for $\widetilde{\Pi}(x^k)$, $k \geq 2$, respectively. We also substitute x^k with $(1 - X^2)^k r^k$. Thus we have

$$\begin{aligned}\widetilde{\pi^+}(x) = \sum_{k\geq 0} \widetilde{\Pi^+}_k X^k + Z_D\left(\sum_{k\geq 0} \widetilde{\Pi^+}_k X^k, \widetilde{\Pi^+}\left((1 - X^2)^2 r^2\right), \widetilde{\Pi^+}\left((1 - X^2)^3 r^3\right), \dots\right) \\ - Z_V\left(\sum_{k\geq 0} \widetilde{\Pi^+}_k X^k, \widetilde{\Pi^+}\left((1 - X^2)^2 r^2\right), \widetilde{\Pi^+}\left((1 - X^2)^3 r^3\right), \dots\right)\end{aligned} \tag{4.14}$$

By developing Equation 4.14 in terms of X around $X = 0$ we have an asymptotic expansion

$$\widetilde{\pi}(x) = \sum_{k\geq 0} \widetilde{\pi}_k X^k.$$

Observe that from Equation 4.14, we have the following equation for the coefficient of X in $\widetilde{\pi}$'s singular expansion at ρ

$$\widetilde{\pi}_1 = \widetilde{\Pi}_1 + \widetilde{\Pi}_1 \frac{\partial}{\partial x_1} Z_D - \widetilde{\Pi}_1 \frac{\partial}{\partial x_1} Z_V. \tag{4.15}$$

We now show that $\widetilde{\pi}_1 = 0$. To this end, let us first introduce a slight variation the function F. Let $H(x, y) = F(x, y) - y$ and observe that the following hold

$$\begin{aligned} H(x, \widetilde{\Pi}(x)) &= \widetilde{\Pi}(x) \\ H(\rho, \sigma) &= 0 \\ \frac{\partial}{\partial y} H(\rho, \sigma) &= 0. \end{aligned}$$

Observe also, that $H(x, y)$ may be rewritten as

$$H(x, y) = xexp\left(\frac{Z_V(y, \widetilde{\Pi}(x^2))}{y} + \sum_{i=2}^{\infty} \frac{Z_V(\widetilde{\Pi}(x^i), \widetilde{\Pi}(x^{2i})}{i\widetilde{\Pi}(x^i)}\right) - y.$$

By noting that V's structures are rooted D structures, i.e $D^\bullet = V$, we have that:

$$x_1 \frac{\partial}{\partial x_1} Z_D = Z_V,$$

and therefore

$$\widetilde{\pi}_1 = \widetilde{\Pi}_1 \left(1 + \frac{Z_D(\sigma, \widetilde{\Pi}(\rho^2))}{\sigma} - \frac{\partial}{\partial x_1} Z_V \bigg|_{(x_1, x_2) = (\sigma, \widetilde{\Pi}(\rho^2))}\right).$$

Now, from the definition of $H(x, y)$ and its aforementioned properties, we have

$$\begin{aligned} 0 &= H_y(r, s) \\ &= (H(\rho, \sigma) + \sigma) \frac{\partial}{\partial y} \frac{Z_V(y, \widetilde{\Pi}(x^2))}{y} \bigg|_{(x,y)=(\rho,\sigma))} - 1 \\ &= \sigma \frac{1}{\sigma^2} \left(\frac{d}{dx_1} Z_V(y, \widetilde{\Pi}(\rho^2)) \bigg|_{y=\sigma} \sigma - Z_V(\sigma, \widetilde{\Pi}(\rho^2)) \right) - 1 \\ &= \frac{d}{dx_1} Z_V \bigg|_{(x_1,x_2)=(\sigma,\widetilde{\Pi}(\rho^2))} - \frac{1}{\sigma} Z_V\left(\sigma, \widetilde{\Pi}(\rho^2))\right) - 1 \\ &= \frac{-1}{\widetilde{\Pi}_1} \widetilde{\pi}_1, \end{aligned}$$

which proves $\widetilde{\pi}_1 = 0$ since $\frac{-1}{\widetilde{\Pi}_1} \neq 0$, as can be seen by solving the characteristic system for F. □

Lemma 4.2.7. *The function $\widetilde{\pi^+}(x)$, at each dominant singularity $p \in \{r, ir, -ir, r\}$, has asymptotic expansions of the form*

$$\widetilde{\pi^+}(x) = \widetilde{\pi^+}(p) + \sum_{k \geq 2} \widetilde{\pi^+}_k X^k,$$

where $X = \sqrt{1 - \frac{x}{r}}$. That is, the singular exponent of the singular expansion of $\widetilde{\pi^+}$ at each p is 3/2.

Proof. Assume, towards a contradiction, that the singular exponent of the singular expansion of $\widetilde{\pi^+}$ at each p is not 3/2.

Observe that for $n \geq 5$ with $n \equiv 1 \pmod 4$, we have $[x^n]\widetilde{\pi^+}(x) = [x^{(n - \frac{n-1}{4})}]\widetilde{\pi}(x)$, which reflects the fact that an augmented 4-cactus with k blocks has k more vertices than the corresponding non-augmented 4-cactus on k blocks.

Now, due to Lemma 4.2.6, we know that the (non-zero) coefficients of the analytic expansion of $\widetilde{\pi}$ satisfy

$$[x^n]\widetilde{\pi} \sim \frac{3c}{4\sqrt{\pi n^5}}\rho^{-n}, \tag{4.16}$$

for some constant c, and for $n \geq 4$ such that $n \equiv 1 \pmod 3$. Now, by replacing n with $l = n - \frac{n-1}{4}$ in Equation 4.16, we obtain asymptotics for the (non-zero) coefficients of $\widetilde{\pi^+}(x)$. In particular, observe that after effecting this change of variable, we obtain an expression in which the exponent of l is $-\frac{5}{2}$. Therefore we have arrived at a contradiction, due to Theorem 2.4.9, since by our assumption, the sum of the contributions of the singular expansions of $\widetilde{\pi^+}(x)$ at each of its singularities (yielding the desired asymptotics for its non-zero coefficients) would be an expression in which the exponent of l is not $-\frac{5}{2}$. □

Lemma 4.2.8. *The number of unrooted augmented 4-cacti having n vertices satisfies*

$$[x^n]\widetilde{\pi^+} = \frac{3c}{4\sqrt{\pi n^5}}r^{-n}\left(2sin\left(\frac{n\pi}{2}\right) - e^{in\pi} + 1\right) \cdot (1 + O(n^{-1})), \tag{4.17}$$

where $c \doteq 1.372658593$ and $r \doteq 0.6317267748$. We also have, approximately, $[x^n]\widetilde{\pi^+} \bowtie 1.58296^n$.

Proof. Our plan is to obtain an asymptotic estimate for the coefficients of $\widetilde{\pi^+}(x)$ using Equation 4.2. First note that $r, ir, -ir, -r$ are the dominant singularities of $\widetilde{\pi^+}(x)$, since $\widetilde{\Pi^+}(x^2)$ and $\widetilde{\Pi^+}(x^4)$ are analytic at $r, ir, -ir$, and $-r$.

From Lemma 4.2.7 we have that the coefficients of $\sqrt{1 - \frac{x}{x_0}}$ vanish and therefore the actual singularity type of $\widetilde{\pi^+}$ is $X^{3/2}$.

To continue our analysis, we must first obtain a singular expansion of $\widetilde{\Pi^+}(x)$ of the form $a_0 - a_1X + a_2X^{3/2} + a_3X^2$ where $a_0 = s$, $a_1 = \gamma$, and $X = (1 - \frac{x}{x_0})$. To do this we make use of the fact that, due to Theorem 2.4.13, $\widetilde{\Pi^+}(x)$ can be written as

$$\widetilde{\Pi^+}(x) = g(x) - h(x)\sqrt{1 - \frac{x}{x_0}}.$$

By comparing the coefficients of the expansions of $\widetilde{\Pi^+}$ and $G(x, \widetilde{\Pi^+}(x))$ at $x_0 = r$ one obtains systems whose solutions give a_1, a_2, etc. This is done as follows, as indicated in the proof of Theorem 2.4.13 found in [26].

First we observe that $\widetilde{\Pi^+}(x) - y_0$, where $y_0 = g(x_0) = G(x_0, y_0)$, is of the form

$$\begin{aligned}\widetilde{\Pi^+}(x) - y_0 &= (g'(x_0)(x - x_0) + \dots) - (h(x_0) + h'(x_0)(x - x_0) + \dots)\sqrt{1 - \frac{x}{x_0}} \\ &= -x_0g'(x_0)(1 - \frac{x}{x_0}) - h(x_0)\sqrt{1 - \frac{x}{x_0}} + x_0h'(x_0)\left(1 - \frac{x}{x_0}\right)^{\frac{3}{2}} + O((1 - \frac{x}{x_0})^2)\end{aligned} \tag{4.18}$$

Then, by substituting the right-hand part of Equation 4.18 in place of $(y - y_0)$ in a suitable truncation of the analytic expansion of $G(x, y) - y$, we obtain two equations for $a_2 = -x_0h'(x_0)$ and $a_3 = -x_0g'(x_0)$. This have been determined, using the computational environment Maple, to be:

$$\begin{aligned}a_2 &= -\frac{1}{24}\frac{G_{yyyy}a_1^4 - 12G_{xyyy}a_1^2x_0 + 12G_{yyy}a_3a_1^2 + 12G_{xx}x_0^2 - 24G_{xy}a_3x_0 + 12G_{yy}a_3^2}{G_{yy}a_1} \\ a_3 &= \frac{1}{6}\frac{-G_{yyy}a_1^2 + 6G_{xy}x_0}{2G_{yy}},\end{aligned}$$

where all partial derivatives of G are evaluated at $(x_0 = r, y_0 = s)$.

One can then compute the values of a_2, a_3 using appropriate truncations of $G(x,y)$ and its derivatives accordingly. Using Maple we find that

$$a_2 \doteq 0.1353187619,$$
$$a_3 \doteq 0.4737827445.$$

Equipped with this higher-order singular expansion of $\widetilde{\Pi^+}$ we can now proceed in a manner similar to our proof of Lemma 4.2.4. From Equation 4.2, after replacing $\widetilde{\Pi^+}(x)$ with its singular expansion and $\widetilde{\Pi^+}(x^2)$, $\widetilde{\Pi^+}(x^4)$ with their regular analytic expansions at $x_0 = r$, we obtain that $\widetilde{\pi^+}(x)$'s singularities are of $X^{3/2}$ type and that $X^{3/2}$'s coefficient is $c \doteq 1.372658593$. The result then follows from singularity analysis of $\widetilde{\pi^+}/x$ and finally by multiplying with the appropriate singularities to recover the asymptotic for $\widetilde{\pi^+}$ itself. □

Once again, by rephrasing the asymptotic estimate of Lemma 4.2.8 in terms of number of Z-subgraphs, we have the following.

Proof of Theorem 4.2.1. From Corollary 4.1.13, Lemma 4.2.8, and the fact that a graph in $\mathcal{Z}_k$ with k Z-subgraphs has $4k+1$ vertices we have that:

$$|\mathcal{Z}_k| \sim \frac{3c}{\sqrt{\pi(1+4k)^5}} r^{-1-4k},$$

where $c \doteq 1.372658593$ and $r \doteq 0.6317267748$. From this we obtain the result in the statement by straightforward computations. □

Using the above we can now prove Theorem 4.2.2.

Proof of Theorem 4.2.2. Consider the generating series $\widetilde{C}(x)$ given in Theorem 4.1.9. We have that the exponential function is entire and therefore the dominant singularities of $\widetilde{C}(x)$ are the same as those of $G(x) = \widetilde{\pi^+}(x) - x$. Now, if some $H(x)$ has some singular expansion at ρ of the form

$$h_0 + \sum_{k\geq 1} h_k X^k,$$

where $X = \sqrt{1 - \frac{x}{\rho}}$, then $H(x) - x$ has a respective singular expansion of the form

$$(h_0 - \rho) \sum_{k\geq 1} h_k X^k - \rho(1-X)^2.$$

From this, we have that $G(x)$ has an asymptotic expansion, at r, of the form

$$(r-s) + (\gamma + r)X^2 + cX^3 + \dots,$$

where $X = \sqrt{1 - \frac{x}{r}}$ and γ and c are as in Lemma 4.2.8. Therefore by replacing $G(x)$ with its singular expansion at r, $\widetilde{\pi^+}(x^i)$ (for $i \geq 2$) with their analytic expansions, and x^k by $\left(1 - X^2\right)^k r^k$, we have

$$\widetilde{C}(x) = exp\left(G(r) + \sum_{k\geq 2} g_k X^k + \sum_{k\geq 2} \frac{1}{k} G(\left(1-X^2\right)^k r^k)\right), \tag{4.19}$$

where g_k are the coefficients of $G(x)$'s singular expansion at r. From this, we obtain that $\widetilde{C}(x)$ has a singular expansion at r of the form:

$$\widetilde{C}(x) = \widetilde{C}(r) + \sum_{k\geq 2} c_k X^k, \tag{4.20}$$

where the constants c_k can be computed from those of G. In particular, we compute that for the singularity r, $c_3 = \widetilde{C}(r)g_3 = \widetilde{C}(r)c$, where c is as in Lemma 4.2.8. For the asymptotic expansions of $\widetilde{C}(x)$ at $\rho \in \{ir, -ir, -r\}$, arguments analogous to the above show the corresponding coefficients of X^3 are of the form $\widetilde{C}(\rho)c$. The result then follows via the process of singularity analysis. □

CHAPTER 5

CONCLUSION

In this thesis, we studied the structure of a subset of obstructions for the families $\mathcal{A}_k(\mathcal{S})$ and all $k \in \mathbb{N}^+$. This subset was that of cactus-obstructions, that is, obstructions which are also cacti. By exploiting this structural characterisation and the tree-like nature of these obstructions, we have also produced exact enumerations of both connected, disconnected, and general cactus obstructions. We also have derived asymptotic estimates for the number of connected and general graphs in these families.

While asymptotic estimates for connected cactus-obstructions were derived in terms of both the number of vertices of a graph and its Z-subgraphs, this was not the case for disconnected obstructions, for which no asymptotic estimates are given, or general obstructions, for which only asymptotic estimates in terms of vertex counts are given. As such, a possible extension of the work presented here is the derivation of asymptotic estimates for the number of disconnected and general cactus-obstructions in terms of the number of their Z-subgraphs. A possible route towards this goal is to perform an analysis, similar to the one we have presented here, for some combinatorial species describing the same cactus-obstructions, but defined explicitly in terms of Z-subgraphs.

Another potential extension of the work presented here would be to apply a similar analysis to cactus-obstructions for other minor-closed families. Provided that these cactus-obstructions can be structurally characterised in a manner similar to the one presented in this work, an analogue of the analysis detailed here could be used to enumerate them and give bounds for the sizes of the obstruction sets for these minor-closed families.

Appendices

APPENDIX A

EXACT AND APPROXIMATE VALUES FOR $|\mathbf{OBS}(\mathcal{A}_K(\mathcal{S})) \cap \mathcal{K}|$

k	Num. of connected cactus-obstructions in $\mathbf{obs}(\mathcal{A}_{k-1}(\mathcal{S}))$	Estimate	Relative Error
1	1	0.4130830925	0.5869169075
2	1	0.5966766188	0.4033233812
3	3	1.494065976	0.5019780080
4	7	4.797209845	0.3146843079
5	25	17.76010980	0.2895956080
6	88	72.11518546	0.1805092561
7	366	312.4385507	0.1463427577
8	1583	1420.226537	0.1028259400
9	7336	6699.170415	0.08680883111
10	34982	32542.32341	0.06974091218
11	172384	$1.619048198\ 10^{5}$	0.06078974963
12	867638	$8.216440698\ 10^{5}$	0.05301050692
13	4452029	$4.240012280\ 10^{6}$	0.04762249302
14	23194392	$2.219486523\ 10^{7}$	0.04309346716
15	122462546	$1.176245371\ 10^{8}$	0.03950602905
16	653957197	$6.301181455\ 10^{8}$	0.03645353489
17	3527218134	$3.407732639\ 10^{9}$	0.03387527804
18	19192275883	$1.858505942\ 10^{10}$	0.03163858543
19	105248481503	$1.021238442\ 10^{11}$	0.02968819365
20	581223149532	$5.649685636\ 10^{11}$	0.02796617085
21	3230039198628	$3.144650462\ 10^{12}$	0.02643582066
22	18053111982952	$1.760060272\ 10^{13}$	0.02506544359
23	101426901301489	$9.900976933\ 10^{13}$	0.02383127098
24	572554846192811	$5.595500612\ 10^{14}$	0.02271360567
25	3246191706162233	$3.175760276\ 10^{15}$	0.02169663297
26	18478844801342495	$1.809509060\ 10^{16}$	0.02076721809
27	105581213907494538	$1.034786199\ 10^{17}$	0.01991447079
28	605329494353309352	$5.937500056\ 10^{17}$	0.01912923277
29	3481649579280451060	$3.417574139\ 10^{18}$	0.01840375906
30	20084998303567318415	$1.972886207\ 10^{19}$	0.01773145433
31	116189504986232518358	$1.142018903\ 10^{20}$	0.01710666295
32	673896759853960666124	$6.627609512\ 10^{20}$	0.01652450251
33	3918152650332387218639	$3.855537655\ 10^{21}$	0.01598074414
34	22833226905494054842291	$2.247995807\ 10^{22}$	0.01547170014
35	133350049991009834558718	$1.313505804\ 10^{23}$	0.01499414211
36	780379656729571601182290	$7.690288553\ 10^{23}$	0.01454522975
37	4575692800123975913062523	$4.511072775\ 10^{24}$	0.01412245704
38	26878259957579427590302227	$2.650939341\ 10^{25}$	0.01372360229
39	158160314856181220120808389	$1.560493986\ 10^{26}$	0.01334668751
40	932197271564918963765058029	$9.200880783\ 10^{26}$	0.01298994716

Table A.1: Exact and approximate values for number of graphs in $\mathbf{obs}(\mathcal{A}_k(\mathcal{S}))\cap\mathcal{K}\cap\mathcal{C}$, as computed using Maple with a precision setting of 10 digits.

n	Num. of cactus-obstructions on n vertices	Estimate	Relative Error
5	1	0.41314214750848070929	0.5868578527
20	1	0.017987152877518395869	0.9820128468
35	148	42.985035962004456173	0.7095605669
50	253673	1.6398678791005710818 10^5	0.3535504851
65	654239743	6.3020822833781193499 10^8	0.03673197029
80	1028866780	5.2246282567341113171 10^8	0.4921958370
95	4901864788225	3.2917082765326720655 10^{12}	0.3284783589
110	25859013680621594	2.1232205284702042908 10^{16}	0.1789243962
125	116217578778409174392	1.1421821683853260900 10^{20}	0.01720361171
140	174140260308755987681	1.1986798934854854481 10^{20}	0.3116583661
155	1146282277649195315360298	8.9979599260097119399 10^{23}	0.2150310508
170	7560121877197584306458759240	6.6465681387041570005 10^{27}	0.1208384940
185	40293871416858098340774697972287	3.9840431603568674333 10^{31}	0.01125332002
200	59133561827905407516512908735404	4.5676336945663207743 10^{31}	0.2275733738
215	439286840835386953744794297320186950	3.6907964791845465435 10^{35}	0.1598208402
230	3193270540030745526087659346391935756570	2.9016372784491662213 10^{39}	0.09132745201
245	18502412839113834025548699382883110825100515	1.8347677256473918108 10^{43}	0.008362994672
260	26841328298867820076729296469344792174144289	2.2033111621031308507 10^{43}	0.1791348132
275	212422772692190161266970976637786266867481217811	1.8540756926385970375 10^{47}	0.1271765859
290	1630557244232634953958050733933796638157553920114052	1.5108128320331671916 10^{51}	0.07343772348
305	992862824042406919715842467813886037577468388376167336 7	9.8625598574362581587 10^{54}	0.006654331233
320	14298022059230299644165959911981633085973571257483252323	1.2186449864568687665 10^{55}	0.1476828047
335	1176431861060954030860376930795872662910013024666518302796 80	1.0521801991614768935 10^{59}	0.1056173869
350	934998443003615751719022027701742824512871432599272598915113437	8.7756338787492998657 10^{62}	0.06142796871
365	5883779653238784438352904063711675899099019634937389816781964942533	5.8512686264550948584 10^{66}	0.005525534421
380	8430232120297086779564782520108201191221046170631704611134220702680	7.3711645754415786948 10^{66}	0.1256273146
395	71213637058553975800924877989850909638753394607366396427431213943857438	6.4781701483649125420 10^{70}	0.09031887256

Table A.2: Exact and approximate values for graphs on n vertices belonging to $\bigcup_{k\in\mathbb{N}^+} \mathbf{obs}(\mathcal{A}_k(\mathcal{S}))\cap\mathcal{K}$, as computed using Maple with a precision setting of 20 digits. Error values truncated to their 10 first digits.

k	Num. of disconnected cactus-obstructions in $\mathbf{obs}(\mathcal{A}_{k-1}(\mathcal{S}))$
2	1
3	2
4	6
5	16
6	58
7	195
8	790
9	3254
10	14804
11	67886
12	331190
13	1625824
14	8293433
15	42480079
16	223323793
17	1177824147
18	6332855124
19	34127357788
20	186659744847
21	1022933862466
22	5672080094063
23	31502392564219
24	176648460926642
25	991915348184998
26	5614278525919369
27	31815766997056353
28	181508189558402364
29	1036615871209001977
30	5954191129636943667

Table A.3: Exact values for disconnected graphs in $\mathbf{obs}(\mathcal{A}_k(\mathcal{S})) \cap \mathcal{K}$, as computed using Maple.

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