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Graph-theoretical enumeration and digital expansions: an analytic approach

Dissertation*

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Preface

Analytical tools certainly belong to the most powerful methods in combinatorics and number theory. Especially the use of generating functions has applications to a whole variety of questions of an enumerative kind.
Besides their obvious theoretical value, enumeration problems, especially in connection with graphs, have proved to be of a certain interest in other parts of science, such as chemistry and physics. For instance, graphs provide a simple and understandable yet powerful tool to describe the structure of molecules. So it is not surprising that some problems of enumerative type are of interest in chemistry – in theory as well as in practice.
The first part of this thesis is devoted to the study of so-called "topological indices", whose history begins in the middle of the 20th century, when the connection between physicochemical properties and certain combinatorial quantities was discovered. Since that time, several hundreds of papers dealing with the mathematical and chemical properties of these quantities have been written. Nevertheless, a lot of open questions remain, some of which are discussed and solved within this thesis.
The second part is devoted to two problems arising from the study of digital systems. Despite their important role in the development of number theory and mathematics in general, the investigation of digital representations and their arithmetical properties has not become very popular before the second half of the 20th century. The arithmetical structure of digitally restricted sets was specifically studied in a series of papers by Erdős, Mauduit and Sárközy in the 90's. Here, we are going to consider two specific problems dealing with sets of natural numbers given by restrictions on their digital expansions.
Even though the two parts of this thesis seem to have not much in common, they are in fact methodologically connected. Combinatorial tools, the use of generating functions and of several asymptotic methods will appear frequently within both parts. Especially chapters 2 and 3 will show how closely graph theory and number theory can be related – it is certainly one of the most fascinating aspects of mathematics how different fields and methods interact.
At this point, I want to thank all people who contributed directly or indirectly to the making of this thesis; in particular, my thanks go to my advisor, Professor Robert Tichy, for his valuable support, and to my reviewer Jörg Thuswaldner. Furthermore, I am grateful to my colleagues Volker Ziegler, Philipp Mayer and Manfred Madritsch for the bright and pleasant working climate, and to my co-authors Elmar Teufl, Hua Wang and Gang Yu. I am also highly indebted to the Austrian Science Fund for the financial support which enabled me to write this thesis. Finally, special thanks go to Gunther Schweitzer, whose delicacies not only sweetened up my day several times, but also led to the investigations of chapter 7.

Part I

The combinatorics of graph-theoretical indices

Chapter 1

Introduction and historical notes

There is a variety of quantities to describe the structure of graphs, such as the diameter, radius, minimal and maximal degrees, the eigenvalues of a graph, planarity of graphs, and others. In applications, such as molecular chemistry, where graphs are taken as simple mathematical models for complex molecular structures, it has proven useful to define several so-called “topological indices”. Formally, a topological index is mainly a map from the set of graphs to the real numbers. The purpose of a topological index is a quantification of structural properties in a sufficiently large scale.
The notion of a “topological” index appears first in a paper of the Japanese chemist Hosoya [49], who investigated the surprising relation between the physicochemical properties of a molecule and the number of its independent edge subsets (matchings). For instance, Hosoya was able to prove a relation between the number of matchings (which is called the “Hosoya index” in his honor now) of a molecular graph and the boiling point or the heat of vaporization.
However, he was not the first to explore such a property. In 1947, Harold Wiener [110] studied the relation between the sum of distances in a graph and the chemical properties of the corresponding molecules. This index is known as the Wiener index of a graph now – it will be the subject of investigation of the first three chapters of this thesis. The Wiener index $W(G)$ of a graph G is defined by

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u, v), \tag{1.1}$$

where $d_G(u, v)$ denotes the distance of u and v. Obviously, $W(G)/\binom{|V(G)|}{2}$ gives the average distance between the vertices of G. There is a lot of mathematical and chemical literature on the Wiener index, especially on the Wiener index of trees – [19] gives a summary of known results and open problems and conjectures.
Further topological indices include the Merrifield-Simmons index (the number of independent vertex subsets of a graph), the Randić index (defined as the sum of $(\deg u \deg v)^{-1/2}$ over all edges (u, v)) or the number of connected subgraphs of a graph (which was called the ρ-index by Merrifield and Simmons [82]). A typical property of all these indices is the fact that the trees of extremal (minimal/maximal) index, given the number of vertices, are the star and the path.
For example, Prodinger and Tichy [93] were able to prove that the inequality

$$F_{n+2} = \sigma(P_n) \leq \sigma(T) \leq \sigma(S_n) = 2^{n-1} + 1 \tag{1.2}$$

holds for all trees T with n vertices, where $\sigma(T)$ is the Merrifield-Simmons index (which was introduced by them in a mathematical context before the chemical work of Merrifield and Simmons), P_n is the path and S_n the star with n vertices. The fact that the number of independent vertex subsets of a path is exactly the Fibonacci number F_{n+2} is the reason why Prodinger and Tichy used the name “Fibonacci number” of a graph.
Apart from their obvious graph-theoretical value, these indices provide a useful tool in theoretical chemistry as well as in practical applications. They are used as structure descriptors for predicting

physicochemical properties of organic compounds (often those significant for pharmacology, agriculture, environment-protection, etc.). For instance, the biochemical community has been using the Wiener index and others to correlate a compound's molecular graph with experimentally gathered data regarding the compound's characteristics. In the drug design process, one wants to construct chemical compounds with certain properties, so the basic idea is to construct chemical compounds from the most common molecules so that the resulting compound has the expected index. For example, larger aromatic compounds can be made from fused benzene rings as follows (Figure 1.1):

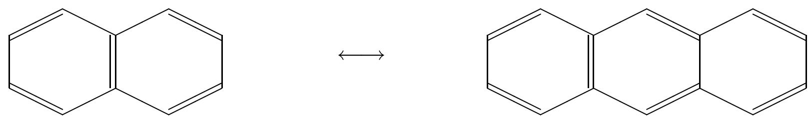

Figure 1.1: Larger aromatic compounds can be made from fused benzene rings.

Compounds with different structures (and different Wiener indices), even with the same chemical formula, can have different properties. For example, cocaine and scopolamine, both with chemical formula $C_{17}H_{21}NO_4$, have different properties and different Wiener indices. Hence it is indeed important to study the structure (and thus the various indices) of the molecular graph besides the chemical formula.

Bearing this in mind, it is certainly a reasonable question to ask for a construction to obtain molecules given a specific index. These inverse problems have been investigated – from an algorithmic point of view – in [70] for instance. A question posed by Lepović and Gutman asks for all values that are the Wiener index of some tree – the solution of this problem and a related one will be the topic of the following two chapters.

Another problem of chemical interest is to determine the average behavior of topological indices. One reason for the importance of this problem is that one wants to define a "normalized" index, which is the index of a graph belonging to a certain class (typically, the class of trees) divided by the average index of all graphs of the class with a certain number of vertices. For this purpose, it is necessary to compute the average number as easily as possible or at least to give the asymptotic behavior. Problems of this type will be considered in chapters 4 and 5.

In chapter 6, we will ask for the correlation of the cited topological indices for trees. The results of this chapter suggest intimate relations between the Hosoya- and Merrifield-Simmons-index resp. the Wiener index and number of subtrees, which are not fully understood yet.

In chapter 7, graph-theoretical indices for classes of self-similar trees are considered. It turns out that there are some interesting connections to other aspects of these graph classes and to the theory of dynamical systems.

In all of the following chapters, we are going to use the graph-theoretical notation from [18].

Chapter 2

A class of trees and its Wiener index

As was explained before, the inverse Wiener index problem asks for a way to construct a graph from a certain class, given its Wiener index. Goldman et al. [38] solved this problem for general graphs: they showed that for every positive integer $n \neq 2, 5$ there exists a graph G such that the Wiener index of G is n.
Since the majority of the chemical applications of the Wiener index deals with chemical compounds that have acyclic organic molecules, whose molecular graphs are trees, the inverse Wiener index problem for trees attracts more attention and, actually, most of the prior work on Wiener indices deals with trees (cf. [19]). For trees, the inverse problem becomes more complicated. Gutman and Yeh [45] solved the problem for bipartite graphs and conjectured that, for all but a finite set of integers n, one can find a tree with Wiener index n.
Lepović and Gutman [68] checked the integers up to 1206 and found that the following numbers are not Wiener indices of any trees:

2, 3, 5, 6, 7, 8, 11, 12, 13, 14, 15, 17, 19, 21, 22, 23, 24, 26, 27, 30, 33, 34, 37, 38, 39, 41, 43, 45, 47, 51, 53, 55, 60, 61, 69, 73, 77, 78, 83, 85, 87, 89, 91, 99, 101, 106, 113, 147, 159.

They claimed that the listed were the only "forbidden" integers and posed the following conjecture.

Conjecture. There are exactly 49 positive integers that are not Wiener indices of trees, namely the numbers listed above.

A recent computational experiment by Ban, Bespamyatnikh and Mustafa [3] shows that every integer $n \in [10^3, 10^8]$ is the Wiener index of some caterpillar tree. Thus, the conjecture is proved if one is able to show that every integer greater than 10^8 is the Wiener index of a tree.
The proof of conjecture 2 will be the main result of this chapter. It was achieved independently by Wang and Yu in [108] as well by different means. To prove our result, we investigate a class of trees we will call "star-like". It is the class of all trees with diameter ≤ 4. However, there is another class of trees – the trees with only one vertex of degree > 2 – that is also called "star-like" in some papers, e.g. [44]. The star-like trees we are considering here have been studied in [62] for another topological index, and they turned out to be quite useful in that context. Here, we will even be able to give an easy and explicit construction of a tree T, given its Wiener index $W(T)$.

Definition 2.1 Let $(c_1, \ldots, c_d)$ be a partition of n. The star-like tree assigned to this partition is the tree shown in Figure 2, where $v_1, \ldots, v_d$ have degree $c_1, \ldots, c_d$ respectively. It has exactly n edges. The tree itself is denoted by $S(c_1, \ldots, c_d)$, its Wiener index by $W(c_1, \ldots, c_d)$.

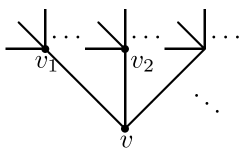

Figure 2.1: A star-like tree.

Lemma 2.1

$$W(c_1, \ldots, c_d) = 2n^2 - (d-1)n - \sum_{i=1}^{d} c_i^2. \tag{2.1}$$

Proof. For all pairs (x, y) of vertices in $S(c_1, \ldots, c_d)$, we have $d(x, y) \leq 4$. Thus we only have to count the number of pairs (x, y) with $d(x, y) = k$, for $1 \leq k \leq 4$. We divide the vertices into three groups - the center v, the neighbors $v_1, \ldots, v_d$ of the center, and the leaves $w_1, \ldots, w_{n-d}$.

- Obviously, there are n pairs with $d(x, y) = 1$.
- All pairs of the form $(x, y) = (v, w_i)$, $(x, y) = (v_i, v_j)$ or $(x, y) = (w_i, w_j)$ (where w_i, w_j are neighbors of the same v_k) satisfy $d(x, y) = 2$. There are
$$(n-d) + \binom{d}{2} + \sum_{i=1}^{d} \binom{c_i - 1}{2}$$
such pairs.
- For all pairs of the form $(x, y) = (v_i, w_j)$ with $v_i \not\sim w_j$ we have $d(x, y) = 3$. The number of these pairs is
$$\sum_{i=1}^{d} (n - d - c_i + 1).$$
- Finally, $d(w_i, w_j) = 4$ if w_i, w_j are not neighbors of the same v_k. There are
$$\binom{n-d}{2} - \sum_{i=1}^{d} \binom{c_i - 1}{2}$$
such pairs.

Summing up, the Wiener index of $S(c_1, \ldots, c_d)$ is

$$\begin{aligned} W(c_1, \ldots, c_d) = n &+ 2\left((n-d) + \binom{d}{2} + \sum_{i=1}^{d} \binom{c_i - 1}{2}\right) + 3\sum_{i=1}^{d}(n - d - c_i + 1) \\ &+ 4\left(\binom{n-d}{2} - \sum_{i=1}^{d} \binom{c_i - 1}{2}\right). \end{aligned}$$

Simple algebraical manipulations yield

$$\begin{aligned}
W(c_1,\dots,c_d) &= n + 2(n-d) + d^2 - d + \sum_{i=1}^{d}(c_i^2 - 3c_i + 2) + 3d(n-d+1) \\
&\quad - 3\sum_{i=1}^{d} c_i + 2(n-d)(n-d-1) - 2\sum_{i=1}^{d}(c_i^2 - 3c_i + 2) \\
&= 2n^2 + n + 2d - dn - \sum_{i=1}^{d}(c_i^2 + 2) \\
&= 2n^2 - (d-1)n - \sum_{i=1}^{d} c_i^2.
\end{aligned}$$

■

2.1 An extremal result

Clearly, as the star is the tree of minimal Wiener index, it is also the star-like tree of minimal Wiener index. Now, this section will be devoted to the characterization of the star-like tree of maximal Wiener index. First, we note the following:

Lemma 2.2 If a partition contains two parts c_1, c_j such that $c_i \geq c_j + 2$, the corresponding Wiener index increases if they are replaced by $c_i - 1, c_j + 1$.

Proof. Obviously, n and d remain unchanged. The only term that changes is the sum $\sum_i c_i^2$, and the difference is

$$c_i^2 + c_j^2 - (c_i - 1)^2 - (c_j + 1)^2 = 2(c_i - c_j - 1) > 0.$$

■

Therefore, if a partition satisfies the condition of the lemma, its Wiener index cannot be maximal. So we only have to consider partitions consisting of two different parts k and $k+1$. Let $r < d$ be the number of $k+1$'s and $d-r$ the number of k's. Then $n = kd + r$ and we have to maximize

$$2n^2 + n - dn - r(k+1)^2 - (d-r)k^2.$$

We neglect the constant part $2n^2+n$ and arrive – after some easy manipulations – at the minimization of the expression

$$n(k+d) + r(k+1)$$

subject to the restrictions that $kd + r = n$ and $r < d$. We assume that $k \leq d$ – otherwise, we may change the roles of k and d, decreasing the term $r(k+1)$. Next, we note that $k+d$ is an integer and $r(k+1) = kr + r < kd + r = n$. Therefore, the expression can only be minimal if $k+d$ is. But

$$k + d = \left\lfloor \frac{n}{d} \right\rfloor + d = \left\lfloor \frac{n}{d} + d \right\rfloor,$$

and the function $f(x) = \frac{n}{x} + x$ is convex and attains its minimum at $x = \sqrt{n}$. So $k+d$ is minimal if either $d = \lfloor \sqrt{n} \rfloor$ or $d = \lceil \sqrt{n} \rceil$ (and perhaps, for other values of d, too). If we write $n = Q^2 + R$, where $0 \leq R \leq 2Q$, we see that the minimum of $k+d$ is

$$\begin{cases} 2Q & R < Q \\ 2Q+1 & Q \leq R \leq 2Q. \end{cases}$$

In the first case, we write $d = Q + S$ and $k = Q - S$. Then we have $r = S^2 + R$ and thus

$$r(k+1) = (S^2 + R)(Q - S + 1) = -S^3 + (Q+1)S^2 - RS + (Q+1)R.$$

For $1 \leq S \leq Q$, we have

$$S^2 - (Q+1)S + R = (S - (Q+1)/2)^2 - (Q+1)^2/4 + R \leq (Q-1)^2/4 - (Q+1)^2/4 + R = R - Q < 0$$

and thus

$$-S^3 + (Q+1)S^2 - RS > 0.$$

So the minimum in this case is obtained when $S = 0$ or $k = d = Q = \lfloor\sqrt{n}\rfloor$. Analogously, we write $d = Q + 1 + S$ and $k = Q - S$ in the second case. Again, we obtain the minimum for $S = 0$ or $d = Q + 1 = \lceil\sqrt{n}\rceil$ and $k = Q = \lfloor\sqrt{n}\rfloor$. Summing up, we have the following theorem:

Theorem 2.3 *The star-like tree with n edges of maximal Wiener index is the tree corresponding to the partition*

$$(k, \dots, k, k+1, \dots, k+1),$$

where $k = \lfloor\sqrt{n}\rfloor$. The part k appears $k^2 + k - n$ times if $k^2 + k > n$ and $k^2 + 2k + 1 - n$ times otherwise. The part $k+1$ appears $n - k^2$ times if $k^2 + k > n$ and $n - k^2 - k$ times otherwise.

Remark. A short calculation shows that the maximal Wiener index of a star-like tree is asymptotically

$$2n^2 - 2n\sqrt{n} + n + O(\sqrt{n}).$$

2.2 The inverse problem

Lepović and Gutman [68] conjectured that there are only finitely many "forbidden values" for the Wiener index of trees. In particular, they claimed that all natural numbers, except 2, 3, 5, 6, 7, 8, 11, 12, 13, 14, 15, 17, 19, 21, 22, 23, 24, 26, 27, 30, 33, 34, 37, 38, 39, 41, 43, 45, 47, 51, 53, 55, 60, 61, 69, 73, 77, 78, 83, 85, 87, 89, 91, 99, 101, 106, 113, 147 and 159, are Wiener indices of trees. By an extensive computer search, they were able to prove that any other "forbidden value" must exceed 1206.

This chapter deals with the proof of their conjecture. We will even show a stronger result: every integer ≥ 470 is the Wiener index of a star-like tree. By Lemma 2.1, this is equivalent to showing that every integer ≥ 470 is of the form

$$2n^2 - (d-1)n - \sum_{i=1}^{d} c_i^2$$

for some partition $(c_1, \dots, c_d)$ of n. First, we consider the special case of partitions of the form

$$p(l,k) = (\underbrace{2, \dots, 2}_{l \text{ times}}, \underbrace{1, \dots, 1}_{k \text{ times}}).$$

By Lemma 2.1, the Wiener index of the corresponding star-like tree is

$$w(l,k) = 2 \cdot (2l+k)^2 - (l+k-1) \cdot (2l+k) - (4l+k) = 6l^2 + (5k-2)l + k^2.$$

Next, we need a simple lemma similar to Lemma 2.2.

Lemma 2.4 If a partition contains the part $c \geq 2$ twice, and if these parts are replaced by $c+1$ and $c-1$, the corresponding Wiener index decreases by 2.

Proof. Obviously, n and d remain unchanged. The only term that changes is the sum $\sum_i c_i^2$, and the difference is $(c+1)^2 + (c-1)^2 - 2c^2 = 2$. ∎

Definition 2.2 Replacing a pair (c, c) by $(c+1, c-1)$ is called a "splitting step". By $s(l)$, we denote the number of splitting steps that one can take beginning with a sequence of l 2's.

Applying Lemma 2.4 $s(l)$ times, beginning with the partition $p(l, k)$, one can construct star-like trees of Wiener index $w(l, k), w(l, k) - 2, \ldots, w(l, k) - 2s(l)$. Our next goal is to show that there is a $c > 1$ such that $s(l) > cl$ if l is large enough (indeed, one can prove that $s(l)/l$ tends to infinity for $l \to \infty$).

Lemma 2.5 For all $l \geq 0$, $s(l) \geq \frac{19l-77}{16}$.

Proof. First, $\lfloor \frac{l}{2} \rfloor \geq \frac{l-1}{2}$ splitting steps can be taken using pairs of 2's. Then, $\lfloor \frac{l}{4} \rfloor \geq \frac{l-3}{4}$ splitting steps can be taken using pairs of 3's. Now, we may split the 4's and 2's ($\lfloor \frac{l}{8} \rfloor \geq \frac{l-7}{8}$ pairs each), and finally the 5's and 3's ($\lfloor \frac{l}{16} \rfloor \geq \frac{l-15}{16}$ and $\lfloor \frac{l}{8} \rfloor \geq \frac{l-7}{8}$ pairs respectively). This gives a total of at least $\frac{19l-77}{16}$ splitting steps, all further possible steps are ignored. ■

It is not difficult to determine $s(l)$ explicitly for small l. We obtain the following table:

l	2	3	4	5	6	7	8	9	10	11	12	13	14	15
$s(l)$	1	1	3	4	4	7	9	10	10	14	17	19	20	20
l	16	17	18	19	20	21	22	23	24	25	30	50	75	100
$s(l)$	25	29	32	34	35	35	41	46	50	53	69	155	283	445

Table 2.1: Table of $s(l)$.

Trivially, $s(l)$ is a non-decreasing function. Therefore, this table, together with Lemma 2.5, shows that $s(l) \geq l + 5$ for $l \geq 12$ and $s(l) \geq l + 9$ for $l \geq 16$.

Now, we are able to prove the following propositions:

Proposition 2.6 Every even integer $W \geq 1506$ is the Wiener index of a star-like tree.

Proof. It was mentioned that one can always construct star-like trees of Wiener index $w(l, k)$, $w(l, k) - 2, \ldots, w(l, k) - 2s(l)$. For $k = 0, 2, 4, 6, 8, 10$ and $l = x + 1 - k/2$, we have $w(l, k) = 6x^2 + (10 - k)x + 4$. For $x \geq 16$, $l \geq 12$ and thus $s(l) \geq l + 5 \geq l + k/2 = x + 1$. Thus, all even numbers in the interval

$$[6x^2 + (10 - k)x + 4 - 2(x + 1), 6x^2 + (10 - k)x + 4] = [6x^2 + (8 - k)x + 2, 6x^2 + (10 - k)x + 4]$$

are Wiener indices of star-like trees. The union of these intervals (over k) is

$$[6x^2 - 2x + 2, 6x^2 + 10x + 4] = [6x^2 - 2x + 2, 6(x + 1)^2 - 2(x + 1)]$$

Finally, the union of these intervals (over all $x \geq 16$) is $[1506, \infty)$. Thus, all even integers ≥ 1506 are Wiener indices of star-like trees. ■

Proposition 2.7 Every odd integer $W \geq 2385$ is the Wiener index of a star-like tree.

Proof. First, let x be an even number, and let $k = 15, 1, 11, 21, 7, 17$ and $l = x - 6, x, x - 4$, $x - 8, x - 2, x - 6$ respectively. Then we obtain the following table:

k	l	$w(l, k)$
15	$x - 6$	$6x^2 + x + 3$
1	x	$6x^2 + 3x + 1$
11	$x - 4$	$6x^2 + 5x + 5$
21	$x - 8$	$6x^2 + 7x + 1$
7	$x - 2$	$6x^2 + 9x + 7$
17	$x - 6$	$6x^2 + 11x + 7$

For $x \geq 20$, we have $l \geq 12$ in all cases and thus $s(l) \geq l+5$. Using the same argument as in the previous proof, all odd numbers (as x is even, the terms $w(l,k)$ are indeed all odd) in the following intervals are Wiener indices of star-like trees:

k	l	Interval
15	$x-6$	$[6x^2-x+5, 6x^2+x+3]$
1	x	$[6x^2+x-9, 6x^2+3x+1]$
11	$x-4$	$[6x^2+3x+3, 6x^2+5x+5]$
21	$x-8$	$[6x^2+5x+7, 6x^2+7x+1]$
7	$x-2$	$[6x^2+7x+1, 6x^2+9x+7]$
17	$x-6$	$[6x^2+9x+9, 6x^2+11x+7]$

The union over all these intervals (considering odd numbers only) is $[6x^2-x+5, 6x^2+11x+7]$.

Now, on the other hand, let x be odd, and take $k = 3, 13, 23, 9, 19, 5$ and $l = x-1, x-5, x-9, x-3, x-7, x-1$ respectively. Then we obtain the following table:

k	l	$w(l,k)$
3	$x-1$	$6x^2+x+2$
13	$x-5$	$6x^2+3x+4$
23	$x-9$	$6x^2+5x-2$
9	$x-3$	$6x^2+7x+6$
19	$x-7$	$6x^2+9x+4$
5	$x-1$	$6x^2+11x+8$

Now, for $x \geq 21$, we have $l \geq 12$ in all cases and thus $s(l) \geq l+5$; furthermore, $x-3 \geq 18$ and thus $s(x-3) \geq (x-3)+9 = x+6$. Therefore, all odd numbers in the following intervals are Wiener indices of star-like trees:

k	l	Interval
3	$x-1$	$[6x^2-x-6, 6x^2+x+2]$
13	$x-5$	$[6x^2+x+4, 6x^2+3x+4]$
23	$x-9$	$[6x^2+3x+6, 6x^2+5x-2]$
9	$x-3$	$[6x^2+5x-6, 6x^2+7x+6]$
19	$x-7$	$[6x^2+7x+8, 6x^2+9x+4]$
5	$x-1$	$[6x^2+9x, 6x^2+11x+8]$

The union over all these intervals (considering odd numbers only) is $[6x^2-x-6, 6x^2+11x+8]$. Combining the two results, we see that for any $x \geq 20$, all odd integers in the interval

$$[6x^2-x+4, 6x^2+11x+8] = [6x^2-x+4, 6(x+1)^2-(x+1)+3]$$

are Wiener indices of star-like trees. The union of these intervals (over all $x \geq 20$) is $[2384, \infty)$. ■

It is not difficult to check (by means of a computer) that all integers $470 \leq W \leq 2384$ can be written as $W = W(S)$ for a star-like tree S with ≤ 40 edges. Therefore, we obtain

Theorem 2.8 *The list of Lepović and Gutman is complete, and all integers not appearing in their list are Wiener indices of trees.*

Remark. There are only 55 further values which are Wiener indices of trees, but not of star-like trees, namely 35, 50, 52, 56, 68, 71, 72, 75, 79, 92, 94, 98, 119, 123, 125, 127, 129, 131, 133, 135, 141, 143, 149, 150, 152, 156, 165, 181, 183, 185, 187, 193, 195, 197, 199, 203, 217, 219, 257, 259, 261, 263, 267, 269, 279, 281, 285, 293, 351, 355, 357, 363, 369, 453 and 469.

Example 2.1 Suppose we want to construct a star-like tree of Wiener index 9999. This number is odd, and it is contained in the interval

$$[9564 = 6 \cdot 40^2 - 40 + 4, 6 \cdot 40^2 + 11 \cdot 40 + 8 = 10048].$$

40 is even, so we use the first case of proposition 2.7. 9999 is contained in

$$[9969 = 6 \cdot 40^2 + 9 \cdot 40 + 9, 6 \cdot 40^2 + 11 \cdot 40 + 7 = 10047],$$

so we start with the partition $(2, \ldots, 2, 1, \ldots, 1)$ consisting of $40 - 6 = 34$ 2's and 17 1's. As $10047 - 9999 = 48$, 24 splitting steps are necessary. After 17 splitting steps, we obtain the partition containing 17 3's and 34 1's. After 7 further steps, we arrive at the partition

$$(\underbrace{4, \ldots, 4}_{7 \text{ times}}, \underbrace{3, \ldots, 3}_{3 \text{ times}}, \underbrace{2, \ldots, 2}_{7 \text{ times}}, \underbrace{1, \ldots, 1}_{34 \text{ times}}).$$

Indeed, the Wiener index of the corresponding star-like tree with 85 edges is

$$2 \cdot 85^2 - (51 - 1) \cdot 85 - 7 \cdot 4^2 - 3 \cdot 3^2 - 7 \cdot 2^2 - 34 \cdot 1^2 = 9999.$$

Remark. The proof of the theorem generalizes in some way to the modified Wiener index of the form

$$W_\lambda(G) := \sum_{\{u,v\} \subseteq V(G)} d_G(u, v)^\lambda$$

for positive integers λ. Using essentially the same methods together with the fact that $s(l)$ grows faster than any linear polynomial, one can show the following: if there is some star-like tree T such that $W(T) \equiv r \mod 2^\lambda(2^\lambda - 1)$, then all members of the residue class r modulo $2^\lambda(2^\lambda - 1)$ – with only finitely many exceptions – are Wiener indices of trees. For $\lambda = 2, 3, 5, 6, 7, 9, 10$, this implies that all integers, with finitely many exceptions, can be written as $W_\lambda(T)$ for some star-like tree T, as all residue classes modulo $2^\lambda(2^\lambda - 1)$ are covered. Unfortunately, for $\lambda = 4$ and all other multiples of 4, this is not the case any more.

2.3 The average Wiener index of a star-like tree

Finally, one might ask for the average size of $W(T)$ for a star-like tree with n edges. First we note that the correlation between partitions of n and star-like trees with n edges is almost bijective: given a tree of diameter 4, the center is uniquely defined, being the center of a path of length 4. For trees of diameter 3 (which have the form of "double-stars", there are two possible centers, giving the representations $S(k, 1, \ldots, 1)$ and $S(n + 1 - k, 1, \ldots, 1)$. The star (with diameter 2) has the two representation $S(n)$ and $S(1, \ldots, 1)$. It follows that there are only $\lfloor \frac{n}{2} \rfloor$ exceptional trees belonging to two different partitions. This number, as well as the sum of their Wiener indices, is small compared to $p(n)$, So, we mainly have to determine the asymptotics of

$$\frac{1}{p(n)} \left(\sum_c \left(2n^2 - (d - 1)n - \sum_{i=1}^d c_i^2 \right) \right),$$

where the sum goes over all partitions c of n and d denotes the length of c. For the average length of a partition, an asymptotic formula is known (see [55]):

$$\frac{1}{p(n)} \sum_c d = \frac{\sqrt{n}}{\nu} \Big(\log n + 2\gamma - 2 \log(\nu/2) \Big) + O\Big((\log n)^3 \Big), \tag{2.2}$$

where $\nu = \sqrt{2/3}\,\pi$ and γ is Euler's constant. Thus, our main problem is to find the asymptotics of the sum

$$\sum_c \sum_{i=1}^d c_i^2. \tag{2.3}$$

First, we have the following generating function for this expression:

Lemma 2.9 The generating function of (2.3) is given by $S(z)F(z)$, where

$$S(z) = \sum_{i=1}^{\infty} \frac{i^2 z^i}{1 - z^i}$$

is the generating function of $\sigma_2(n) = \sum_{d|n} d^2$ and

$$F(z) = \prod_{i=1}^{\infty} (1 - z^i)^{-1}$$

is the generating function of the partition function $p(n)$.

Proof. This is simply done by some algebraic transformations: the number of k's in all partitions of n is $p(n-k) + p(n-2k) + \dots$. Therefore,

$$\begin{aligned}\sum_c \sum_{i=1}^{d} c_i^2 &= \sum_{k \geq 1} k^2 \sum_{i \geq 1} p(n - ik) \\ &= \sum_{m \geq 1} \sum_{d|m} d^2 p(n-m) \\ &= \sum_{m \geq 1} \sigma_2(m) p(n-m).\end{aligned}$$

So the expression (2.3) is indeed the convolution of σ_2 and p, which proves the lemma. ■

Now, we can proceed along the same lines as in [55]. We use the following lemmas:

Lemma 2.10 (Newman [87]) Let

$$\phi(z) = \sqrt{\frac{1-z}{2\pi}} \exp\left(\frac{\pi^2}{12}\Big(-1 + \frac{2}{1-z}\Big)\right).$$

Then we have

$$|F(z)| < \exp\left(\frac{1}{1-|z|} + \frac{1}{|1-z|}\right) \tag{2.4}$$

for $|z| < 1$ and

$$F(z) = \phi(z)(1 + O(1-z)) \tag{2.5}$$

for $|1-z| \leq 2(1-|z|)$ and $|z| < 1$.

Lemma 2.11 Let

$$\psi(z) = \frac{2\zeta(3)}{(1-z)^3},$$

where $\zeta(s)$ denotes the Riemann ζ-function. Then we have

$$|S(z)| \leq \frac{4}{(1-|z|)^3} \tag{2.6}$$

for $|z| < 1$ and

$$S(z) = \psi(z) + O(|1-z|^{-2}) \tag{2.7}$$

for $|1-z| \leq 2(1-|z|)$ and $\frac{1}{3} \leq |z| < 1$.

Proof. For $|z| < 1$, we obtain

$$
\begin{aligned}
|S(z)| &\le \frac{1}{1-|z|} \sum_{i=1}^{\infty} \frac{i^2|z|^i}{1+|z|+\ldots+|z|^{i-1}} \\
&= \frac{1}{1-|z|} \sum_{i=1}^{\infty} \frac{i^2|z|^{(i+1)/2}}{|z|^{-(i-1)/2}+|z|^{-(i-1)/2+1}+\ldots+|z|^{(i-1)/2}} \\
&\le \frac{1}{1-|z|} \sum_{i=1}^{\infty} \frac{i^2|z|^{(i+1)/2}}{i} = \frac{1}{1-|z|} \sum_{i=1}^{\infty} i|z|^{(i+1)/2} \\
&= \frac{|z|}{(1-|z|)(1-\sqrt{|z|})^2} \le \frac{4}{(1-|z|)^3}.
\end{aligned}
$$

Now, let $z = e^{-u}$. By the Euler-Maclaurin summation formula, we have

$$
S(e^{-u}) = \sum_{i=1}^{\infty} \frac{i^2}{e^{iu}-1} = \int_0^{\infty} \frac{t^2}{e^{tu}-1}\,dt - \int_0^{\infty} \Big(\{t\} - \frac{1}{2}\Big) \frac{-2t+e^{ut}(2t-ut^2)}{(e^{ut}-1)^2}\,dt.
$$

Now

$$
\int_0^{\infty} \frac{t^2}{e^{tu}-1}\,dt = \frac{1}{u^3}\int_0^{\infty} \frac{s^2}{e^s-1}\,ds = \frac{1}{u^3}\int_0^{\infty} \sum_{i=1}^{\infty} s^2 e^{-is}\,ds = \frac{1}{u^3}\sum_{i=1}^{\infty}\frac{2}{i^3} = \frac{2\zeta(3)}{u^3}
$$

and, for $v = \operatorname{Re} u$,

$$
\begin{aligned}
\Big|\int_0^{\infty} \Big(\{t\} - \frac{1}{2}\Big) \frac{-2t+e^{ut}(2t-ut^2)}{(e^{ut}-1)^2}\,dt\Big| &\le \frac{1}{2}\int_0^{\infty} \left|\frac{-2t+e^{ut}(2t-ut^2)}{(e^{ut}-1)^2}\right| dt \\
&\le \frac{1}{2}\int_0^{\infty} \left|\frac{2t}{e^{ut}-1}\right| dt + \frac{1}{2}\int_0^{\infty} \left|\frac{ut^2e^{ut}}{(e^{ut}-1)^2}\right| dt \\
&\le \int_0^{\infty} \frac{t}{e^{vt}-1}\,dt + \frac{|u|}{2}\int_0^{\infty} \frac{t^2e^{vt}}{(e^{vt}-1)^2}\,dt \\
&= \frac{1}{v^2}\int_0^{\infty} \frac{s}{e^s-1}\,ds + \frac{|u|}{2v^3}\int_0^{\infty} \frac{s^2e^s}{(e^s-1)^2}\,ds \\
&= O(v^{-2}) + O(|u|v^{-3}) = O(|u|v^{-3}).
\end{aligned}
$$

If $|1-z| \le 2(1-|z|)$ and $\frac{1}{3} \le |z| < 1$, $|u|/v$ is bounded by some constant K. Therefore, the latter expression is $O(|u|^2)$. Replacing u by $-\log z = 1 - z + O(|1-z|^2)$ gives us the desired result. ■

Proposition 2.12 If $s(n) = \sum_c \sum_{i=1}^d c_i^2$ and $F(z)\psi(z) = \sum_{n=0}^{\infty} s'(n)z^n$, then

$$
s(n) = s'(n) + O\Big(n^{1/4}\exp(\pi\sqrt{2n/3})\Big). \tag{2.8}
$$

Proof. Let $\mathcal{C} = \{z \in \mathbb{C} \mid |z| = 1 - \pi/\sqrt{6n}\}$. Then, by Cauchy's residue theorem,

$$
s(n) - s'(n) = \frac{1}{2\pi i}\int_{\mathcal{C}} \frac{(FS - F\psi)(z)}{z^{n+1}}\,dz.
$$

We split $\mathcal{C}$ into two parts: $\mathcal{A} = \{z \in \mathcal{C}\ |1-z| < \pi\sqrt{2/(3n)}\}$ and $\mathcal{B} = \mathcal{C} \setminus \mathcal{A}$. On $\mathcal{A}$, we use the approximations (2.5) and (2.7) from Lemmas 2.10 and 2.11:

$$\begin{aligned}
I_{\mathcal{A}} &= \Big|\frac{1}{2\pi i}\int_{\mathcal{A}} \frac{(FS - F\psi)(z)}{z^{n+1}}\,dz\Big| \\
&\ll \int_{\mathcal{A}} \frac{|\phi(z)|}{|1-z|^2|z|^{n+1}}\,dz \\
&\ll \int_{\mathcal{A}} |1-z|^{-3/2}\exp\Big(\frac{\pi^2}{6(1-|z|)}\Big)|z|^{-n}\,dz \\
&\ll n^{3/4}\exp(\pi\sqrt{n/6})\exp(\pi\sqrt{n/6})n^{-1/2} \\
&= n^{1/4}\exp(\pi\sqrt{2n/3}).
\end{aligned}$$

Similarly, on $\mathcal{B}$, we use (2.4) together with the estimate $\psi(z), S(z) \ll (1-|z|)^{-3}$ from Lemma 2.11:

$$\begin{aligned}
I_{\mathcal{B}} &= \Big|\frac{1}{2\pi i}\int_{\mathcal{B}} \frac{(FS - F\psi)(z)}{z^{n+1}}\,dz\Big| \\
&\ll \int_{\mathcal{B}} \exp\Big(\frac{1}{|1-z|} + \frac{1}{1-|z|}\Big)\cdot\frac{1}{(1-|z|)^3}\cdot|z|^{-n}\,dz \\
&\ll \exp\Big(\sqrt{\frac{3n}{2\pi^2}} + \sqrt{\frac{6n}{\pi^2}}\Big)n^{3/2}\exp\Big(\sqrt{\frac{\pi^2 n}{6}}\Big) \\
&= \exp\Big(\frac{9+\pi^2}{\pi\sqrt{6}}\sqrt{n}\Big)n^{3/2} \\
&\ll \exp\Big(\frac{2\pi^2}{\pi\sqrt{6}}\sqrt{n}\Big) = \exp(\pi\sqrt{2n/3}).
\end{aligned}$$

Thus

$$|s(n) - s'(n)| \le I_{\mathcal{A}} + I_{\mathcal{B}} = O\Big(n^{1/4}\exp(\pi\sqrt{2n/3})\Big).$$

■

Proposition 2.13

$$s'(n) = \frac{12\sqrt{6}\zeta(3)}{\pi^3}p(n)(n^{3/2} + O(n(\log n)^2)). \tag{2.9}$$

Proof. From the definition of $s'(n)$, we have

$$s'(n) = 2\zeta(3)\sum_{k=0}^{n}\binom{k+2}{2}p(n-k).$$

We divide the sum into three parts and use the well-known estimate

$$p(n) = \frac{e^{\nu\sqrt{n}}}{4\sqrt{3}n} + O\Big(\frac{e^{\nu\sqrt{n}}}{n^{3/2}}\Big),$$

which follows directly from Rademachers asymptotic formula ([94], cf. also [55]). The first sum is

$$A_1 = \sum_{k>n/2}\binom{k+2}{2}p(n-k) \ll n^3 p(n/2) \ll n^2 e^{\nu\sqrt{n/2}},$$

the second sum is

$$\begin{aligned}
A_2 &= \sum_{n/2 \geq k > \sqrt{n}\log n/\nu} \binom{k+2}{2} p(n-k) \\
&\ll \sum_{n/2 \geq k > \sqrt{n}\log n/\nu} k^2 \frac{e^{\nu\sqrt{n-k}}}{n-k}\Big(1 + O\Big(\frac{1}{\sqrt{n-k}}\Big)\Big) \\
&\ll \frac{1}{n} e^{\nu\sqrt{n}} \sum_{k > \sqrt{n}\log n/\nu} k^2 e^{\nu(\sqrt{n-k}-\sqrt{n})} \leq \frac{1}{n} e^{\nu\sqrt{n}} \sum_{k > \sqrt{n}\log n/\nu} k^2 e^{-(\nu k)/(2\sqrt{n})} \\
&\sim \frac{1}{n} e^{\nu\sqrt{n}} \int_{\sqrt{n}\log n/\nu}^{\infty} t^2 e^{-(\nu t)/(2\sqrt{n})}\, dt = \frac{1}{n} e^{\nu\sqrt{n}} e^{-(\log n)/2} \frac{2 + \log n + (\log n)^2/4}{(\nu/(2\sqrt{n}))^3} \\
&\ll (\log n)^2 e^{\nu\sqrt{n}},
\end{aligned}$$

and the third sum, which gives the main part,

$$\begin{aligned}
A_3 &= \sum_{k \leq \sqrt{n}\log n/\nu} \binom{k+2}{2} p(n-k) \\
&= \sum_{k \leq \sqrt{n}\log n/\nu} \binom{k+2}{2} \frac{e^{\nu\sqrt{n-k}}}{4\sqrt{3}(n-k)}\Big(1 + O\Big(\frac{1}{\sqrt{n-k}}\Big)\Big) \\
&= \frac{e^{\nu\sqrt{n}}}{4\sqrt{3}n} \sum_{k \leq \sqrt{n}\log n/\nu} \binom{k+2}{2} e^{\nu(\sqrt{n-k}-\sqrt{n})}\Big(1 + O\Big(\frac{\log n}{\sqrt{n}}\Big)\Big) \\
&= \frac{e^{\nu\sqrt{n}}}{4\sqrt{3}n} \sum_{k \leq \sqrt{n}\log n/\nu} \binom{k+2}{2} e^{-(\nu k)/(2\sqrt{n}) + O(k^2 n^{-3/2})}\Big(1 + O\Big(\frac{\log n}{\sqrt{n}}\Big)\Big) \\
&= \frac{e^{\nu\sqrt{n}}}{4\sqrt{3}n} \sum_{k \leq \sqrt{n}\log n/\nu} \binom{k+2}{2} e^{-(\nu k)/(2\sqrt{n})}\Big(1 + O\Big(\frac{(\log n)^2}{\sqrt{n}}\Big)\Big).
\end{aligned}$$

The last sum has the form

$$\sum_{k=0}^{N} \binom{k+2}{2} q^k = \frac{1}{2(1-q)^3}\Big(2 - q^{N+1}(N^2(1-q)^2 + N(1-q)(5-3q) + 2(q^2-3q+3))\Big)$$

with $N = \sqrt{n}\log n/\nu + O(1)$, $q = e^{-\nu/(2\sqrt{n})} = 1 - \nu/(2\sqrt{n}) + O(n^{-1})$ and $q^N \sim 1/\sqrt{n}$, which gives us

$$A_3 = \frac{e^{\nu\sqrt{n}}}{4\sqrt{3}n} \cdot \frac{8n^{3/2}}{\nu^3}\Big(1 + O\Big(\frac{(\log n)^2}{\sqrt{n}}\Big)\Big) = p(n) \cdot \frac{6\sqrt{6}n^{3/2}}{\pi^3}\Big(1 + O\Big(\frac{(\log n)^2}{\sqrt{n}}\Big)\Big).$$

Summing A_1, A_2 and A_3 yields the desired result. ■

Combining Propositions 2.12 and 2.13 with the expression (2.2), we arrive at our final result:

Theorem 2.14 *The average Wiener index* $\mathrm{av}(n)$ *of a star-like tree with* n *edges is given by*

$$\mathrm{av}(n) = 2n^2 - \frac{\sqrt{6}n^{3/2}}{2\pi}\Big(\log n + 2\gamma - \log\frac{\pi^2}{6} + \frac{24\zeta(3)}{\pi^2}\Big) + O(n(\log n)^3). \tag{2.10}$$

Remark. We have noted that the maximal Wiener index of a star-like tree is aymptotically $2n^2 - 2n\sqrt{n} + n + O(\sqrt{n})$. On the other hand, the minimal Wiener index is n^2. This shows that "most" star-like trees have a Wiener index close to the maximum.

Chapter 3

Molecular graphs and the inverse Wiener index problem

In the preceding chapter, we gave, among other results, a solution of the inverse Wiener index problem for trees. However, the molecular graphs of most practical interest have natural restrictions on their degrees corresponding to the valences of the atoms and are typically trees or have hexagonal or pentagonal cycles ([105] and [43]).
In this chapter, we go one step further and study the inverse Wiener index problem for the following two kinds of structures:

- trees with degree ≤ 3 (Figure 3.1),
- hexagon type graphs (Figure 3.2).

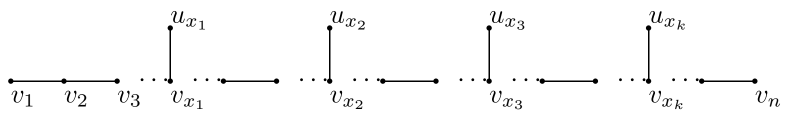

Figure 3.1: Caterpillar tree with degree ≤ 3

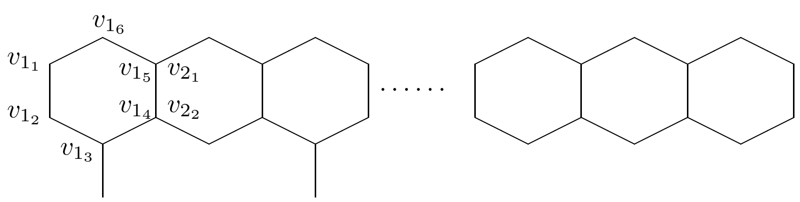

Figure 3.2: The hexagon type graph.

We define a family of trees $T = T(n, x_1, x_2, \ldots, x_k)$ by

$$V = \{v_1, \ldots, v_n\} \cup \{u_{x_1}, \ldots, u_{x_k}\},$$

$$E = \{(v_i, v_{i+1}), 1 \leq i \leq n-1\} \cup \{(v_{x_i}, u_{x_i}), 1 \leq i \leq k\},$$

where n and $x_i, 1 \leq i \leq k$, are integers such that $1 \leq x_1 \leq \ldots \leq x_k \leq n$ (Figure 3.1).
We also define a family of hexagon type graphs $G = G(n, x_1, x_2, \ldots, x_k)$, where we have n adjacent hexagons $v_{i_1} v_{i_2} \ldots v_{i_6}$, for $i = 1, 2, \ldots, n$. The edges $v_{i_4} v_{i_5}, v_{(i+1)_2} v_{(i+1)_1}$ are indentified for $i = 1, 2, \ldots, n-1$. On the x_jth hexagon there is a pendant edge incident to v_{j_3}, for $j = 1, \ldots, k$ (Figure 3.2). Another popular structure involves pentagons. We note that our proofs can be easily modified to solve the inverse Wiener index problem in that case. For the two kinds of graphs (Figure 3.1 and Figure 3.2) to be considered, we shall prove the following results:

Theorem 3.1 *Every sufficiently large integer n is the Wiener index of a caterpillar tree with maximal degree* ≤ 3.

Theorem 3.2 *Every sufficiently large integer n is the Wiener index of a hexagon type graph.*

Remark. Even though our proofs are not algorithmic, they can be turned into algorithms by merely checking all the possible cases. Unfortunately, the complexity is quite high; the running time for finding a graph from our graph classes with given Wiener index W is pseudo-polynomial in W.

First of all, we give explicit formulas for the Wiener index of the graphs we defined above. For $T = T(n, x_1, x_2, \ldots, x_k)$, as shown in Figure 3.1, we have

$$W(T) = \frac{n^3 - n}{6} + \sum_{i=1}^{n} \sum_{j=1}^{k} (1 + |x_j - i|) + \sum_{1 \leq i < j \leq k} (2 + x_j - x_i),$$

which can be rewritten as

$$\frac{n^3}{6} + \frac{kn^2}{4} + \frac{(6k-1)n}{6} - \frac{k^3 - 12k^2 + 14k}{12} + \sum_{j=1}^{k} \left(x_j + j - 1 - \frac{k+n}{2} \right)^2 \tag{3.1}$$

after some elementary simplification steps. For $G = G(n, x_1, x_2, \ldots, x_k)$ as shown in Figure 3.2, we have

$$\begin{aligned} W(G) = {} & \frac{16n^3 + 36n^2 + 26n + 3}{3} + \sum_{1 \leq i < j \leq k} (2 + 2(x_j - x_i)) \\ & + \sum_{i=1}^{k} (4n^2 + 8{x_i}^2 - 8nx_i + 12n - 8x_i + 7). \end{aligned} \tag{3.2}$$

We note that, from (3.2), $W(G)$ and k have opposite parity. Due to this (somewhat annoying) phenomenon, the Wiener indices of our hexagon type graphs with a fixed number of “leaves” comprise at most half of positive integers. To show that every large integer is the Wiener index of such a graph, one should consider at least two different k, with different parities. Expanding the last sum in (3.2) and collecting terms, we see that $W(G)$ is equal to

$$\frac{16n^3 + 36n^2 + 26n + 3}{3} + k(4n^2 + 12n + k + 6) + \sum_{i=1}^{k} (8{x_i}^2 - (8n + 2k - 4i + 10)x_i).$$

Completing squares is not necessary for our proof of Theorem 3.2, but it may make the expression look better. By doing so, we have

$$\begin{aligned} W(G) = {} & \frac{16n^3 + 36n^2 + 26n + 3}{3} + k\left(2n^2 + 8n + k + 4 - \frac{k^2 - 1}{24}\right) \\ & + \frac{1}{8} \sum_{i=1}^{k} (8x_i - 4n - k - 5 + 2i)^2. \end{aligned} \tag{3.3}$$

3.1 The inverse problem for chemical trees

We will use formula (3.1) in the special case $k = 8$ and show that all sufficiently large integers can be written as $W(T(n, x_1, \dots, x_8))$. Taking $k = 8$ and $n = 2s$, we can rewrite (3.1) as

$$W(T(n, x_1, \dots, x_8)) = \frac{4s^3}{3} + 8s^2 + \frac{47s}{3} + 12 + \sum_{j=1}^{k} (x_j + j - 5 - s)^2. \tag{3.4}$$

If we now set $y_j := x_j + j - 5 - s$, we obtain

$$W(T(n, x_1, \dots, x_8)) = \frac{4s^3}{3} + 8s^2 + \frac{47s}{3} + 12 + \sum_{j=1}^{k} y_j^2. \tag{3.5}$$

subject to the restrictions

$$-3 - s \leq y_1 < y_2 < \ldots < y_8 \leq 3 + s$$

and without any two consecutive y_j (since no two of the x_j may be equal). Now we need the following lemma, which is a slight modification of Lagrange's famous four-square theorem:

Lemma 3.3 Let $N > 103$ and $4 \nmid N$. Then N can be written as $a_1^2 + a_2^2 + a_3^2 + a_4^2$ with nonnegative integers $a_1 < a_2 < a_3 < a_4$ and $a_2 \geq 2$.

Proof. It is well known (see [47, Theorem 386]) that the number of representations of a positive integer N as the sum of 4 squares (representations which differ only in order or sign counting as different) is

$$r_4(N) = 8 \sum_{\substack{d \mid N \\ 4 \nmid d}} d,$$

while the number of representations of N as the sum of 2 squares is

$$r_2(N) = 4 \prod_{\substack{p^r \| N \\ p \equiv 1 \mod 4}} (r + 1).$$

if every prime factor $\equiv 3 \mod 4$ appears with an even power in the factorization of N (and 0 otherwise). The representations violating the first condition correspond to representations of the form $2a^2 + b^2 + c^2$. For each fixed $a \geq 0$ and each representation $b^2 + c^2$ of $N - 2a^2$, we have at most 24 representations of N as a sum of 4 squares (six possible choices for the positions of the two a's, and two additional choices of sign). The representations violating the second condition correspond to representations of the form $1 + a^2 + b^2$. For each representation $a^2 + b^2$ of $N - 1$, this gives us at most 24 representations of N as a sum of 4 squares (twelve possible choices for the positions of 0 and 1, and one additional choice of sign). So the number of representations violating any of the conditions is at most

$$24 \sum_{a \leq \sqrt{N/2}} r_2(N - 2a^2) + 24 r_2(N - 1).$$

Now,

$$r_2(k) \leq 4 \cdot \frac{3}{\sqrt{5}} \cdot \frac{2}{\sqrt[4]{13}} \cdot k^{1/4}$$

(cf. [47]; in fact, $r_2(k) \ll k^{\delta}$ for every fixed $\delta > 0$). Therefore, if $4 \nmid N$ and $N \geq 28561 = 13^4$, the number of representations violating one of the conditions is at most

$$24\Big(\sqrt{N/2} + 2\Big) \cdot \frac{24}{\sqrt[4]{325}} N^{1/4} \leq 96\sqrt{2}\Big(\sqrt{N/2} + 2\Big) N^{1/4} < 104 N^{3/4} < 8N < r_4(N).$$

So there must be some representation not violating any of the conditions. This proves the lemma for $N > 28560$, but it turns out that it also holds true for $N \in [104, 28560]$ by explicit testing. ■

Remark. The condition $4 \nmid N$ may not be skipped – for example, 4^k cannot be represented as a sum of four squares without violating the conditions.

Corollary 3.4 If $4 \nmid N$, $N > 103$, one can always find integers z_1, z_2, z_3, z_4 such that $N = z_1^2 + \ldots + z_4^2$, $z_1 < \ldots < z_4$ and no two of the z_i are consecutive.

Proof. Let $a_1 < a_2 < a_3 < a_4$ satisfy the conditions of the lemma. Choose $z_1 = -a_3$, $z_2 = -a_1$, $z_3 = a_2$ and $z_4 = a_4$. Then,

$$z_1 < -a_2 < z_2 < 1 < z_3 < a_3 < z_4,$$

which already proves the claim. ■

Remark. Obviously, $z_4 \leq \lfloor \sqrt{N} \rfloor$ and $|z_1| \leq \lfloor \sqrt{N} \rfloor - 1$.

Proposition 3.5 Let $K \geq 15$. Then any integer N in the interval $[4K^2 - 8K + 112, 5K^2 - 16K + 21]$ can be written as $y_1^2 + \ldots y_8^2$, where the y_i are integers satisfying

$$-K \leq y_1 < y_2 < \ldots < y_8 \leq K$$

and no two of them are consecutive.

Proof. Take $y_1 = -K$, $y_7 = K - 2$, $y_8 = K$ and either $y_2 = -K + 2$ or $y_2 = -K + 3$. By the corollary and the subsequent remark, any integer $M \in [104, (K-3)^2 - 1]$, $4 \nmid M$, can be written as $y_3^2 + \ldots + y_6^2$, where

$$-K = y_1 < y_2 < -K + 4 < y_3 < y_4 < y_5 < y_6 < K - 3 < y_7 < y_8 = K$$

(no two of them being consecutive). Now

$$(-K)^2 + (-K+2)^2 + (K-2)^2 + K^2 = 4K^2 - 8K + 8 \equiv 0 \mod 4$$

and

$$(-K)^2 + (-K+3)^2 + (K-2)^2 + K^2 = 4K^2 - 10K + 13 \equiv 2K + 1 \mod 4.$$

So all integers $\not\equiv 0 \mod 4$ in the interval $[4K^2 - 8K + 112, 5K^2 - 14K + 16]$ and all integers $\not\equiv 2K + 1 \mod 4$ in the interval $[4K^2 - 10K + 117, 5K^2 - 16K + 21]$ can be written in the required way. Since $0 \not\equiv 2K + 1 \mod 4$, this means that in fact all integers in the interval $[4K^2 - 8K + 112, 5K^2 - 16K + 21]$ can be written in the required way, which proves the claim. ■

Theorem 3.6 *All integers* ≥ 3856 *are Wiener indices of trees of the form* $T(n, x_1, \ldots, x_8)$ $(x_1 < x_2 < \ldots < x_8)$ *and thus Wiener indices of chemical trees.*

Proof. By the preceding proposition, any integer in the interval $[4K^2 - 8K + 112, 5K^2 - 16K + 21]$ can be written as $y_1^2 + \ldots + y_8^2$, where the y_i satisfy our requirements and $-K \leq y_1 < \ldots < y_8 \leq K$. If we take the union of these intervals over $21 \leq K \leq s + 3$, we see that in fact any integer in the interval $[1708, 5s^2 + 14s + 18]$ can be written as $y_1^2 + \ldots y_8^2$, where the y_i satisfy our requirements and $-3 - s \leq y_1 < \ldots < y_8 \leq s + 3$. Short computer calculations show that, for $s \geq 7$, even any integer in the interval $[224, 5s^2 + 14s + 18]$ can always be written that way. But this means that for any $s \geq 7$, all integers in the interval

$$\left[\frac{4s^3}{3} + 8s^2 + \frac{47s}{3} + 236, \frac{4s^3}{3} + 13s^2 + \frac{89s}{3} + 30\right]$$

are Wiener indices of trees of the form $T(n, x_1, \ldots, x_8)$. Taking the union over all these intervals, we see that all integers ≥ 12567 are contained in an interval of that type. By an additional computer search ($n \leq 40$ will do) in the remaining interval, one can reduce this number further to 3856. ■

Remark. By checking $k = 4, 5, 6, 7$ and finally all $n \leq 17$, one obtains a list of 250 integers (the largest being 927) that are not Wiener indices of trees of the form $T(n, x_1, \ldots, x_k)$ with maximal degree ≤ 3. Further computer search gives a list of 127 integers that are not Wiener indices of trees with maximal degree ≤ 3 – these are 16, 25, 28, 36, 40, 42, 44, 49, 54, 57, 58, 59, 62, 63, 64, 66, 80, 81, 82, 86, 88, 93, 95, 97, 103, 105, 107, 109, 111, 112, 115, 116, 118, 119, 126, 132, 139, 140, 144, 148, 152, 155, 157, 161, 163, 167, 169, 171, 173, 175, 177, 179, 181, 183, 185, 187, 189, 191, 199, 227, 239, 251, 255, 257, 259, 263, 267, 269, 271, 273, 275, 279, 281, 283, 287, 289, 291, 405 and the 49 values that cannot be represented as the Wiener index of any tree. This list reduces to the following values if one considers also trees with maximal degree = 4: 25, 36, 40, 49, 54, 57, 59, 80, 81, 93, 95, 97, 103, 105, 107, 109, 132, 155, 157, 161, 163, 167, 169, 171, 173 and 177.

3.2 The inverse problem for hexagon type graphs

We shall show that every sufficiently large integer N is the Wiener index of a hexagon type graph. As we have noticed that the parity of N determines the parity of k, we have to prove the theorem in two cases separately subject to the parity of N. We shall sketch a proof only for odd N, in which case we take $k = 10$. The argument for even N (in which case we can take $k = 9$) is similar and much simpler, thus we shall omit the proof. Actually, for even N, an elementary discussion would suffice for a proof with $k = 17$.

Suppose N is a sufficiently large odd integer. Let $k = 10$, then from (3.3) we have

$$W(G) = \frac{16}{3}n^3 + 32n^2 + \frac{266}{3}n + \frac{399}{4} + \frac{1}{8}\sum_{i=1}^{10}(8x_i - 4n - 15 + 2i)^2.$$

We thus want to show that

$$N = \frac{16}{3}n^3 + 32n^2 + \frac{266}{3}n + \frac{399}{4} + \frac{1}{8}\sum_{i=1}^{10}(8x_i - 4n - 15 + 2i)^2$$

for certain integers x_i, $i = 1, 2, ..., 10$ satisfying

$$1 \leq x_1 < x_2 < \cdots < x_9 < x_{10} \leq n. \tag{3.6}$$

Let

$$f(x) = \frac{16}{3}x^3 + 32x^2 + \frac{266}{3}x + \frac{399}{4},$$

and $\alpha(N)$ be the positive real root of $f(x) = N - N^{\frac{1}{3}}$. It is quite easy to see that $\alpha(N) = \left(\frac{3}{16}N\right)^{\frac{1}{3}} + 2 + O(N^{-\frac{1}{3}})$. Let $n = [\alpha(N)]$. Then we have $n = \left(\frac{3}{16}N\right)^{\frac{1}{3}} + O(1)$, and thus $n < N^{\frac{1}{3}} < 2n$. Also, we have

$$0 \leq N - f(n) - N^{\frac{1}{3}} < f(n+1) - f(n) = 16n^2 + 80n + 126. \tag{3.7}$$

We note that $8f(n) \equiv -2 (\bmod 16)$. To settle the theorem for large odd N, we thus want to show that, for every integer M satisfying

$$8n \leq M \leq 8(16n^2 + 82n + 126) \quad \text{and} \quad M \equiv 10 \pmod{16}, \tag{3.8}$$

we have

$$M = \sum_{i=1}^{10}(8x_i - 4n - 15 + 2i)^2$$

for some x_i ($i = 1, 2, ..., 10$) satisfying (3.6). Let $K = [\sqrt{M}/24]$, and

$$x_i = [n/2] + K + i, \quad i = 6, \ldots, 10. \tag{3.9}$$

Since $K \le \sqrt{8(16n^2+82n+126)}/24 < \frac{12}{25}n$, we have

$$n/2+\sqrt{M}/24 < x_6 < x_7 < x_8 < x_9 < x_{10} \le n. \tag{3.10}$$

Note then

$$\sum_{i=6}^{10}(8x_i-4n-15+2i)^2 = 320K^2+5200K-320K(n-2[n/2])+80(n-2[n/2])^2+2600(n-2[n/2])+22125.$$

It is very easy to check that

$$\sum_{i=6}^{10}(8x_i-4n-15+2i)^2 \equiv 8n+13 \pmod{16} \tag{3.11}$$

and, noticing that M is sufficiently large,

$$\frac{5}{9}M < \sum_{i=6}^{10}(8x_i-4n-15+2i)^2 < \frac{3}{5}M. \tag{3.12}$$

From (3.11), (3.12) and (3.8), we see that it is sufficient to show that

$$\sum_{i=1}^{5}(8x_i-4n-15+2i)^2 = L \tag{3.13}$$

for an integer L satisfying

$$\frac{2}{5}M \le L \le \frac{4}{9}M \quad \text{and} \quad L \equiv 8n+13 \pmod{16} \tag{3.14}$$

with

$$1 \le x_1 < x_2 < x_3 < x_4 < x_5 \le n/2+\sqrt{M}/24. \tag{3.15}$$

Lemma 3.7 Suppose $g_i(y) = a_iy^2+b_iy+c_i$ $(i=1,\ldots,5)$ are integer-valued quadratic polynomials, $a_i > 0$ for $i=1,\ldots,5$. d_i and D_i $(i=1,\ldots,5)$ are positive constants satisfying

$$d_i < D_i, \;\; i=1,\ldots,5, \quad \sum_{i=1}^{5} a_i{d_i}^2 < 1-\epsilon < 1+\epsilon < \sum_{i=1}^{5} a_i{D_i}^2$$

for some constant $\epsilon > 0$. Suppose L is a sufficiently large integer. If

$$g_1(y_1)+g_2(y_2)+\cdots+g_5(y_5) \equiv L \pmod{p^s}$$

is solvable for every prime power p^s, then the equation

$$g_1(y_1)+g_2(y_2)+\cdots+g_5(y_5) = L \tag{3.16}$$

with $d_i\sqrt{L} < y_i \le D_i\sqrt{L}$ has at least $cL^{\frac{3}{2}}$ integer solutions, where c is a certain positive constant depending only on a_i, d_i and D_i, $i=1,\ldots,5$.

Proof. This is the most trivial case of representing large integers as a sum of integer valued polynomials. A straightforward application of the Hardy-Littlewood method (with an argument similar to [51]) yields the lemma. ■

Proof of Theorem 3.2. With the aid of Lemma 3.7, we shall show that there exists some integer solution to (3.13) subject to conditions (3.14), (3.15). Let

$$g_i(y) = (8y-4(n-2[n/2])-15+2i)^2, \quad i=1,\ldots,5.$$

It is easy to see that for every prime $p \geq 3$,

$$g_1(y_1) + g_2(y_2) + \cdots + g_5(y_5) \equiv L \pmod{p}$$

is solvable, and each solution can be lifted by Hensel's Lemma to a solution modulo p^s for any $s \geq 2$. Note that $\theta(2) = 4$ is the largest integer such that

$$2^4 \mid {g_i}'(y) \quad \text{for all} \;\; y,$$

so to show that the congruence condition for $p = 2$ holds, it suffices to show that

$$g_1(y_1) + g_2(y_2) + \cdots + g_5(y_5) \equiv L \pmod{2^6} \tag{3.17}$$

is solvable. (If (3.17) is solvable, then by Hensel's Lemma, every non-trivial solution can be lifted to a solution of the congruence modulo any higher power of 2.) Expanding the left-hand side of (3.17), we see that

$$\sum_{i=1}^{5} g(y_i) \equiv 16\left(\sum_{i=1}^{5}(-1)^i y_i + (n - 2[n/2] + 1)^2\right) + 8(n - 2[n/2]) + 45 \pmod{64}.$$

It is then easy to check that (3.17) has a non-trivial solution

$$y_1 = 0, \;\; y_2 = y_3 = 1, \;\; y_4 = \frac{L - 8(n - 2[n/2]) + 19}{16}, \;\; y_5 = (n - 2[n/2] + 1)^2.$$

Let

$$d_i = \frac{1}{18} + \frac{3^i}{4 \cdot 10^5}, \qquad D_i = \frac{1}{18} + \frac{3^i}{2 \cdot 10^5}, \;\; i = 1, \ldots, 5. \tag{3.18}$$

Then we have

$$\sum_{i=1}^{5}(8d_i)^2 = 0.9941\ldots < 1, \quad \sum_{i=1}^{5}(8D_i)^2 = 1.0006\ldots > 1.$$

Now all conditions required by Lemma 3.7 are satisfied, thus, for the integer L satisfying (3.14), the equation (3.16) has solutions with $d_i\sqrt{L} < y_i \leq D_i\sqrt{L}$, $i = 1, \ldots, 5$. Let $x_i = [n/2] + y_i$ $(i = 1, \ldots, 5)$, and note that

$$d_i < D_i, \;\; i = 1, \ldots, 5, \;\; \text{and} \;\; D_i + 10^{-6} < d_{i+1} \;\; i = 1, \ldots, 4,$$

Lemma 3.7 guarantees a solution for (3.13) with

$$[n/2] < x_1 < x_2 < x_3 < x_4 < x_5 \leq [n/2] + D_5\sqrt{L} < n/2 + \sqrt{M}/24.$$

Theorem 3.2 thus follows. ■

Chapter 4

The average Wiener index of degree-restricted trees

In this chapter, we turn to another important problem in connection with the Wiener index. As it was mentioned in the introduction to this part, it is of interest to determine the average behavior of the Wiener index, especially for trees.
The average behaviour of the Wiener index was first studied by Entringer et al. [26], who considered so-called simply generated families of trees (introduced by Meir and Moon, cf. [78]). They were able to prove that the average Wiener index is asymptotically $Kn^{5/2}$, where the constant K depends on the specific family of trees. Thus, the average value of the Wiener index is, apart from a constant factor, the geometric mean of the extremal values, which are given for the star S_n and the path P_n respectively:

$$(n-1)^2 = W(S_n) \leq W(T) \leq W(P_n) = \binom{n+1}{3} \tag{4.1}$$

for all trees T with n vertices (s. [25]). In more recent articles, Neininger [86] studied recursive and binary search trees, and Janson [53] determined moments of the Wiener index of random rooted trees. Dobrynin and Gutman [20] calculated numerical values for the average Wiener index of trees and chemical trees of small order by direct computer calculation.
The average Wiener index of a tree (taking isomorphies into account) has been determined, in a different context, in a paper of Moon [83] – it is given asymptotically by $0.56828n^{5/2}$.
However, for chemical application, it is more interesting to know the average behavior for graphs with restricted degrees (typically restricted by 3 or 4, as in the previous chapter). The aim of this chapter is to extend the cited result to trees with restricted degree, especially chemical trees. In fact, the enumeration method for chemical trees is older than the analogous result of Otter for trees and goes back to Cayley (cf. [15]) and Pólya [92].
Let $Z(A)$ denote the cycle index of a permutation group A, and write $Z(A, f(z))$ for the cycle index $Z(A)$ with $f(z^l)$ substituted for the variable s_l belonging to an l-cycle. If $T_{\mathcal{G}}(z)$ and $T_{\mathcal{G}_k}(z)$ are the counting series for two classes $\mathcal{G}$, $\mathcal{G}_k$ of rooted trees, where $\mathcal{G}_k$ is constructed by attaching a collection of k trees from the family $\mathcal{G}$ to a common root (ignoring the order), we have (cf. [46])

$$T_{\mathcal{G}_k}(z) = z \cdot Z(S_k, T_{\mathcal{G}}(z)), \tag{4.2}$$

where S_k denotes the symmetric group. Additionally, we define $Z(S_0, f(z)) = 1$ and $Z(S_k, f(z)) = 0$ for $k < 0$. This gives us, for example, the functional equation for the counting series $T_3(z)$ of rooted trees with maximal outdegree ≤ 3:

$$T_3(z) = z \cdot \sum_{k=0}^{3} Z(S_k, T_3(z)).$$

4.1 Functional equations for the total height and Wiener index

Our method will be the same one as in Entringer et al. [26]. First, we consider an auxiliary value, $D(T)$, denoting the sum of the distances of all vertices from the root. This is also known as the *total height* of the tree T, cf. [97]. The value $D(T)$ can be calculated recursively from the branches $T_1, \dots, T_k$ of T, viz.

$$D(T) = \sum_{i=1}^{k} D(T_i) + |T| - 1, \tag{4.3}$$

where $|T|$ is the size (number of vertices) of T. Now we have to translate this recursive property into a functional equation. Again, we suppose that the branches come from a certain family $\mathcal{G}$, and denote the corresponding generating function for $D(T)$ by

$$D_{\mathcal{G}}(z) = \sum_{T \in \mathcal{G}} D(T) z^{|T|}.$$

Let $\mathcal{G}_k$ be defined as before and define $D_{\mathcal{G}_k}(z)$ analogously. There is an obvious bijection between the elements of $\mathcal{G}_{k-j}$ and the elements of $\mathcal{G}_k$ which contain a certain tree $T \in \mathcal{G}$ at least j times as a branch. Therefore, if $g_{k,n}$ denotes the number of trees of size n in $\mathcal{G}_k$, the branch B appears

$$\sum_{j=1}^{k} g_{k-j,n-j|B|}$$

times in all rooted trees of size n belonging to $\mathcal{G}_k$. Together with (4.3), this gives us

$$\begin{aligned} D_{\mathcal{G}_k}(z) &= \sum_{B \in \mathcal{G}} D(B) \sum_{j=1}^{k} \sum_{n \geq 1} g_{k-j,n-j|B|} z^n + z T'_{\mathcal{G}_k}(z) - T_{\mathcal{G}_k}(z) \\ &= z \sum_{j=1}^{k} D_{\mathcal{G}}(z^j) Z(S_{k-j}, T_{\mathcal{G}}(z)) + z T'_{\mathcal{G}_k}(z) - T_{\mathcal{G}_k}(z). \end{aligned} \tag{4.4}$$

Similarly, we introduce generating functions for the Wiener index:

$$W_{\mathcal{G}}(z) = \sum_{T \in \mathcal{G}} W(T) z^{|T|},$$

and $W_{\mathcal{G}_k}(z)$ is defined analogously. Now, we use the following recursive relation from [26], which relates the Wiener index of a rooted tree T with the Wiener indices of its branches $T_1, \dots, T_k$:

$$W(T) = D(T) + \sum_{i=1}^{k} W(T_i) + \sum_{i \neq j} \Big(D(T_i) + |T_i| \Big) |T_j|, \tag{4.5}$$

where the last sum goes over all $k(k-1)$ pairs of different branches. Now, we have to determine the number of times the pair $(B_1, B_2) \in \mathcal{G}^2$ appears in trees with n vertices belonging to $\mathcal{G}_k$. By the same argument that was applied before, this number is given by

$$\sum_{j=1}^{k-1} \sum_{i=1}^{k-j} g_{k-j-i,n-j|B_1|-i|B_2|}$$

if B_1 and B_2 are distinct elements from $\mathcal{G}$. If, on the other hand, $B_1 = B_2 = B$ are equal, the number is

$$\sum_{j=1}^{k} j(j-1) \Big(g_{k-j,n-j|B|} - g_{k-j-1,n-(j+1)|B|} \Big) = \sum_{j=1}^{k} 2(j-1) g_{k-j,n-j|B|}.$$

Together with (4.5), this yields

$$
\begin{aligned}
W_{\mathcal{G}_k}(z) &= D_{\mathcal{G}_k}(z) + \sum_{B \in \mathcal{G}} W(B) \sum_{j=1}^{k} \sum_{n \geq 1} g_{k-j,n-j|B|} z^n \\
&+ \sum_{B_1 \in \mathcal{G}} \sum_{B_2 \in \mathcal{G}} \Big(D(B_1) + |B_1| \Big) |B_2| \sum_{j=1}^{k-1} \sum_{i=1}^{k-j} \sum_{n \geq 1} g_{k-j-i,n-j|B_1|-i|B_2|} z^n \\
&+ \sum_{B \in \mathcal{G}} \Big(D(B) + |B| \Big) |B| \sum_{j=1}^{k} \sum_{n \geq 1} (j-1) g_{k-j,n-j|B|} z^n
\end{aligned}
$$

or

$$
\begin{aligned}
W_{\mathcal{G}_k}(z) &= D_{\mathcal{G}_k}(z) + z \sum_{j=1}^{k} W_{\mathcal{G}}(z^j) Z(S_{k-j}, T_{\mathcal{G}}(z)) \\
&+ z \sum_{j=1}^{k-1} \sum_{i=1}^{k-j} \Big(D_{\mathcal{G}}(z^j) + z^j T'_{\mathcal{G}}(z^j) \Big) \cdot z^i T'_{\mathcal{G}}(z^i) Z(S_{k-j-i}, T_{\mathcal{G}}(z)) \qquad (4.6) \\
&+ z \sum_{j=1}^{k} (j-1) z^j \Big(D'_{\mathcal{G}}(z^j) + T'_{\mathcal{G}}(z^j) + z^j T''_{\mathcal{G}}(z^j) \Big) Z(S_{k-j}, T_{\mathcal{G}}(z)).
\end{aligned}
$$

These functional equations (and combinations of them for different values of k) enable us to calculate the average Wiener indices for various sorts of degree-restricted rooted trees. For the study of unrooted trees, however, we need yet another tool. In particular, we want to determine the average Wiener index of trees with maximal degree ≤ 4, also known as chemical trees (cf. [20]).
For this purpose, let $\mathcal{F}_{\mathcal{D}}$ denote the family of rooted trees with the property that the outdegree of every vertex lies in $\mathcal{D}_0 = \mathcal{D} \cup \{0\}$, where $\mathcal{D} \subseteq \mathbb{N}$, and let $\tilde{\mathcal{F}}_{\mathcal{D}}$ be the family of trees with the property that all degrees lie in the set $\tilde{\mathcal{D}} = \{d+1 : d \in \mathcal{D}_0\}$. By a theorem of Otter (cf. [46]), the number of different representations of a tree as a rooted tree equals 1 plus the number of representations as a pair of two unequal rooted trees (the order being irrelevant), with their roots joined by an edge. Thus, for counting the trees in $\tilde{\mathcal{F}}_{\mathcal{D}}$, one has to take

- rooted trees with $k \in \tilde{\mathcal{D}}$ branches from $\mathcal{F}_{\mathcal{D}}$

minus

- pairs of unequal rooted trees from $\mathcal{F}_{\mathcal{D}}$, joined by an edge.

If $T_{\mathcal{D}}$ and $\tilde{T}_{\mathcal{D}}$ are the respective generating functions for the number of trees in $\mathcal{F}_{\mathcal{D}}$ and $\tilde{F}_{\mathcal{D}}$, this means that

$$
\tilde{T}_{\mathcal{D}}(z) = z + z \sum_{k \in \mathcal{D}_0} Z(S_{k+1}, T_{\mathcal{D}}(z)) - \frac{1}{2} \Big(T_{\mathcal{D}}^2(z) - T_{\mathcal{D}}(z^2) \Big). \qquad (4.7)
$$

The first summand, corresponding to the tree with only a single vertex, can be included or not, as it makes no real difference. The generating function for the Wiener index of trees from $\tilde{\mathcal{F}}_{\mathcal{D}}$ is also a difference of the respective generating functions for the two possibilities of representing a tree from $\tilde{\mathcal{F}}_{\mathcal{D}}$ which were given above. If we denote it by $\tilde{W}_{\mathcal{D}}(z) = \tilde{W}^{(1)}_{\mathcal{D}}(z) - \tilde{W}^{(2)}_{\mathcal{D}}(z)$, the first summand is given by equation (4.8), which is easily deduced from (4.4) and (4.6).

$$
\begin{aligned}
\tilde{W}_{\mathcal{D}}^{(1)}(z) = \sum_{k\in\tilde{D}} \Bigg(& z\sum_{j=1}^{k} D_{\mathcal{D}}(z^j) Z(S_{k-j}, T_{\mathcal{D}}(z)) + z\left(\frac{d}{dz} z \cdot Z(S_k, T_{\mathcal{D}}(z))\right) - z \cdot Z(S_k, T_{\mathcal{D}}(z)) \\
& + z\sum_{j=1}^{k} W_{\mathcal{D}}(z^j) Z(S_{k-j}, T_{\mathcal{D}}(z)) \\
& + z\sum_{j=1}^{k-1}\sum_{i=1}^{k-j} \Big(D_{\mathcal{D}}(z^j) + z^j T'_{\mathcal{D}}(z^j)\Big) \cdot z^i T'_{\mathcal{D}}(z^i) Z(S_{k-j-i}, T_{\mathcal{D}}(z)) \\
& + z\sum_{j=1}^{k} (j-1) z^j \Big(D'_{\mathcal{D}}(z^j) + T'_{\mathcal{D}}(z^j) + z^j T''_{\mathcal{D}}(z^j)\Big) Z(S_{k-j}, T_{\mathcal{D}}(z)) \Bigg),
\end{aligned}
\tag{4.8}
$$

On the other hand, if two rooted trees T_1 and T_2 are joined by an edge, the Wiener index of the resulting tree T is given by

$$W(T) = W(T_1) + W(T_2) + D(T_1)|T_2| + D(T_2)|T_1| + |T_1||T_2|.$$

Therefore, we obtain

$$
\begin{aligned}
\tilde{W}_{\mathcal{D}}^{(2)}(z) &= \frac{1}{2}\sum_{T_1\in\mathcal{F}_{\mathcal{D}}}\sum_{T_2\in\mathcal{F}_{\mathcal{D}}} \Big(W(T_1) + W(T_2) + D(T_1)|T_2| + D(T_2)|T_1| + |T_1||T_2|\Big) z^{|T_1|+|T_2|} \\
&\quad - \frac{1}{2}\sum_{T\in\mathcal{F}_{\mathcal{D}}} \Big(2W(T) + 2D(T)|T| + |T|^2\Big) z^{2|T|} \\
&= \frac{1}{2}\Big(2W_{\mathcal{D}}(z)T_{\mathcal{D}}(z) + 2D_{\mathcal{D}}(z)\cdot zT'_{\mathcal{D}}(z) + z^2 T'_{\mathcal{D}}(z)^2 \\
&\quad - 2W_{\mathcal{D}}(z^2) - 2z^2 D'_{\mathcal{D}}(z^2) - z^2(z^2 T''_{\mathcal{D}}(z^2) + T'_{\mathcal{D}}(z^2))\Big).
\end{aligned}
\tag{4.9}
$$

4.2 Wiener index of trees and chemical trees

Equations (4.4), (4.6), (4.8) and (4.9) enable us to calculate the exact average Wiener index of all trees of size n from a certain family $\mathcal{F}$ with degree restrictions for considerably high n. As an example, we calculate the average Wiener index of all chemical trees (i.e. maximal degree ≤ 4) up to $n = 100$. We have to start with the generating function T_3 for $\mathcal{F}_3$, the class of rooted trees with maximal outdegree ≤ 3, whose functional equation is given by

$$T_3(z) = z \cdot \sum_{k=0}^{3} Z(S_k, T_3(z)).$$

Then, the generating function for the number of trees with degree ≤ 4 is given by

$$\tilde{T}_3(z) = z\sum_{k=0}^{4} Z(S_k, T_3(z)) - \frac{1}{2}\Big(T_3^2(z) - T_3(z^2)\Big).$$

From (4.4), we know that the corresponding generating function for $D(T)$ satisfies

$$D_3(z) = z\sum_{k=1}^{3}\sum_{j=1}^{k} D_3(z^j) Z(S_{k-j}, T_3(z)) + zT'_3(z) - T_3(z).$$

Analogously, from (4.6), we obtain

$$W_3(z) = D_3(z) + \sum_{k=1}^{3} \Bigg(z \sum_{j=1}^{k} W_3(z^j) Z(S_{k-j}, T_3(z))$$
$$+ z \sum_{j=1}^{k-1} \sum_{i=1}^{k-j} \Big(D_3(z^j) + z^j T_3'(z^j) \Big) \cdot z^i T_3'(z^i) Z(S_{k-j-i}, T_3(z))$$
$$+ z \sum_{j=1}^{k} (j-1) z^j \Big(D_3'(z^j) + T_3'(z^j) + z^j T_3''(z^j) \Big) Z(S_{k-j}, T_3(z)) \Bigg).$$

$\tilde{W}_3$, the generating function for the sum of the Wiener indices of all trees with maximal degree ≤ 4, is then given by (4.8) and (4.9). Easy computer calculations yield us the following table – up to $n = 20$, the values were given in [20] by direct computation; $\tilde{t}_{4,n}$ denotes the number of trees of size n with maximal degree ≤ 4, $\tilde{w}_{4,n}$ the total of their Wiener indices:

n	$\tilde{t}_{4,n}$	$\tilde{w}_{4,n}$	$\tilde{w}_{4,n}/\tilde{t}_{4,n}$
1	1	0	0
2	1	1	1
3	1	4	4
4	2	19	9.5
5	3	54	18
6	5	155	31
7	9	432	48
8	18	1252	69.56
9	35	3384	96.69
10	75	9714	129.52
20	366319	310884129	848.67
50	$1.11774 \cdot 10^{18}$	$1.05659 \cdot 10^{22}$	9452.93
100	$5.92107 \cdot 10^{39}$	$3.34957 \cdot 10^{44}$	56570.38

Table 4.1: Some numerical values for chemical trees.

Things are somewhat easier in the case of ordinary trees. If $\mathcal{D} = \mathbb{N}$, the functional equations reduce to

$$D(z) = T(z) \sum_{j \geq 1} D(z^j) + zT'(z) - T(z),$$
$$W(z) = D(z) + T(z) \sum_{j \geq 1} W(z^j) + \sum_{j \geq 1} \sum_{i \geq 1} \Big(D(z^j) + z^j T'(z^j) \Big) \cdot z^i T'(z^i) \cdot T(z)$$
$$+ \sum_{j \geq 1} (j-1) z^j \Big(D'(z^j) + T'(z^j) + z^j T''(z^j) \Big) \cdot T(z),$$
$$\tilde{W}(z) = W(z) - \frac{1}{2} \Big(2W(z)T(z) + 2D(z) \cdot zT'(z) + z^2 T'(z)^2$$
$$- 2W(z^2) - 2z^2 D'(z^2) - z^2 (z^2 T''(z^2) + T'(z^2)) \Big).$$

These equations are also given in Moon [83]. They yield the list of values given in Table 4.2.

4.3 Asymptotic analysis

Now, we study the asymptotic behavior of the Wiener index for rooted trees and trees with degree restrictions. In particular, we will prove the following fairly general theorem:

n	w_n	$\tilde{w}_n$	w_n/t_n	$\tilde{w}_n/\tilde{t}_n$
1	0	0	0	0
2	1	1	1	1
3	8	4	4	4
4	38	19	9.5	9.5
5	164	54	18.22222	18
6	609	180	30.45	30
7	2256	508	47	46.18182
8	7815	1533	67.95652	66.65217
9	26892	4332	94.02797	92.17021
10	90146	13041	125.37691	123.02830
20	10319401978	655274837	804.55470	796.13984
50	$3.73537 \cdot 10^{24}$	$9.20871 \cdot 10^{22}$	8768.95009	8732.57790
100	$2.66359 \cdot 10^{48}$	$3.25933 \cdot 10^{46}$	51836.59972	51724.32112

Table 4.2: Some numerical values for trees.

Theorem 4.1 *Let $\mathcal{D} \subseteq \mathbb{N}$ be an arbitrary subset of the positive integers such that $\mathcal{D} \neq \{1\}$ and* $\gcd(d : d \in \mathcal{D}) = 1$. *Then the average total height $D(T_n)$ of a tree $T_n \in \mathcal{F}_\mathcal{D}$ with n vertices is asymptotically $2Kn^{3/2}$, the average Wiener index is asymptotically $Kn^{5/2}$, where K is given by*

$$K = \frac{\sqrt{\pi}}{2\alpha b \rho^{3/2}}$$

and α, b and ρ are defined as follows:

- *ρ is the radius of convergence of $T_\mathcal{D}(z)$,*
- *The expansion of $T_\mathcal{D}(z)$ around ρ is given by*

$$T_\mathcal{D}(z) = t_0 - b\sqrt{\rho - z} + O(\rho - z), \tag{4.10}$$

- $\alpha = \sum_{k \in \mathcal{D}} Z(S_{k-2}, T_\mathcal{D}(z))|_{z=\rho}$.

Remark. If $\mathcal{D} = \mathbb{N}$, we have $\alpha = \frac{1}{\rho} = 2.95576528\ldots$, $\rho = 0.33832185\ldots$ and $b = 2.68112814\ldots$, the constants given by Otter [88].

In the proof of the theorem, we will make use of the following property of the cycle indices of symmetric groups:

Lemma 4.2 If the cycle index $Z(S_k)$ of the symmetric group S_k is written in terms of $s_1, s_2, \ldots$, we have

$$\frac{\partial}{\partial s_l} Z(S_k) = \frac{1}{l} Z(S_{k-l}).$$

Proof. From [46], we know that the cycle index of S_k has the explicit representation

$$Z(S_k) = \frac{1}{k!} \sum_{(j)} h(j) \prod_{r=1}^{k} s_r^{j_r},$$

where the sum runs over all partitions $(j) = (j_1, \ldots, j_k)$ of k (j_r denotes the number of parts equal to r) and $h(j)$ is given by

$$h(j) = \frac{k!}{\prod_{r=1}^{k} r^{j_r} j_r!}.$$

There is an obvious bijection between the partitions of k which contain l and the partitions of $k-l$. For a partition (j) of k that contains l, let (j') be the partition of $k-l$ which results from replacing j_l by $j_l - 1$. Then it is easy to see that

$$h(j') = \frac{(k-l)! l j_l h(j)}{k!}.$$

This shows that

$$\frac{\partial}{\partial s_l} Z(S_k) = \frac{1}{k!} \sum_{(j)} \frac{j_l h(j)}{s_l} \prod_{r=1}^{k} s_r^{j_r} = \frac{1}{(k-l)!} \sum_{(j')} \frac{h(j')}{l} \prod_{r=1}^{k} s_r^{j'_r} = \frac{1}{l} Z(S_{k-l}).$$

■

Corollary 4.3

$$\frac{d}{dz} Z(S_k, f(z)) = \sum_{l=1}^{k} z^{l-1} f'(z^l) Z(S_{k-l}, f(z)).$$

Proof. This follows trivially upon application of the chain rule. ■

Proof of the theorem. We fix $\mathcal{D}$ and use the abbreviations T, D, W for $T_{\mathcal{D}}$, $D_{\mathcal{D}}$, $W_{\mathcal{D}}$. We start with the equation

$$T(z) = z \sum_{k \in \mathcal{D}_0} Z(S_k, T(z)). \tag{4.11}$$

The gcd-condition for $\mathcal{D}$ ensures that all but finitely many coefficients of T are positive. Following [46, pp. 208–214], one can prove that T has positive radius of convergence $1 > \rho \geq 0.33832\ldots$ (the lower bound being given by the case $\mathcal{D} = \mathbb{N}$), that T converges at $z = \rho$ and that ρ is the only singularity on the circle of convergence. Furthermore, T has an expansion of the form (4.10) around ρ, giving an asymptotic formula for the number $t_{\mathcal{D},n}$ of trees of size n in $\mathcal{F}_{\mathcal{D}}$:

$$t_{\mathcal{D},n} \sim \frac{b}{2\sqrt{\pi}} \rho^{-n+1/2} n^{-3/2}.$$

The values of ρ, t_0 and b can be determined numerically. Differentiating (4.11) yields, by Corollary 4.3,

$$\begin{aligned} T'(z) &= \frac{T}{z} + z \sum_{k \in \mathcal{D}} \sum_{l=1}^{k} z^{l-1} T'(z^l) Z(S_{k-l}, T(z)) \\ &= \frac{T}{z} + zT'(z) \sum_{k \in \mathcal{D}} Z(S_{k-1}, T(z)) + \sum_{k \in \mathcal{D}} \sum_{l=2}^{k} z^l T'(z^l) Z(S_{k-l}, T(z)) \end{aligned}$$

and thus

$$T'(z) \left(1 - z \sum_{k \in \mathcal{D}} Z(S_{k-1}, T(z)) \right) = \frac{T}{z} + \sum_{k \in \mathcal{D}} \sum_{l=2}^{k} z^l T'(z^l) Z(S_{k-l}, T(z)). \tag{4.12}$$

We set

$$\beta := \sum_{k \in \mathcal{D}} \sum_{l=2}^{k} z^l T'(z^l) Z(S_{k-l}, T(z)) \Big|_{z=\rho}.$$

Note, at this occasion, that $T(z^l)$ is holomorphic within a larger circle than $T(z)$ if $l > 1$, and that the sum over l can be uniformly bounded by a geometric sum on any compact subset of this larger circle. Furthermore, since it is a well-known fact that

$$\sum_{k \geq 0} Z(S_k, f(z)) = \exp\left(\sum_{m \geq 1} \frac{1}{m} f(z^m) \right),$$

we know that the sum over all $k \in \mathcal{D}$ converges as the sum $\sum_{m\geq 1} \frac{1}{m} T(\rho^m)$ is bounded. This argument will be used quite frequently in the following steps without being mentioned explicitly. Now, expanding around ρ gives us

$$1 - z \sum_{k\in\mathcal{D}} Z(S_{k-1}, T(z)) \sim \frac{2}{b}\left(\frac{t_0}{\rho} + \beta\right)\sqrt{\rho - z}. \tag{4.13}$$

On the other hand, we have

$$\begin{aligned}\frac{d}{dz}\left(1 - z\sum_{k\in\mathcal{D}} Z(S_{k-1}, T(z))\right) = &- \sum_{k\in\mathcal{D}} Z(S_{k-1}, T(z)) - zT'(z)\sum_{k\in\mathcal{D}} Z(S_{k-2}, T(z)) \\ &- z\sum_{k\in\mathcal{D}}\sum_{l=2}^{k-1} z^{l-1}T'(z^l)T(S_{k-1-l}, T(z)).\end{aligned}$$

The first and the last summand are bounded, therefore, if we set

$$\alpha := \sum_{k\in\mathcal{D}} Z(S_{k-2}, T(z))\Big|_{z=\rho},$$

we obtain

$$\frac{d}{dz}\left(1 - z\sum_{k\in\mathcal{D}} Z(S_{k-1}, T(z))\right) \sim -\frac{\rho b\alpha}{2}(\rho - z)^{-1/2},$$

giving us $\alpha = \frac{2}{b^2\rho}\left(\frac{t_0}{\rho} + \beta\right)$. Next, we turn to the functional equation for $D(z)$:

$$D(z) = zT'(z) - T(z) + zD(z)\sum_{k\in\mathcal{D}} Z(S_{k-1}, T(z)) + z\sum_{k\in\mathcal{D}}\sum_{l=2}^{k} D(z^l)Z(S_{k-l}, T(z)). \tag{4.14}$$

The last summand is bounded around ρ – note that $D(z)$ has the same radius of convergence as $T(z)$, since $D(T) \leq \frac{|T|(|T|-1)}{2}$ for all trees T; the same argument holds true for the generating function of the Wiener index by inequality (4.1). Solving for $D(z)$ yields

$$D(z) = \frac{zT'(z) - T(z) + z\sum_{k\in\mathcal{D}}\sum_{l=2}^{k} D(z^l)Z(S_{k-l}, T(z))}{1 - z\sum_{k\in\mathcal{D}} Z(S_{k-1}, T(z))}.$$

Therefore, the expansion of $D(z)$ around ρ is given by

$$D(z) \sim \frac{b^2\rho^2}{4(t_0 + \beta\rho)}(\rho - z)^{-1} = \frac{1}{2\alpha}(\rho - z)^{-1}, \tag{4.15}$$

which follows upon combining (4.10), (4.13) and (4.14). Finally, we consider the function $W(z)$:

$$\begin{aligned}W(z) = D(z) &+ zW(z)\sum_{k\in\mathcal{D}} Z(S_{k-1}, T(z)) + z\sum_{k\in\mathcal{D}}\sum_{j=2}^{k} W(z^j)Z(S_{k-j}, T(z)) \\ &+ z\sum_{k\in\mathcal{D}}\sum_{j=1}^{k-1}\sum_{i=1}^{k-j}\left(D(z^j) + z^jT'(z^j)\right)\cdot z^iT'(z^i)Z(S_{k-j-i}, T(z)) \\ &+ z\sum_{k\in\mathcal{D}}\sum_{j=1}^{k}(j-1)z^j\left(D'(z^j) + T'(z^j) + z^jT''(z^j)\right)Z(S_{k-j}, T(z)).\end{aligned} \tag{4.16}$$

We extract the asymptotically relevant terms to obtain

$$W(z)\left(1 - z\sum_{k\in\mathcal{D}} Z(S_{k-1}, T(z))\right) = z^2D(z)T'(z)\sum_{k\in\mathcal{D}} Z(S_{k-2}, T(z)) + O((\rho - z)^{-1}).$$

The right hand side of this equation behaves like $\frac{\rho^2 b}{4}(\rho - z)^{-3/2}$, so this yields

$$W(z) \sim \frac{\rho}{4\alpha}(\rho - z)^{-2}. \tag{4.17}$$

Thus, if $t_{\mathcal{D},n}$, $d_{\mathcal{D},n}$ and $w_{\mathcal{D},n}$ denote the coefficients of $T(z)$, $D(z)$ and $W(z)$ respectively, we have

$$t_{\mathcal{D},n} \sim \frac{b}{2\sqrt{\pi}}\rho^{-n+1/2}n^{-3/2},\ d_{\mathcal{D},n} \sim \frac{1}{2\alpha}\rho^{-n-1},\ w_{\mathcal{D},n} \sim \frac{1}{4\alpha}\rho^{-n-1}n.$$

So the average values of $D(T_n)$ and $W(T_n)$ for $T_n \in \mathcal{F}_{\mathcal{D}}$ are given by

$$\frac{d_{\mathcal{D},n}}{t_{\mathcal{D},n}} \sim \frac{\sqrt{\pi}}{\alpha b \rho^{3/2}}n^{3/2},\ \frac{w_{\mathcal{D},n}}{t_{\mathcal{D},n}} \sim \frac{\sqrt{\pi}}{2\alpha b \rho^{3/2}}n^{5/2},$$

which finally proves the claim. ■

In the same manner, we prove our second main theorem:

Theorem 4.4 *Let $\mathcal{D} \subset \mathbb{N}$ be a subset of the positive integers as in Theorem 4.1. Then the average Wiener index of a tree $T_n \in \tilde{\mathcal{F}}_{\mathcal{D}}$ is asymptotically $Kn^{5/2}$, where K is defined as in Theorem 4.1.*

Proof. We use the abbreviations T, D, W again and write $\tilde{T}$, $\tilde{W}$ for $\tilde{T}_{\mathcal{D}}$, $\tilde{W}_{\mathcal{D}}$. We consider the generating function $\tilde{T}(z)$ first:

$$\tilde{T}(z) = z + z\sum_{k\in\mathcal{D}_0} Z(S_{k+1}, T(z)) - \frac{1}{2}\Big(T^2(z) - T(z^2)\Big). \tag{4.18}$$

Clearly, $\tilde{T}(z)$ must have the same radius of convergence as T, and ρ is the only singularity of $\tilde{T}(z)$ on the circle of convergence. Thus we have to determine the expansion of $\tilde{T}(z)$ around ρ. First, we differentiate (4.18):

$$\begin{aligned}
\tilde{T}'(z) &= 1 + \sum_{k\in\mathcal{D}_0} Z(S_{k+1}, T(z)) + z\sum_{k\in\mathcal{D}_0}\sum_{l=1}^{k+1} z^{l-1}T'(z^l)Z(S_{k+1-l}, T(z)) - T(z)T'(z) + zT'(z^2)\\
&= 1 + \sum_{k\in\mathcal{D}_0} Z(S_{k+1}, T(z)) + T'(z)\left(z\sum_{k\in\mathcal{D}_0} Z(S_k, T(z)) - T(z)\right)\\
&\quad + z\sum_{k\in\mathcal{D}_0}\sum_{l=2}^{k+1} z^{l-1}T'(z^l)Z(S_{k+1-l}, T(z)) + zT'(z^2)\\
&= 1 + \sum_{k\in\mathcal{D}_0} Z(S_{k+1}, T(z)) + z\sum_{k\in\mathcal{D}}\sum_{l=2}^{k+1} z^{l-1}T'(z^l)Z(S_{k+1-l}, T(z)) + zT'(z^2).
\end{aligned}$$

Thus the derivative of $\tilde{T}(z)$ is bounded at $z = \rho$. Differentiating again yields

$$\tilde{T}''(z) = \sum_{k\in\mathcal{D}_0} T'(z)Z(S_k, T(z)) + z\sum_{k\in\mathcal{D}}\sum_{l=2}^{k+1} z^{l-1}T'(z^l)T'(z)Z(S_{k-l}, T(z)) + \dots,$$

the remaining terms being bounded at $z = \rho$. We find that

$$\tilde{T}''(z) \sim \left(\beta + \frac{t_0}{\rho}\right)T'(z) = \frac{b^2\alpha\rho}{2}T'(z)$$

around $z = \rho$. This means that $\tilde{T}(z)$ has an expansion of the form

$$T(z) = \tilde{t}_0 + a_1(\rho - z) + \frac{b^3\alpha\rho}{3}(\rho - z)^{3/2} + O((\rho - z)^2), \tag{4.19}$$

giving the asymptotic formula for the number $\tilde{t}_{\mathcal{D},n}$ of trees of size n in $\tilde{F}_{\mathcal{D}}$:

$$t_{\mathcal{D},n} \sim \frac{b^3\alpha}{4\sqrt{\pi}}\rho^{-n+5/2}n^{-5/2}.$$

We only have to determine the expansion of $\tilde{W}(z)$ now. This function is given by $\tilde{W}(z) = \tilde{W}^{(1)}(z) - \tilde{W}^{(2)}(z)$, where $\tilde{W}^{(1)}$ and $\tilde{W}^{(2)}$ are given by (4.8) and (4.9) respectively. We extract all asymptotically relevant parts and obtain

$$\begin{aligned}
\tilde{W}^{(1)}(z) &= z(D(z)+W(z))\sum_{k\in\tilde{\mathcal{D}}} Z(S_{k-1},T(z)) + z^2T'(z)(D(z)+zT'(z))\sum_{k\in\tilde{\mathcal{D}}} Z(S_{k-2},T)\\
&\quad + zD(z)\sum_{k\in\tilde{\mathcal{D}}}\sum_{l=2}^{k-1} z^lT'(z^l)Z(S_{k-1-l},T(z)) + O((\rho-z)^{-1/2})\\
&= z(D(z)+W(z))\sum_{k\in\mathcal{D}_0} Z(S_k,T(z)) + z^2T'(z)(D(z)+zT'(z))\sum_{k\in\mathcal{D}} Z(S_{k-1},T)\\
&\quad + zD(z)\sum_{k\in\mathcal{D}}\sum_{l=2}^{k} z^lT'(z^l)Z(S_{k-l},T(z)) + O((\rho-z)^{-1/2}).
\end{aligned} \tag{4.20}$$

and

$$\tilde{W}^{(2)}(z) = W(z)T(z) + zT'(z)D(z) + \frac{z^2}{2}T'(z)^2 + O((\rho-z)^{-1/2}). \tag{4.21}$$

Now, we make use of equations (4.11) and (4.12). Some algebraic manipulations then lead us to

$$\begin{aligned}
\tilde{W}(z) &= (D(z)+W(z))T(z) - W(z)T(z) + zT'(z)D(z)\left(z\sum_{k\in\mathcal{D}} Z(S_{k-1},T) - 1\right)\\
&\quad + \frac{z^2}{2}T'(z)^2 + z^2T'(z)^2\left(z\sum_{k\in\mathcal{D}} Z(S_{k-1},T) - 1\right)\\
&\quad + zD(z)\sum_{k\in\mathcal{D}}\sum_{l=2}^{k} z^lT'(z^l)Z(S_{k-l},T(z)) + O((\rho-z)^{-1/2})\\
&= D(z)T(z) + \frac{z^2}{2}T'(z)^2 - (D(z)+zT'(z))\left(T(z) + z\sum_{k\in\mathcal{D}}\sum_{l=2}^{k} z^lT'(z^l)Z(S_{k-l},T(z))\right)\\
&\quad + zD(z)\cdot\beta + O((\rho-z)^{-1/2})\\
&= D(z)\cdot t_0 + \frac{z^2}{2}T'(z)^2 - (D(z)+zT'(z))(t_0+\rho\beta) + D(z)\cdot\rho\beta + O((\rho-z)^{-1/2})\\
&= \frac{z^2}{2}T'(z)^2 + O((\rho-z)^{-1/2}).
\end{aligned}$$

Therefore, the expansion of $\tilde{W}$ around ρ is given by

$$\tilde{W}(z) \sim \frac{\rho^2b^2}{8}(\rho-z)^{-1}, \tag{4.22}$$

giving us an asymptotic formula for the coefficients of $\tilde{W}(z)$:

$$\tilde{w}_{\mathcal{D},n} \sim \frac{b^2}{8}\rho^{-n+1}.$$

Dividing by $\tilde{t}_{\mathcal{D},n}$ finally yields the theorem. ∎

As a conclusion, we give numerical values of K for $\mathcal{D} = \{1, \dots, M\}$ in some special cases:

M	$K(M)$
2	0.7842482154
3	0.6418839467
4	0.5962854459
5	0.5790571390
10	0.5683583008
∞	0.5682799594

Table 4.3: Some numerical values of K.

Remark. The theorem still holds – mutatis mutandis – when the gcd-condition for $\mathcal{D}$ is violated. In this case, there are several singularities of equal behavior on the circle of convergence. If, for example, $\mathcal{D} = \{3\}$ (in this case, $\tilde{\mathcal{F}}_{\mathcal{D}}$ corresponds to saturated hydrocarbons), there are only trees in $\mathcal{F}_{\mathcal{D}}$ with a number of vertices $n \equiv 1 \mod 3$, and their average Wiener index is asymptotically $0.3705918694 n^{5/2}$.

Remark. It is also possible to determine the moments of the Wiener index of a random tree as well by the same methods. For instance, in the case $\mathcal{D} = \mathbb{N}$, we have

$$\begin{aligned} D(T)^2 &= \left(\sum_{i=1}^{k} D(T_i) + |T| - 1 \right)^2 = 2D(T)(|T|-1) - (|T|-1)^2 + \left(\sum_{i=1}^{k} D(T_i) \right)^2 \\ &= 2D(T)(|T|-1) - (|T|-1)^2 + \sum_{i=1}^{k} D(T_i)^2 + \sum_{i \neq j} D(T_i) D(T_j), \end{aligned}$$

which yields the functional equation

$$\begin{aligned} D_2(z) &= 2zD'(z) - 2D(z) - z^2 T''(z) + zT'(z) - T(z) \\ &\quad + \left(\sum_{i \geq 1} \sum_{j \geq 1} D(z^i) D(z^j) + \sum_{i \geq 1} i D_2(z^i) \right) T(z) \end{aligned} \tag{4.23}$$

for the generating function

$$D_2(z) := \sum_T D(T)^2 z^{|T|}.$$

Similarly, one derives the following formulas for the generating functions of $D(T)W(T)$, denoted $DW(z)$, and $W(T)^2$, denoted $W_2(z)$:

$$\begin{aligned} DW(z) &= zW'(z) - W(z) - zD'(z) + D(z) + D_2(z) \\ &+ \Bigg(\sum_{i \geq 1} \sum_{j \geq 1} \sum_{k \geq 1} D(z^i)(D(z^j) + z^j T'(z^j)) z^k T'(z^k) + \sum_{i \geq 1} \sum_{j \geq 1} (i-1) \Big((D_2(z^i) + z^i D'(z^i)) z^j T'(z^j) \\ &\quad + z^i D'(z^i)(D(z^j) + z^j T'(z^j)) + z^i (D'(z^i) + T'(z^i) + z^i T''(z^i)) D(z^j) \Big) \\ &+ \sum_{i \geq 1} \sum_{j \geq 1} (D_2(z^i) + z^i D'(z^i)) z^j T'(z^j) + z^i D'(z^i)(D(z^j) + z^j T'(z^j)) \\ &+ \sum_{i \geq 1} \sum_{j \geq 1} D(z^i) W(z^j) + \sum_{i \geq 1} i(i-1) z^i (D_2(z^i) + D'(z^i) + z^i D''(z^i)) + \sum_{i \geq 1} i DW(z^i) \Bigg) T(z), \end{aligned}$$

$$
\begin{aligned}
W_2(z) = {} & 2DW(z) - D_2(z) + \sum_{i\geq 1} iW_2(z^i)T(z) + \sum_{i\geq 1}\sum_{j\geq 1} W(z^i)W(z^j)T(z) \\
& + 2T(z)\Big(\sum_{i\geq 1}\sum_{j\geq 1}\sum_{k\geq 1} W(z^i)(D(z^j)+z^jT'(z^j))z^kT'(z^k) \\
& \quad + \sum_{i\geq 1}\sum_{j\geq 1} (i-1)\Big((DW(z^i)+z^iW'(z^i))z^jT'(z^j) + z^iW'(z^i)(D(z^j)+z^jT'(z^j)) \\
& \quad + z^i(D'(z^i)+T'(z^i)+z^iT''(z^i))W(z^j)\Big) \\
& \quad + \sum_{i\geq 1}\sum_{j\geq 1} (DW(z^i)+z^iW'(z^i))z^jT'(z^j) + z^iW'(z^i)(D(z^j)+z^jT'(z^j)) \\
& \quad + \sum_{i\geq 1} i(i-1)z^i(DW'(z^i)+W'(z^i)+z^iW''(z^i))\Big) \\
& + T(z)\Big(\sum_{i\geq 1}\sum_{j\geq 1} (D_2(z^i)+2z^iD'(z^i)+z^iT'(z^i)+z^{2i}T''(z^i))(z^jT'(z^j)+z^{2j}T''(z^j)) \\
& \quad + (z^iD'(z^i)+z^iT'(z^i)+z^{2i}T''(z^i))(z^jD'(z^j)+z^jT'(z^j)+z^{2j}T''(z^j)) \\
& \quad + \sum_{i\geq 1} i(i-1)^2(z^iD_2'(z^i)+z^{2i}D_2''(z^i)+2z^iD'(z^i)+6z^{2i}D''(z^i)+2z^{3i}D'''(z^i) \\
& \quad + z^iT'(z^i)+7z^{2i}T''(z^i)+6z^{3i}T'''(z^i)+z^{4i}T''''(z^i))\Big) \\
& + 2T(z)\Big(\sum_{i\geq 1}\sum_{j\geq 1}\sum_{k\geq 1} (z^iD'(z^i)+z^iT'(z^i)+z^{2i}T''(z^i))(D(z^j)+z^jT'(z^j))z^kT'(z^k) \\
& \quad + \sum_{i\geq 1}\sum_{j\geq 1} (i-1)((z^iD_2'(z^i)+2z^iD'(z^i)+2z^{2i}D''(z^i)+z^iT'(z^i)+3z^{2i}T''(z^i)+z^{3i}T'''(z^i))z^jT'(z^j) \\
& \quad + (z^iD'(z^i)+z^{2i}D''(z^i)+z^iT'(z^i)+3z^{2i}T''(z^i)+z^{3i}T'''(z^i))(D(z^j)+z^jT'(z^j)) \\
& \quad + (z^iD'(z^i)+z^iT'(z^i)+z^{2i}T''(z^i))(z^jD'(z^j)+z^jT'(z^j)+z^{2j}T''(z^j)))\Big) \\
& + T(z)\Big(\sum_{i\geq 1}\sum_{j\geq 1}\sum_{k\geq 1} (D_2(z^i)+2z^iD'(z^i)+z^iT'(z^i)+z^{2i}T''(z^i))z^jT'(z^j)z^kT'(z^k) \\
& \quad + \sum_{i\geq 1}\sum_{j\geq 1} (i-1)(2(z^iD_2'(z^i)+2z^iD'(z^i)+2z^{2i}D''(z^i)+z^iT'(z^i)+3z^{2i}T''(z^i)+z^{3i}T'''(z^i))z^jT'(z^j) \\
& \quad + (z^iT'(z^i)+z^{2i}T''(z^i))(D_2(z^j)+2z^jD'(z^j)+z^jT'(z^j)+z^{2j}T''(z^j)))\Big) \\
& + T(z)\Big(\sum_{i\geq 1}\sum_{j\geq 1}\sum_{k\geq 1} (z^iT'(z^i)+z^{2i}T''(z^i))(D(z^j)+z^jT'(z^j))(D(z^k)+z^kT'(z^k)) \\
& \quad + \sum_{i\geq 1}\sum_{j\geq 1} (i-1)(2(z^iD'(z^i)+z^{2i}D''(z^i)+z^iT'(z^i)+3z^{2i}T''(z^i)+z^{3i}T'''(z^i))(D(z^j)+z^jT'(z^j)) \\
& \quad + (D_2(z^i)+2z^iD'(z^i)+z^iT'(z^i)+z^{2i}T''(z^i))(z^jT'(z^j)+z^{2j}T''(z^j)))\Big) \\
& + T(z)\Big(\sum_{i\geq 1}\sum_{j\geq 1}\sum_{k\geq 1}\sum_{l\geq 1} (D(z^i)+z^iT'(z^i))z^jT'(z^j)(D(z^k)+z^kT'(z^k))z^lT'(z^l) \\
& \quad + \sum_{i\geq 1}\sum_{j\geq 1}\sum_{k\geq 1} 4(i-1)(z^iD'(z^i)+z^iT'(z^i)+z^{2i}T''(z^i))z^jT'(z^j)(D(z^k)+z^kT'(z^k)) \\
& \quad + \sum_{i\geq 1}\sum_{j\geq 1}\sum_{k\geq 1} (i-1)(D_2(z^i)+2z^iD'(z^i)+z^iT'(z^i)+z^{2i}T''(z^i))z^jT'(z^j)z^kT'(z^k) \\
& \quad + \sum_{i\geq 1}\sum_{j\geq 1}\sum_{k\geq 1} (i-1)(z^iT'(z^i)+z^{2i}T''(z^i))(D(z^j)+z^jT'(z^j))(D(z^k)+z^kT'(z^k)) \\
& \quad + 2\sum_{i\geq 1}\sum_{j\geq 1} (i-1)(i-2)((z^iD_2'(z^i)+2z^iD'(z^i)+2z^{2i}D''(z^i)+z^iT'(z^i)+3z^{2i}T''(z^i)+z^{3i}T'''(z^i))z^jT'(z^j) \\
& \quad + (z^iD'(z^i)+z^{2i}D''(z^i)+z^iT'(z^i)+3z^{2i}T''(z^i)+z^{3i}T'''(z^i))(D(z^j)+z^jT'(z^j))) \\
& \quad + \sum_{i\geq 1}\sum_{j\geq 1} (i-1)(j-1)(2(z^iD'(z^i)+z^iT'(z^i)+z^{2i}T''(z^i))(z^jD'(z^j)+z^jT'(z^j)+z^{2j}T''(z^j)) \\
& \quad + (D_2(z^i)+2z^iD'(z^i)+z^iT'(z^i)+z^{2i}T''(z^i))(z^jT'(z^j)+z^{2j}T''(z^j)))\Big)
\end{aligned}
$$

Certainly, calculations become quite complex and tedious at this point, but an asymptotic analysis of the functional equations is still possible by deleting all terms which give only an asymptotically irrelevant contribution. This will yield the following results:

Theorem 4.5 *Let T_n be a random rooted tree on n vertices. Then we have, for the variance of $D(T_n)$ and $W(T_n)$ and the covariance of the two,*

$$\begin{aligned}\mathrm{Var}(D(T_n)) &\sim \frac{10-3\pi}{3\alpha^2 b^2\rho^3}n^3,\\ \mathrm{Cov}(D(T_n),W(T_n)) &\sim \frac{16-5\pi}{10\alpha^2 b^2\rho^3}n^4,\\ \mathrm{Var}(W(T_n)) &\sim \frac{16-5\pi}{20\alpha^2 b^2\rho^3}n^5.\end{aligned}$$

Also, if $\tilde{T}_n$ is a random tree on n vertices, we have

$$\mathrm{Var}(W(\tilde{T}_n)) \sim \frac{16-5\pi}{20\alpha^2 b^2\rho^3}n^5.$$

Here, $\alpha = 2.95576528\ldots$, $\rho = 0.33832185\ldots$ and $b = 2.68112814\ldots$ as in Theorem 4.1.

Chapter 5

Subset counting on trees

Now, we turn to different topological indices, namely those which are defined as the number of some specific type of subsets of a graph. The typical instances for this kind of index are the Merrifield-Simmons index (number of independent vertex subsets) and the Hosoya index (number of independent edge subsets), which were mentioned in the introductional chapter. Their growth is, unlike that of the Wiener index, exponential, so we need a slightly different approach to determine the average behavior of these indices.
Things are comparatively easy for the aforementioned simply generated families introduced by Meir and Moon [78], which have been investigated in a lot of papers, such as [26, 79, 80]. A simply generated family is determined by a sequence $c_0 = 1, c_1, c_2, \ldots$ of weights. The weight of a rooted ordered tree is then given by

$$c(T) = \prod c_i^{N_i(T)},$$

where $N_i(T)$ is the number of vertices in T with exactly i children. One can define a generating function for the total weight of all trees on n vertices via

$$Y(x) = \sum_T c(T)x^{|T|}.$$

It is easy to see now that $Y(x)$ must satisfy a functional equation of the form $Y(x) = x\Phi(Y(x))$, where $\Phi(t) = \sum_{i=0}^{\infty} c_i t^i$. Special cases include ordinary rooted ordered trees ($\Phi(t) = \frac{1}{1-t}$) and rooted labelled trees ($\Phi(t) = e^t$). Because of the simple functional equation for $Y(x)$, enumeration problems of various kind can be solved by an appropriate study of generating functions. For example, the average number of independent or maximal independent subsets, connected subsets or matchings have been studied by various authors [22, 58, 60, 61, 79, 80, 99]. None of them investigates the average behavior for rooted trees or trees; however, it seems certainly desirable to obtain information on the average behaviour of certain combinatorial indices for trees with consideration of isomorphisms. As an example, we will determine the average number of independent vertex subsets for trees and binary rooted trees. However, our method works for other enumeration problems, for example the number of matchings or connected subsets, just as well with the appropriate modifications.
As in the preceding chapter, we start with the well-known functional equation that is satisfied by the generating function $T(x)$ for the number of rooted trees (s. [46]):

$$T(x) = x\sum_{m=0}^{\infty} Z(S_m, T(x)) = x\exp\left(\sum_{m=1}^{\infty}\frac{1}{m}T(x^m)\right). \tag{5.1}$$

The generating function $\tilde{T}(x)$ for the number of trees is connected to $T(x)$ via

$$\tilde{T}(x) = T(x) - \frac{1}{2}\Big(T^2(x) - T(x^2)\Big). \tag{5.2}$$

Thus, rooted trees do not belong to the class of simply generated families of trees. This also complicates the analysis of enumeration problems.
We introduce some notation first. Let $|T|$ be the size (number of vertices) of a tree, and let $\sigma(T)$ denote the number of independent vertex subsets (i.e. subsets which contain no pair of adjacent vertices) of a tree T. Furthermore, for a rooted tree T, let $\sigma_1(T)$ and $\sigma_2(T)$ denote the number of independent vertex subsets containing resp. not containing the root. Then, if $T_1, \dots, T_r$ are the branches of a rooted tree T, it is easy to see that

$$\sigma_1(T) = \prod_{i=1}^{r} \sigma_2(T_i)$$

and

$$\sigma_2(T) = \prod_{i=1}^{r} (\sigma_1(T_i) + \sigma_2(T_i)).$$

5.1 The average number of independent subsets of a rooted tree

For a simply generated family of trees as defined in the introduction, it is not difficult to determine functional equations for the generating functions $S_1(x)$ and $S_2(x)$ of σ_1 and σ_2. In fact, from the recursive relations for σ_1 and σ_2, it follows that

$$S_1(x) = x\Phi(S_2(x)), \; S_2(x) = x\Phi(S_1(x) + S_2(x)).$$

For rooted trees, things are a little more difficult. Note that terms of type $T(x^k)$ appear in equation (5.1). These belong to k-tuples of isomorphic rooted trees among the branches. In the equations for σ_1 and σ_2, these give a contribution of the form $\sigma_1(T_i)^k$ resp. $(\sigma_1(T_i) + \sigma_2(T_i))^k$. Therefore, it is necessary to introduce some more generating functions of the form

$$S_{k,l}(x) = \sum_{T} \sigma_1(T)^k \sigma_2(T)^l x^{|T|},$$

where the sum is over all rooted trees T. Now, it is not difficult to see that

$$S_1(x) := S_{1,0}(x) = x \exp\left(\sum_{m=1}^{\infty} \frac{1}{m} S_{0,m}(x^m) \right) \tag{5.3}$$

and

$$S_2(x) := S_{0,1}(x) = x \exp\left(\sum_{m=1}^{\infty} \frac{1}{m} \sum_{k=0}^{m} \binom{m}{k} S_{k,m-k}(x^m) \right). \tag{5.4}$$

Observe in the latter equation that

$$\sum_{k=0}^{m} \binom{m}{k} S_{k,m-k}(x)$$

is, in fact, a generating function for $\sigma(T)^m = (\sigma_1(T) + \sigma_2(T))^m$. In order to find the asymptotic behavior of the average values of σ_1 and σ_2, we have to determine the dominating singularity of S_1 and S_2. For this purpose, we employ the same trick that is used in the asymptotic calculation of the number of trees (in fact, we will almost directly follow the proof of Otter's tree-counting theorem given in [46]): we observe that only the summands corresponding to $m = 1$ in the functional equations are not holomorphic around the singularity. To prove this, we need an a-priori estimate.
Let $s_{n,1}$ and $s_{n,2}$ be the coefficients of S_1 and S_2. Then, we have $s_{n-1,2} \le s_{n,1} \le s_{n,2}$. These relations follow easily from the recurrences, but can also be proved by a combinatorial argument: for the former inequality, note that a rooted tree T with a single branch T_1 satisfies $\sigma_1(T) = \sigma_2(T_1)$; for the latter, note that removing the root from an independent subset containing the root always results in another independent set.

Therefore, S_1 and S_2 have a common radius of convergence ρ_S; as the coefficients of S_1 and S_2 are positive, ρ_S is a singularity of both of them. Let us denote the radius of convergence of T by ρ. It is known (cf. [46]) that $\rho \approx 0.338322 < \frac{1}{2}$. Now, define $C_{m,n} := \sum_{|T|=n} \sigma(T)^m$. From estimate (1.2), we obtain $\sigma(T) \leq 2^{|T|}$ and thus

$$C_{m,n} \leq C_{1,n} 2^{(m-1)n} \ll \rho_S^{(-1-\epsilon)n} 2^{(m-1)n}$$

for any $\epsilon > 0$. On the other hand, $\frac{\rho}{2} \leq \rho_S \leq \rho < \frac{1}{2}$. Now, we are ready to prove two auxiliary lemmas:

Lemma 5.1 The series

$$\sum_{m=2}^{\infty} \frac{1}{m} S_{0,m}(x^m)$$

and

$$\sum_{m=2}^{\infty} \frac{1}{m} \sum_{k=0}^{m} \binom{m}{k} S_{k,m-k}(x^m)$$

define analytic functions within a circle of radius $\eta_S > \rho_S$.

Proof. We have to prove that the convergence radius of both series is larger than ρ_S. In fact, this is only necessary for the second series, since the first is a partial sum of the second and all coefficients are positive. Now, let $\eta \in (\rho_S, \sqrt{\frac{\rho_S}{2}})$. Since $\rho_S < \frac{1}{2}$, this interval is nonempty and $2\eta < \sqrt{2\rho_S} < 1$. Furthermore, choose $\epsilon > 0$ in such a way that $\alpha = 2\eta^2 \rho_S^{-1-\epsilon} < 1$. There exists some constant $A > 0$ such that $C_{1,n} \leq A\rho_S^{(-1-\epsilon)n}$ for all n. Therefore, we have

$$\begin{aligned}
\sum_{m=2}^{\infty} \frac{1}{m} \sum_{k=0}^{m} \binom{m}{k} S_{k,m-k}(\eta^m) &= \sum_{m=2}^{\infty} \frac{1}{m} \sum_{n=1}^{\infty} C_{m,n} \eta^{mn} \leq \sum_{m=2}^{\infty} \frac{1}{m} \sum_{n=1}^{\infty} C_{1,n} 2^{(m-1)n} \eta^{mn} \\
&\leq \sum_{m=2}^{\infty} \frac{1}{m} \sum_{n=1}^{\infty} A\rho_S^{(-1-\epsilon)n} 2^{(m-1)n} \eta^{mn} = \sum_{m=2}^{\infty} \frac{A}{m} \frac{\rho_S^{-1-\epsilon} 2^{m-1} \eta^m}{1 - \rho_S^{-1-\epsilon} 2^{m-1} \eta^m} \\
&\leq \sum_{m=2}^{\infty} \frac{A}{m} \rho_S^{-1-\epsilon} 2^{m-1} \eta^m \frac{1}{1 - 2\rho_S^{-1-\epsilon}\eta^2} \leq \frac{A\rho_S^{-1-\epsilon}}{4(1 - 2\rho_S^{-1-\epsilon}\eta^2)} \sum_{m=2}^{\infty} (2\eta)^m \\
&= \frac{A\rho_S^{-1-\epsilon}\eta^2}{(1 - 2\rho_S^{-1-\epsilon}\eta^2)(1 - 2\eta)} < \infty.
\end{aligned}$$

Hence, the series converges (absoutely, since all summands are positive) for every $\eta < \sqrt{\frac{\rho_S}{2}}$, which means that its radius of convergence is $\eta_S \geq \sqrt{\frac{\rho_S}{2}} > \rho_S$. So it represents an analytic function within a circle of radius $\eta_S > \rho_S$ around the origin. ■

Lemma 5.2 The limits $\lim_{x \to \rho_S -} S_1(x)$ and $\lim_{x \to \rho_S -} S_2(x)$ exist, and the power series for S_1 and S_2 converge at ρ_S (to the respective limits).

Proof. Note that, for $0 \leq x < \rho_S$, we have $S_1(x) \leq S_2(x)$ and

$$\log\left(\frac{S_2(x)}{x}\right) = \sum_{m=1}^{\infty} \frac{1}{m} \sum_{k=0}^{m} \binom{m}{k} S_{k,m-k}(x^m) \geq S_{0,1}(x) = S_2(x).$$

Thus, it follows that

$$\frac{S_2(x)/x}{\log(S_2(x)/x)} \leq \frac{1}{x},$$

which means that $S_2(x)$ (and thus $S_1(x)$) must be bounded on the interval $(0, \rho_S)$. Since $S_1(x)$ and $S_2(x)$ are monotonous functions on this interval, the left-hand limits must exist. It follows easily that the power series converge at ρ_S. ■

Next, we investigate the values of $S_1(x)$ and $S_2(x)$ at $x = \rho_S$:

Lemma 5.3 ρ_S is the only singularity of S_1 and S_2 on their circle of convergence. The values $s_1 = S_1(\rho_S)$ and $s_2 = S_2(\rho_S)$ satisfy the equation

$$s_2(1 + s_1) = 1. \tag{5.5}$$

Proof. We write the functional equations for $S_1(x)$ and $S_2(x)$ in the following form:

$$F_1(S_1(x), S_2(x), x) = x \exp(S_2(x) + R_1(x)) - S_1(x) = 0,$$
$$F_2(S_1(x), S_2(x), x) = x \exp(S_1(x) + S_2(x) + R_2(x)) - S_2(x) = 0,$$

where $R_1(x)$ and $R_2(x)$ are abbreviations for $\sum_{m=2}^{\infty} \frac{1}{m} S_{0,m}(x^m)$ and $\sum_{m=2}^{\infty} \frac{1}{m} \sum_{k=0}^{m} \binom{m}{k} S_{k,m-k}(x^m)$ respectively. We already know that R_1 and R_2 are analytic within a circle of radius $\eta_S > \rho_S$. The Jacobian determinant of these equations has to vanish at a singularity. Otherwise, by the implicit function theorem, they would have a unique analytic solution in a certain neighborhood. Therefore, we calculate the Jacobian matrix of $F_1(y_1, y_2, x)$ and $F_2(y_1, y_2, x)$:

$$\frac{\partial F}{\partial y} = \begin{pmatrix} -1 & F_1(y_1, y_2, x) + y_1 \\ F_2(y_1, y_2, x) + y_2 & F_2(y_1, y_2, x) + y_2 - 1 \end{pmatrix} = \begin{pmatrix} -1 & y_1 \\ y_2 & y_2 - 1 \end{pmatrix},$$

since both F_1 and F_2 must vanish. The determinant is thus given by

$$\left| \frac{\partial F}{\partial y} \right| = 1 - y_2 - y_1 y_2,$$

which means that equation (5.5) must be satisfied. Now let $\xi \neq \rho_S$ be another point on the circle of convergence. Then, since all coefficients of S_1 and S_2 are positive real numbers, we have $|S_1(\xi)| < s_1$ and $|S_2(\xi)| < s_2$, so the equation $1 - S_2(\xi) - S_1(\xi)S_2(\xi)$ cannot be satisfied. ∎

Therefore, we may make use of the following well-known theorem (cf. [8, 14, 46]):

Theorem 5.4 *Let $F(x, y)$ be analytic in each variable seperately in some neighborhood of (x_0, y_0) and suppose that the following conditions are satisfied:*

1. *$F(x_0, y_0) = 0$,*
2. *$y = f(x)$ is analytic in $|x| < |x_0|$ and x_0 is the unique singularity on the circle of covergence,*
3. *if $f(x) = \sum_{n=0}^{\infty} f_n x^n$ is the expansion of f at the origin, then $y_0 = \sum_{n=0}^{\infty} f_n x_0^n$,*
4. *$F(x, f(x)) = 0$ for $|x| < |x_0|$,*
5. *$\frac{\partial F}{\partial y}(x_0, y_0) = 0$,*
6. *$\frac{\partial^2 F}{\partial y^2}(x_0, y_0) \neq 0$.*

Then $f(x)$ may be expanded about x_0:

$$f(x) = f(x_0) + \sum_{k=1}^{\infty} a_k (x_0 - x)^{k/2},$$

and if $a_1 \neq 0$,

$$f_n \sim \frac{-a_1}{2\sqrt{\pi}} x_0^{-n+1/2} n^{-3/2}.$$

If $a_1 = 0$ and $a_3 \neq 0$,

$$f_n \sim \frac{3a_3}{4\sqrt{\pi}} x_0^{-n+3/2} n^{-5/2}.$$

Note that $S(x) = S_1(x) + S_2(x)$ satisfies the equation

$$S(x) = x\exp(S(x) + R_2(x)) + x\exp(x\exp(S(x) + R_2(x)) + R_1(x)),$$

so the conditions of the theorem are satisfied by the preliminary lemmas with $f(x) = S(x)$ and

$$F(x,y) = x\exp(y + R_2(x)) + x\exp(x\exp(y + R_2(x)) + R_1(x)) - y.$$

They are also satisfied for $f(x) = S_2(x)$ and

$$F(x,y) = x\exp(x\exp(y + R_1(x)) + y + R_2(x)) - y,$$

so S_1, S_2 and S may be expanded around ρ_S in the way that is given by the theorem. We only have to care about the values of the implied constants and their calculation. First of all, ρ_S is uniquely defined by the equations

$$\begin{aligned} s_1 &= \rho_S \exp(s_2 + R_1(\rho_S)), \\ s_2 &= \rho_S \exp(s_1 + s_2 + R_2(\rho_S)), \\ 1 &= s_2(s_1 + 1). \end{aligned} \tag{5.6}$$

Note that $R_1(x)$ and $R_2(x)$ are convergent series within a circle of radius $\eta_S > \rho_S$. Therefore, if we calculate the coefficients of R_1 and R_2 up to some power x^N, we obtain estimates $\overline{R}_1(x)$ and $\overline{R}_2(x)$ which can be uniformly bounded within a circle of radius $\eta_S - \epsilon$. Solving the system with $\overline{R}_i$ instead of R_i thus gives estimates for s_1, s_2 and ρ_S.
The error can even be quantified in the following way: clearly, we have $C_{1,n} \leq 2^n t_n$, where t_n is the number of rooted trees of size n. This shows, following the estimates of Lemma 5.1, that the error can be uniformly and explicitly bounded within the circle of radius $\frac{\sqrt{\rho}}{2} - \epsilon$. On the other hand, by the left-hand estimate in (1.2), we have $\rho_S \leq \frac{\rho(\sqrt{5}-1)}{2} < \frac{\sqrt{\rho}}{2}$, which means that the error can be estimated explicitly. Numerical computation shows that $\rho_S \approx 0.2020447686$, $s_1 \approx 0.4202770330$ and $s_2 \approx 0.7040879890$. Computational details will be discussed in section 5.3. Now, write

$$\begin{aligned} S_1(x) &= s_1 - b_1\sqrt{\rho_S - x} + \ldots, \\ S_2(x) &= s_2 - b_2\sqrt{\rho_S - x} + \ldots, \\ S(x) &= s - b\sqrt{\rho_S - x} + \ldots. \end{aligned}$$

To determine b_1 and b_2 (and thus $b = b_1 + b_2$), we note first that

$$S_1'(x)(1 - S_2(x) - S_1(x)S_2(x)) = \frac{b_1}{2}(s_1 b_2 + s_2 b_1 + b_2) + O((\rho_S - x)^{1/2})$$

and

$$S_2'(x)(1 - S_2(x) - S_1(x)S_2(x)) = \frac{b_2}{2}(s_1 b_2 + s_2 b_1 + b_2) + O((\rho_S - x)^{1/2}),$$

so we have

$$\begin{aligned} \frac{b_1}{2}(s_1 b_2 + s_2 b_1 + b_2) &= \lim_{x \to \rho_S} S_1'(x)(1 - S_2(x) - S_1(x)S_2(x)) =: c_1, \\ \frac{b_2}{2}(s_1 b_2 + s_2 b_1 + b_2) &= \lim_{x \to \rho_S} S_2'(x)(1 - S_2(x) - S_1(x)S_2(x)) =: c_2. \end{aligned} \tag{5.7}$$

The values on the right can be calculated by differentiating the functional equations for S_1 and S_2 first:

$$S_1'(x) = \frac{S_1(x)}{x} + S_1(x)(S_2'(x) + R_1'(x))$$

and

$$S_2'(x) = \frac{S_2(x)}{x} + S_2(x)(S_1'(x) + S_2'(x) + R_2'(x)).$$

Solving this system for $S_1'(x)$ and $S_2'(x)$ yields

$$S_1'(x)(1 - S_2(x) - S_1(x)S_2(x)) = \frac{S_1(x)}{x} + S_1(x)R_1'(x) + S_1(x)S_2(x)(R_2'(x) - R_1'(x))$$

and

$$S_2'(x)(1 - S_2(x) - S_1(x)S_2(x)) = \frac{S_2(x)(1 + S_1(x))}{x} + S_1(x)S_2(x)R_1'(x) + S_2(x)R_2'(x).$$

Therefore,

$$c_1 = \frac{s_1}{\rho_S} + s_1 \sum_{m=2}^{\infty} S_{0,m}'(\rho_S^m)\rho_S^{m-1} + s_1 s_2 \sum_{m=2}^{\infty} \sum_{k=1}^{m} \binom{m}{k} S_{k,m-k}'(\rho_S^m)\rho_S^{m-1}$$

and

$$c_2 = \frac{1}{\rho_S} + s_1 s_2 \sum_{m=2}^{\infty} S_{0,m}'(\rho_S^m)\rho_S^{m-1} + s_2 \sum_{m=2}^{\infty} \sum_{k=0}^{m} \binom{m}{k} S_{k,m-k}'(\rho_S^m)\rho_S^{m-1},$$

which can be calculated numerically. Furthermore, solving the system (5.7) for b_1 and b_2 gives us

$$b_1 = \frac{\sqrt{2}c_1}{\sqrt{s_2 c_1 + c_2 + s_1 c_2}}, \; b_2 = \frac{\sqrt{2}c_2}{\sqrt{s_2 c_1 + c_2 + s_1 c_2}}$$

and thus

$$b = \frac{\sqrt{2}(c_1 + c_2)}{\sqrt{s_2 c_1 + c_2 + s_1 c_2}}. \tag{5.8}$$

Numerical calculations show that $b \approx 3.8130254771$. Noting that the number t_n of rooted trees of size n satisfies $t_n \sim A \cdot n^{-3/2}\rho^{-n}$ with $A \approx 0.4399240126$, we have obtained the following theorem:

Theorem 5.5 *The average number of independent vertex subsets in a rooted tree of size n is given by*

$$\mathrm{av}_n \sim (1.0990334536) \cdot (1.6744895662)^n.$$

5.2 The average number of independent subsets of a tree

Now, having established the asymptotics for rooted trees, we are also able to give them for trees. We will make use of Otter's theorem [88] which states that the number of different representations of a tree as a rooted tree equals 1 plus the number of representations as a pair of two unequal rooted trees (the order being irrelevant), with their roots joined by an edge (see also [46]). It is easy to see that, if two rooted trees T_1, T_2 are joined by an edge connecting their root, the resulting tree T has a total number of

$$\sigma(T) = \sigma_1(T_1)\sigma_2(T_2) + \sigma_2(T_1)\sigma_1(T_2) + \sigma_2(T_1)\sigma_2(T_2)$$

independent vertices. Thus, if we denote the generating function which counts independent subsets in all trees instead of rooted trees by $\tilde{S}$, we have

$$\tilde{S}(x) = S(x) - \frac{1}{2}\left(2S_1(x)S_2(x) + S_2(x)^2 - 2S_{1,1}(x^2) - S_{0,2}(x^2)\right). \tag{5.9}$$

$S_{1,1}(x^2)$ and $S_{0,2}(x^2)$ are holomorphic around ρ_S. Thus, we only have to determine the expansion of the remaining terms around ρ_S. Let

$$\tilde{S}(x) = a_0 - a_1\sqrt{\rho_S - x} + a_2(\rho_S - x) + a_3(\rho_S - x)^{3/2} + \ldots.$$

We know that $s_2(s_1 + 1) = 1$. Furthermore, from the equation

$$S_1(x) = x\exp(S_2(x) + R_1(x)),$$

we obtain $b_1 = s_1 b_2$. Inserting the expansions of S_1 and S_2 in (5.9) and using these relations shows that $a_1 = 0$. To determine a_3, we differentiate twice:

$$\tilde{S}''(x) = \frac{3a_3}{4}(\rho_S - x)^{-1/2} + \dots.$$

On the other hand, we differentiate the functional equations for S_1' and S_2':

$$S_1''(x) = \frac{S_1'(x)}{x} - \frac{S_1(x)}{x^2} + S_1'(x)(S_2'(x) + R_1'(x)) + S_1(x)(S_2''(x) + R_1''(x))$$

and

$$S_2''(x) = \frac{S_2'(x)}{x} - \frac{S_2(x)}{x^2} + S_2'(x)(S_1'(x) + S_2'(x) + R_2'(x)) + S_2(x)(S_1''(x) + S_2''(x) + R_2''(x)).$$

We solve this system for S_1'' and S_2'' and insert it in

$$\tilde{S}''(x) = S_1''(x) + S_2''(x) - S_1''(x)S_2(x) - 2S_1'(x)S_2'(x) - S_1(x)S_2''(x) - S_2'(x)^2 - S_2(x)S_2''(x) + R''(x)$$

together with the expressions for S_1' and S_2'. Note that $R(x) = S_{1,1}(x^2) + \frac{1}{2}S_{0,2}(x^2)$ is holomorphic within the circle of radius $\eta_S > \rho_S$. Then, we use the expansions of S_1 and S_2 together with the relations for s_1, s_2, b_1, b_2 to obtain the final expression for a_3:

$$\frac{3a_3}{4} = \sqrt{\frac{c_2^3}{2s_2(1 + s_2 - s_2^2)}} \approx 11.7914747833.$$

This gives us the asymptotic behavior of the coefficients of $\tilde{S}$ and, together with the asymptotic formula for the number $\tilde{t}_n$ of trees of size n, which is $\tilde{t}_n \sim B \cdot n^{-5/2}\rho^{-n}$ with $B \approx 0.5349496061$, we have established the following theorem:

Theorem 5.6 *The average number of independent vertex subsets in a tree of size n is given by*

$$\tilde{\mathrm{av}}_n \sim (1.1294102715) \cdot (1.6744895662)^n.$$

Thus, interestingly, a tree contains more independent sets on average than a rooted tree. It is not easy to explain this phenomenon in an intuitive or heuristic way. Note, however, that trees with a large number of independent subsets are similar to stars in some way (cf. inequality (1.2)), and these trees usually also have a large number of symmetries. So their contribution to the average number of independent subsets of trees is larger than to the analogous value for rooted trees.

5.3 Efficient computation of the auxiliary functions and numerical values

In the approximate solution of the system (5.6), it was necessary to compute a sufficient number of coefficients of the auxiliary functions $S_{k,l}$. For this purpose, it is possible, of course, to compute the number of independent subsets explicitly for all rooted trees of size $n \leq N$. However, this brute-force method is highly inefficient, so it is desirable to have a better method at hand. It is quite simple to achieve this: we can deduce functional equations for $S_{k,l}$ in the same manner as we did for $S_1 = S_{1,0}$ and $S_2 = S_{0,1}$. These are given by the general formula

$$S_{k,l}(x) = x \exp\left(\sum_{m=1}^{\infty} \frac{1}{m} \sum_{r=0}^{ml} \binom{ml}{r} S_{ml-r,mk+r}(x^m)\right), \tag{5.10}$$

which enables us to compute the coefficients of $S_{k,l}$ in a simple recursive manner. We give the initial values of $S_{1,0}$, $S_{0,1}$ and $S_{2,0}$ for instance:

$$S_{1,0}(x) = x + x^2 + 3x^3 + 10x^4 + 38x^5 + 143x^6 + 577x^7 + 2325x^8 + 9697x^9 + 40853x^{10} + \dots,$$
$$S_{0,1}(x) = x + 2x^2 + 7x^3 + 24x^4 + 91x^5 + 341x^6 + 1370x^7 + 5504x^8 + 22914x^9 + 96457x^{10} + \dots,$$
$$S_{2,0}(x) = x + x^2 + 5x^3 + 30x^4 + 196x^5 + 1267x^6 + 8615x^7 + 58613x^8 + 411209x^9 + 2909597x^{10} + \dots.$$

Note that the functional equation can also be used to calculate higher moments of the number of independent subsets of a random tree. We give some numerical instances of the average values for rooted trees resp. trees in the following table:

n	av_n	$\tilde{\mathrm{av}}_n$	n	av_n	$\tilde{\mathrm{av}}_n$
1	2	2	8	68.08	70.83
2	3	3	9	114.02	119.09
3	5	5	10	190.97	199.02
4	8.5	8.5	15	2512.81	2608.75
5	14.33	14.67	20	33063.90	34210.51
6	24.2	24.83	50	$1.719535 \cdot 10^{11}$	$1.771075 \cdot 10^{11}$
7	40.56	42.09	100	$2.687782 \cdot 10^{22}$	$2.765055 \cdot 10^{22}$

Table 5.1: Some values of av_n and $\tilde{\mathrm{av}}_n$.

5.4 Independent subsets in a degree-restricted tree

It is clear that the methods we established in section 5.1 are easily generalized to other classes of trees or tree-like structures. As an example, we will determine the asymptotic average number of independent subsets in binary rooted trees (maximal outdegree ≤ 2, cf. [46, 88]). The functional equation for $T^{(2)}$, the generating function for the number of such trees, is given by

$$\begin{aligned} T^{(2)}(x) &= x\left(1 + Z(S_1, T^{(2)}(x)) + Z(S_2, T^{(2)}(x))\right) \\ &= x\left(1 + T^{(2)}(x) + \frac{1}{2}\left(T^{(2)}(x) + T^{(2)}(x^2)\right)\right). \end{aligned} \tag{5.11}$$

Next, we define $S_{k,l}^{(2)}$ in the same manner as in section 5.1. The functional equation

$$S_{k,l}^{(2)}(x) = x\left(1 + \sum_{r=0}^{l}\binom{l}{r}S_{l-r,k+r}^{(2)}(x) + \frac{1}{2}\left(\sum_{r=0}^{l}\binom{l}{r}S_{l-r,k+r}^{(2)}(x)\right)^2 + \frac{1}{2}\left(\sum_{r=0}^{2l}\binom{2l}{r}S_{2l-r,2k+r}^{(2)}(x^2)\right)\right)$$

follows at once in the same way as for rooted trees. In particular, we have

$$\begin{aligned} S_1^{(2)}(x) &:= S_{1,0}^{(2)}(x) = x\left(1 + S_2^{(2)}(x) + \frac{1}{2}S_2^{(2)}(x)^2 + \frac{1}{2}S_{0,2}^{(2)}(x^2)\right), \\ S_2^{(2)}(x) &:= S_{0,1}^{(2)}(x) = x\Bigg(1 + S_1^{(2)}(x) + S_2^{(2)}(x) + \frac{1}{2}\left(S_1^{(2)}(x) + S_2^{(2)}(x)\right)^2 \\ &\qquad + \frac{1}{2}\left(S_{0,2}^{(2)}(x^2) + 2S_{1,1}^{(2)}(x^2) + S_{2,0}^{(2)}(x^2)\right)\Bigg). \end{aligned} \tag{5.12}$$

Analogously to Theorem 5.5, we achieve the following result:

Theorem 5.7 *The average number of independent vertex subsets in a rooted tree of size n with maximal outdegree ≤ 2 is given by*

$$\mathrm{av}_n^{(2)} \sim (1.1311298442) \cdot (1.6425223181)^n.$$

It is not surprising that the average number of independent subsets decreases by the degree restriction. Rooted trees with restricted outdegrees are typically more "path-like", so – in view of inequality (1.2) – the number of independent subsets is closer to the minimum. Again, we give some numerical values in the following table:

n	$\mathrm{av}_n^{(2)}$	n	$\mathrm{av}_n^{(2)}$
1	2	8	60.04
2	3	9	98.55
3	5	10	161.91
4	8.33	15	1934.40
5	13.5	20	23121.26
6	22.27	50	$6.748132 \cdot 10^{10}$
7	36.67	100	$4.024331 \cdot 10^{21}$

Table 5.2: Some values of $\mathrm{av}_n^{(2)}$.

Chapter 6

Correlation of graph-theoretical indices

The properties of the indices which were studied in the preceding chapters – especially the common property that the extremal trees are always the path and star – raise the natural question how the various indices are related. It is also worthwhile to find out the distinct properties of each index. For example, the isomer-discriminating power, a measure for the ability of an index to distinguish between isomeric compounds, has been considered in the paper [68].
It seems very natural to ask how the different indices are (statistically) correlated. Obviously, they should be correlated in some way, since they are all supposed to reflect the physicochemical properties of the corresponding molecules. This chapter tries to shed some light on the relations between the various types of indices by proposing measures for the correlation of two indices and discussing them.
The main part of this chapter will deal with the asymptotic discussion of the classical correlation coefficient given by

$$r(X_n, Y_n) = \frac{E(X_n Y_n) - E(X_n)E(Y_n)}{\sqrt{\operatorname{Var}(X_n)\operatorname{Var}(Y_n)}}. \tag{6.1}$$

Here, $X_n = X(T_n)$ and $Y_n = Y(T_n)$ are the X- and Y- index of a random tree T_n on n vertices from some family of trees – for simplicity, we will only consider rooted ordered trees in detail; however, the methods can be extended to other families of simply generated trees (such as binary trees, cf. [78, 26]) quite easily. The methods of the preceding chapter may also be applied for a generalization to rooted trees and trees.
The asymptotic behaviour of the correlation coefficient will give us a measure of the linear correlation of the indices X and Y. Other possibilities to define such a measure are discussed afterwards, but it seems that there is no possibility for a similar asymptotic discussion in these cases.
We are going to investigate the following indices which were introduced in the previous chapters:

(1) The *Merrifield-Simmons-* or σ-index, i.e. the number of independent vertex subsets of a graph.

(2) The *Hosoya-* or Z-index, i.e. the number of independent edge subsets (also referred to as "matchings" by some authors).

(3) The *number of subtrees* or ρ-index.

(4) The *Wiener index*, which were the topic of chapters 2–4.

Section 6.1 will deal with the correlation of (1), (2) and (3). The Wiener index has another growth structure than the other three, so we need a different approach, which will be presented in section 6.2. Finally, we will take a look at some other statistical measures in section 6.3.

6.1 σ-, Z-, and ρ-index

The method to determine the expected values of these indices for rooted ordered trees on n vertices has been given in several papers [58, 60, 61]. In the preceding chapter, it was also explained how to extend it to rooted trees and trees. However, for the sake of completeness, it is repeated here. It is well known that the generating function for the number of rooted ordered trees is given by the functional equation

$$T(z) = \frac{z}{1 - T(z)}, \tag{6.2}$$

which is an immediate consequence of the recursive structure of this family of trees. Now, consider the σ-index for instance. We want to determine the function

$$S(z) = \sum_T \sigma(T) z^{|T|},$$

where the sum goes over all trees T and $|T|$ denotes the number of vertices. Now, we distinguish between independent sets containing the root and those not containing it. If $S_1(z)$ is the generating function for the number of subsets of the first type and $S_2(z)$ the generating function for the number of subsets of the second type, it is easy to obtain the following system of functional equations from the recursive relations introduced in the preceding chapter:

$$\begin{aligned} S_1(z) &= \frac{z}{1 - S_2(z)}, \\ S_2(z) &= \frac{z}{1 - S_1(z) - S_2(z)}. \end{aligned} \tag{6.3}$$

The asymptotic growth of the coefficients of functions satisfying algebraical equations of this kind can be determined by a standard application of Darboux's method, which is discussed in several papers such as [8, 14, 81] (sometimes, one can even find exact expressions by means of Lagrange's inversion formula; this is the case for this example (s. [58, 60]), but we won't need the exact solution, which can be given as a hypergeometric sum). However, the details can be intricate, as will be explained in the following. Here, inserting gives us

$$S_2(z) = \frac{z}{1 - \frac{z}{1 - S_2(z)} - S_2(z)}$$

or

$$S_2(z)^3 - 2S_2(z)^2 + S_2(z) - z = 0.$$

Therefore, the common singularity z_0 of $S_1(z), S_2(z)$ and $S(z) = S_1(z) + S_2(z)$ nearest to the origin is given by the system of equations

$$\begin{aligned} F(s,z) &= s^3 - 2s^2 + s - z = 0, \\ \frac{\partial}{\partial s} F(s,z) &= 3s^2 - 4s + 1 = 0, \end{aligned}$$

giving us $z_0 = \frac{4}{27}$. Using the formula for the number of rooted ordered trees on n vertices,

$$t_n = \frac{1}{n}\binom{2n-2}{n-1} \sim \frac{1}{4\sqrt{\pi}} n^{-3/2} 4^n,$$

it is easy to find out the asymptotics for the expected σ-index:

$$E(\sigma_n) \sim \sqrt{3}\left(\frac{27}{16}\right)^{n-1}.$$

Similarly, for the Z-index, we obtain the functional equations

$$\begin{aligned} Z_1(z) &= \frac{zZ_2(z)}{(1 - Z_1(z) - Z_2(z))^2}, \\ Z_2(z) &= \frac{z}{1 - Z_1(z) - Z_2(z)}, \end{aligned} \tag{6.4}$$

where $Z_1(z)$ and $Z_2(z)$ are the generating functions for the number of independent edge subsets containing resp. not containing an edge incident to the root. This system gives us the asymptotic expression for the average Z-index:

$$E(Z_n) \sim \sqrt{\frac{65 - \sqrt{13}}{78}} \left(\frac{35 + 13\sqrt{13}}{54} \right)^n .$$

Finally, for the ρ-index, the system of equations is

$$\begin{aligned} R_1(z) &= \frac{z}{1 - R_1(z) - T(z)}, \\ R_2(z) &= \frac{z}{(1 - T(z))^2}(R_1(z) + R_2(z)), \end{aligned} \tag{6.5}$$

yielding

$$E(\rho_n) \sim \frac{16}{3\sqrt{15}} \left(\frac{25}{16} \right)^n .$$

All these results have already been given in a paper of Klazar [61]. Now, to find the covariances, one needs four generating functions connected by a system of equations. For the covariance of the σ- and Z-index, for example, we take $\mathrm{SZ}_{11}, \ldots, \mathrm{SZ}_{22}$ to be the generating functions for the product of the number of independent vertex subsets and independent edge subsets such that the root is contained in

- the vertex and the edge subset,
- the vertex, but not the edge subset,
- the edge, but not the vertex subset,
- neither,

respectively. The functional equations can be seen to be a combination of those for S_1 and S_2 resp. Z_1 and Z_2:

$$\begin{aligned} \mathrm{SZ}_{11}(z) &= \frac{z\,\mathrm{SZ}_{22}(z)}{(1 - \mathrm{SZ}_{21}(z) - \mathrm{SZ}_{22}(z))^2}, \\ \mathrm{SZ}_{12}(z) &= \frac{z}{1 - \mathrm{SZ}_{21}(z) - \mathrm{SZ}_{22}(z)}, \\ \mathrm{SZ}_{21}(z) &= \frac{z(\mathrm{SZ}_{12}(z) + \mathrm{SZ}_{22}(z))}{(1 - \mathrm{SZ}_{11}(z) - \mathrm{SZ}_{12}(z) - \mathrm{SZ}_{21}(z) - \mathrm{SZ}_{22}(z))^2}, \\ \mathrm{SZ}_{22}(z) &= \frac{z}{1 - \mathrm{SZ}_{11}(z) - \mathrm{SZ}_{12}(z) - \mathrm{SZ}_{21}(z) - \mathrm{SZ}_{22}(z)}. \end{aligned} \tag{6.6}$$

Since all the functional equations can be written in polynomial form, it is possible to employ the method of Gröbner bases (cf. [35]) and a computer algebra package such as Mathematica® to obtain a single polynomial equation from the system. In this case, we find that $s = \mathrm{SZ}_{22}(z)$ satisfies the polynomial equation

$$s^{10} + 2zs^8 - 3zs^7 + z^2s^6 - 4z^2s^5 + 3z^2s^4 - z^3s^3 + 2z^3s^2 - z^3s + z^4 = 0.$$

Since $\mathrm{SZ}(z) = \mathrm{SZ}_{11}(z) + \mathrm{SZ}_{12}(z) + \mathrm{SZ}_{21}(z) + \mathrm{SZ}_{22}(z) = 1 - \frac{z}{\mathrm{SZ}_{22}(z)}$, the smallest singularity of SZ is either a singularity of SZ_{22} or a zero of SZ_{22}. However, from the functional equation we know that SZ_{22} has only one zero at $z = 0$, where the zero cancels out with the numerator. Therefore, we only have to find the smallest singularity of SZ_{22} to apply Darboux' method. For this purpose, Bender [8] gives a general theorem dealing with functional equations of the type $F(z, w(z)) = 0$. His theorem states that, given a minimal solution (with respect to absolute value) (α, β) of the system

$$F(z, w) = 0, F_w(z, w) = 0,$$

which lies within the region of analyticity of F and satisfies $F_z(\alpha, \beta), F_{ww}(\alpha, \beta) \neq 0$, the asymptotical behavior of the coefficients a_n of $w(z)$ is determined by

$$a_n \sim \sqrt{\frac{\alpha F_z(\alpha, \beta)}{2\pi F_{ww}(\alpha, \beta)}} n^{-3/2} \alpha^{-n}.$$

However, there is a mistake in this theorem, as was pointed out by Canfield [14], and this method might give erroneous results. The theorem only holds true if α is indeed the radius of convergence of $w(z)$ and the only singularity on the circle of convergence. Fortunately, things are comparatively simple in our case since we can bound the range of the singularity by an a-priori estimate. From [48, Th. 12.2.1] (see also [14]), we know that a singularity of an algebraic function $w(z)$ given by a polynomial equation of the form

$$F(z, w) = \sum_{j=0}^{k} p_{k-j}(z) w^j = 0$$

is either a zero of $p_0(z)$ (in the present case, there is no such zero) or given by a solution of the system $F(z, w) = 0$, $F_w(z, w) = 0$. The solutions of this system can be found by the method of Gröbner bases once again – it turns out that a singularity z_0 of SZ must be a solution of

$$5038848z^4 - 221833728z^3 + 5017360096z^2 + 3451610880z - 387420489 = 0.$$

Now we note that, for trivial reasons, $1 \leq \sigma(T), Z(T), \rho(T) \leq 2^{|T|}$ for all trees T. This shows that the coefficients c_n of SZ are bounded by

$$\frac{1}{n}\binom{2n-2}{n-1} \leq c_n \leq \frac{1}{n}\binom{2n-2}{n-1} \cdot 4^n,$$

so the radius of convergence of SZ lies in the interval $\left[\frac{1}{16}, \frac{1}{4}\right]$. Thus we only have to search for a solution whose absolute value lies within this interval. There is only one such solution in this case, which is given by $z_0 \approx 0.0982673$. Expanding SZ_{22} and SZ around this singularity and applying Bender's formula yields us an asymptotic expression for the expected product of σ- and Z-index:

$$E(\sigma_n Z_n) \sim (0.92565) \cdot (2.54408)^n.$$

Of course, the same way of reasoning can also be used to determine the variances of all our random variables. Therefore, we only list all the asymptotics in a table (Table 6.1).

The numerical values given stand for algebraic numbers of higher degree. Now, we can turn to the correlation coefficients. We see that

$$\begin{aligned} r(\sigma_n, Z_n) &\sim (-1.01706) \cdot (0.99405)^n, \\ r(\sigma_n, \rho_n) &\sim (1.05088) \cdot (0.99023)^n, \\ r(Z_n, \rho_n) &\sim (-1.08924) \cdot (0.97853)^n. \end{aligned}$$

We conclude that the σ and ρ-index are positively correlated, whereas they are both negatively correlated to the Z-index. The correlation coefficient tends to zero as $n \to \infty$, but rather slowly. The constant factor as well as the basis of the exponential term can be used as a measure for the correlation. So we may claim that the closest correlation of the three is between the σ- and the Z-index.

moment	asymptotics
$E(\sigma_n)$	$\sqrt{3}\left(\frac{27}{16}\right)^{n-1}$
$E(Z_n)$	$\sqrt{\frac{65-\sqrt{13}}{78}}\left(\frac{35+13\sqrt{13}}{54}\right)^n$
$E(\rho_n)$	$\frac{16}{3\sqrt{15}}\left(\frac{25}{16}\right)^n$
$E(\sigma_n Z_n)$	$(0.92565)\cdot(2.54408)^n$
$E(\sigma_n \rho_n)$	$(1.36653)\cdot(2.66477)^n$
$E(Z_n \rho_n)$	$\frac{1}{116}\sqrt{\frac{5(128985+57683\sqrt{5})}{58}}\cdot\left(8(7-3\sqrt{5})\right)^n$
$\mathrm{Var}(\sigma_n)$	$(1.03802)\cdot(2.86096)^n$
$\mathrm{Var}(Z_n)$	$(0.77227)\cdot(2.31549)^n$
$\mathrm{Var}(\rho_n)$	$\frac{64\sqrt{14}}{147}\cdot\left(\frac{81}{32}\right)^n$

Table 6.1: Asymptotical values for the moments of the considered indices.

6.2 Correlation to the Wiener index

The Wiener index has a different recursive structure than the indices discussed in the preceding section, and its growth is not exponential. We already know that the average Wiener index is asymptotically $K\cdot n^{5/2}$ for a simply generated family of trees, where K is a constant depending on the specific family (Entringer et al. [26]). For rooted ordered trees, the constant K is $\frac{\sqrt{\pi}}{4}$. We repeat the argument that yields this results here since it will be needed for the computation of the covariances.
Again, we consider the auxiliary value, $D(T)$, denoting the sum of the distances of all vertices from the root. Then, we set

$$D(z) := \sum_T D(T) z^{|T|},$$

where the sum runs over all rooted ordered trees T again. The value $D(T)$ can be calculated recursively from the branches of T as in equation 4.3 of chapter 4. In terms of $D(z)$, this gives us

$$D(z) = \frac{zD(z)}{(1-T(z))^2} + zT'(z) - T(z). \tag{6.7}$$

Now, we apply equation 4.3 of chapter 4, yielding

$$W(z) = D(z) + \frac{zW(z)}{(1-T(z))^2} + \frac{2z^2T'(z)(D(z)+zT'(z))}{(1-T(z))^3} \tag{6.8}$$

for the generating function

$$W(z) := \sum_T W(T) z^{|T|}.$$

It turns out that $W(z) = \frac{z^2}{(1-4z)^2}$, giving an average Wiener index of asymptotically $\frac{\sqrt{\pi}}{4}n^{5/2}$. Now, we introduce different generating functions for the correlation of $D(T), W(T)$ and $\sigma(T)$: let $\mathrm{DS}_1, \mathrm{DS}_2, \mathrm{WS}_1$ and WS_2 be the generating functions for the product of $D(T)$ resp. $W(T)$ with the number of independent vertex subsets containing resp. not containing the root. In analogy to the functional equations for $D(z)$ and $W(z)$ we obtain the following system of linear equations:

$$\begin{aligned}
\mathrm{DS}_1(z) &= \frac{z\,\mathrm{DS}_2(z)}{(1-S_2(z))^2} + zS_1'(z) - S_1(z),\\
\mathrm{DS}_2(z) &= \frac{z(\mathrm{DS}_1(z)+\mathrm{DS}_2(z))}{(1-S_1(z)-S_2(z))^2} + zS_2'(z) - S_2(z),\\
\mathrm{WS}_1(z) &= \mathrm{DS}_1(z) + \frac{z\,\mathrm{WS}_2(z)}{(1-S_2(z))^2} + \frac{2z^2S_2'(z)(\mathrm{DS}_2(z)+zS_2'(z))}{(1-S_2(z))^3},\\
\mathrm{WS}_2(z) &= \mathrm{DS}_2(z) + \frac{z(\mathrm{WS}_1(z)+\mathrm{WS}_2(z))}{(1-S_1(z)-S_2(z))^2}\\
&\quad + \frac{2z(zS_1'(z)+zS_2'(z))(\mathrm{DS}_1(z)+\mathrm{DS}_2(z)+zS_1'(z)+zS_2'(z))}{(1-S_1(z)-S_2(z))^3}.
\end{aligned} \tag{6.9}$$

We solve this system for WS_1 and WS_2 (which can be done explicitly in terms of S_1 and S_2 since the system is linear) and write the total generating function $\mathrm{WS}(z) = \mathrm{WS}_1(z) + \mathrm{WS}_2(z)$ in terms of S_1, S_2, S_1', S_2'. Then we make use of the functional equations for S_1 and S_2 and replace $S_1(z)$ by $\frac{z}{1-S_2(z)}$. Implicit differentiation of the equation $S_2(z)^3 - 2S_2(z)^2 + S_2(z) - z = 0$ yields

$$S_2'(z) = \frac{1}{3S_2(z)^2 - 4S_2(z) + 1},$$

so WS can be written in terms of S_2 and z only. In fact, we have

$$\mathrm{WS}(z) = \frac{N}{(1-3S_2(z))^2(1-S_2(z))^3(S_2(z)^2+S_2(z)^3-z)^2},$$

where N is a polynomial in S_2 and z. The denominator only vanishes at 0 and at the dominating singularity $\frac{4}{27}$ of S_2. Therefore, we only have to expand around WS around $\frac{4}{27}$:

$$\mathrm{WS}(z) \sim \frac{5}{81\left(1-\frac{27z}{4}\right)^2},$$

which gives us the expected value $E(W_n\sigma_n)$:

$$E(W_n\sigma_n) \sim \frac{20\sqrt{\pi}}{81} n^{5/2} \left(\frac{27}{16}\right)^n.$$

It was shown by Janson [53] that the variance of the Wiener index for rooted ordered trees is given asymptotically by

$$\mathrm{Var}(W_n) \sim \frac{16-5\pi}{80} n^5,$$

and thus the correlation coefficient of W_n and σ_n is

$$r(W_n, \sigma_n) \sim (-0.27891) \cdot (0.99767)^n.$$

Similarly, we obtain

$$\begin{aligned}
r(W_n, Z_n) &\sim (0.40351) \cdot (0.99637)^n,\\
r(W_n, \rho_n) &\sim (-1.78357) \cdot (0.98209)^n.
\end{aligned}$$

6.3 Some numerical values and their interpretation

We have seen that in all the considered cases, the correlation coefficient was of the form

$$\alpha \cdot \beta^n$$

for some constants α and β. The significance of these constants can be roughly described as follows:

- A large value of α usually means a higher correlation for trees with few vertices.
- A large value of β means that the correlation decreases very slowly – thus, it is a measure for the correlation of the indices when the number of vertices is large.

When the correlation of σ, Z and ρ was considered, β depended on the growth of both indices. If the correlation was negative in these cases (which it was except for the correlation of σ- and ρ-index), the exact asymptotics of the expected value of their product were redundant for the asymptotics of the correlation coefficient. So, in order to exploit this piece of information as well, one should separately consider normalized values of the form

$$\frac{E(X_nY_n)}{\sqrt{\operatorname{Var}(X_n)\operatorname{Var}(Y_n)}} \text{ and } \frac{E(X_n)E(Y_n)}{\sqrt{\operatorname{Var}(X_n)\operatorname{Var}(Y_n)}},$$

where X_n and Y_n are X- and Y-indices of random trees.
Further problems arise in the study of the Wiener index. Since the Wiener index only grows polynomially, β only depends on the expected value and variance of the second index. Again, one should also consider the coefficients given above separately. We have seen that they are of the same asymptotic order except from the constant factors, so one might use their quotient as a correlation measure as well. The following table gives the asymptotic behavior of these coefficients and their quotient:

Indices	$\frac{E(X_nY_n)}{\sqrt{\operatorname{Var}(X_n)\operatorname{Var}(Y_n)}}$	$\frac{E(X_n)E(Y_n)}{\sqrt{\operatorname{Var}(X_n)\operatorname{Var}(Y_n)}}$	$\frac{E(X_nY_n)}{E(X_n)E(Y_n)}$
$\sigma - Z$	$(1.03386)\cdot(0.988448)^n$	$(1.01706)\cdot(0.99405)^n$	$(1.01652)\cdot(0.99436)^n$
$\sigma - \rho$	$(1.05088)\cdot(0.99023)^n$	$(1.08694)\cdot(0.97981)^n$	$(0.96683)\cdot(1.01064)^n$
$Z - \rho$	$(1.14617)\cdot(0.96423)^n$	$(1.08924)\cdot(0.97853)^n$	$(1.05227)\cdot(0.98539)^n$
$\sigma - W$	$(7.10957)\cdot(0.99767)^n$	$(7.38848)\cdot(0.99767)^n$	0.96225
$Z - W$	$(7.80764)\cdot(0.99637)^n$	$(7.40413)\cdot(0.99637)^n$	1.05450
$\rho - W$	$(6.12924)\cdot(0.98209)^n$	$(7.91281)\cdot(0.98209)^n$	0.77460

Table 6.2: $E(X_nY_n)$ and $E(X_n)E(Y_n)$ separated.

In any case, our approach will only yield us quantitative correlation measures; qualitative information on the correlation structure is not provided.
One can calculate the exact correlation coefficients for small values of n quite easily from the functional equations. In Table 6.3, some numerical examples are given – note that the correlation coefficient only makes sense for $n \geq 4$: for $n \leq 3$, all trees are isomorphic.
We see that the correlation coefficient between σ- and Z-index is largest among those investigated in section 6.1. Likewise, the correlation to the Wiener index is highest for the ρ-index. This observation agrees with the asymptotic results of the preceding sections. The following plots (Fig. 6.1) suggest that the correlation is in fact very strong in both cases (much stronger than for the other pairs, which is quite interesting), but not entirely linear, which is clear from the exponential growth of σ-, Z- and ρ-index (this phenomenon will be discussed in detail in the following section). The plots show the values of all trees with 12 vertices.

6.4 Other correlation measures

Unfortunately, there are some drawbacks in our approach. Apart from the obvious fact that asymptotic correlations might only hold for a considerably large number of vertices, the correlation coefficient principally measures linear dependence. But since the $\sigma-$, $Z-$ and $\rho-$ indices grow exponentially with different growth rates, the dependence cannot be completely linear. So, it might be reasonable to study the correlation of their logarithms instead. The problem with that approach is the fact that generating function methods as presented in this chapter will not be applicable any longer.

n	$r(\sigma_n, Z_n)$	$r(\sigma_n, \rho_n)$	$r(Z_n, \rho_n)$	$r(\sigma_n, W_n)$	$r(Z_n, W_n)$	$r(\rho_n, W_n)$
4	-1.000000	1.000000	-1.000000	-1.000000	1.000000	-1.000000
5	-0.991189	0.971494	-0.994334	-0.923381	0.966092	-0.988064
6	-0.970054	0.947369	-0.955649	-0.870581	0.918482	-0.977131
7	-0.959741	0.926080	-0.926321	-0.829908	0.883867	-0.966673
8	-0.950801	0.907123	-0.898558	-0.796570	0.853248	-0.956356
9	-0.943296	0.890225	-0.873371	-0.768197	0.826459	-0.945962
10	-0.936479	0.875159	-0.850213	-0.743446	0.802492	-0.935353
11	-0.930116	0.861703	-0.828817	-0.721477	0.780828	-0.924449
12	-0.924048	0.849641	-0.808906	-0.701723	0.761060	-0.913214
13	-0.918187	0.838772	-0.790246	-0.683782	0.742891	-0.901641
14	-0.912479	0.828909	-0.772640	-0.667357	0.726088	-0.889750
15	-0.906888	0.819890	-0.755923	-0.652218	0.710467	-0.877574
20	-0.880077	0.783214	-0.681768	-0.590624	0.645700	-0.814057
25	-0.854498	0.753917	-0.617683	-0.544547	0.596088	-0.750155

Table 6.3: Correlation coefficients for ordered rooted trees, $n \leq 25$.

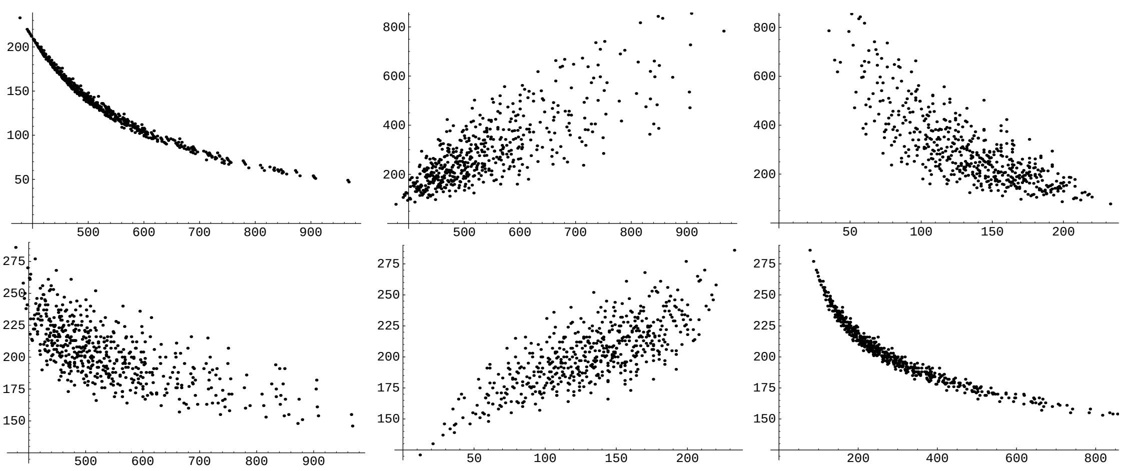

Figure 6.1: From top to bottom: σ- and Z-index, σ- and ρ-index, Z- and ρ-index, σ- and Wiener index, Z- and Wiener index, ρ- and Wiener index.

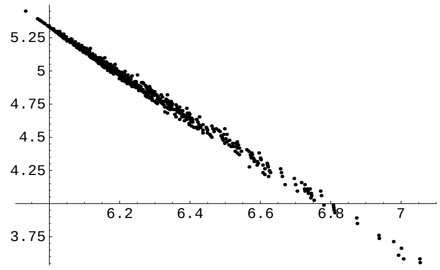

Figure 6.2: σ- and Z-index after logarithmic transformation.

The corresponding plot for the correlation of $\log \sigma_n$ and $\log Z_n$ (the random variables are rescaled in such a way that they are of equal order now!) suggests that it is reasonable to use a logarithmic transformation – it shows an almost linear correspondence (Fig. 6.2). This suggests that a sharp inequality of the form

$$f_n(\sigma(T)) \leq Z(T) \leq g_n(\sigma(T)) \tag{6.10}$$

should hold for all trees T on n vertices, where $f_n(x), g_n(x)$ behave like negative powers of x, i.e. $f_n(x) \sim a_1(n)x^{-c_1}$, $g_n(x) \sim a_2(n)x^{-c_2}$. However, it is not difficult to construct discordant pairs of trees, i.e. two trees T_1, T_2 such that $Z(T_1) > Z(T_2)$ and $\sigma(T_1) > \sigma(T_2)$.
This leads us to an alternative method of measuring correlation – the use of rank statistics (cf. [54, 67]): given two indices X and Y, we assign ranks x_i and y_i to all trees $T_1, \ldots, T_s$ on n vertices such that x_i and y_i range from 1 to s and $x_i < x_j$ if $X(T_i) < X(T_j)$ resp. $y_i < y_j$ if $Y(T_i) < Y(T_j)$. Then, a correlation measure is given by Spearman's ρ:

$$\rho_S(X_n, Y_n) = 1 - \frac{6\sum_{i=1}^{s}(x_i - y_i)^2}{s^3 - s} \tag{6.11}$$

which ranges from -1 (perfect negative correlation) to 1 (perfect positive correlation). Unfortunately, even though rank statistics are an interesting means of measuring the statistical dependence of random variables, it seems virtually impossible to apply them to our problem, since generating function methods are not apt to the treatment of ranks. It seems that rank statictics can only be applied to our problem if the number of vertices is considerably small, so that everything can be calculated explicitly.
Another problem with them is the occurrence of ties – all the random variables under consideration are discrete, and the number of trees grows larger than the maximal index in all our cases, so ties (i.e. several non-isomorphic trees of the same index) are inevitable. There are statistical methods to cope with this problem (cf. [54, 67]) – usually, if ties occur, the average rank is allotted to all tied elements. This method is used in the examples at the end of this section.
The problem of ties leads us to our final remark. The methods of this chapter easily generalize to all simply generated families of trees. However, one would like to apply them to unordered rooted trees or trees (so one can take isomorphies into account). This is possible using the methods of the previous section, but the calculational details are rather intricate.
In Table 6.4, correlation coefficients for trees with ≤ 14 vertices. If we compare them to the values of Table 6.3, we see that the correlation coefficients for ordered rooted trees provide suitable estimates.
Finally, we examine the rank correlation. Table 6.4 shows the numerical values of Spearman's ρ for all trees with ≤ 14 vertices.
Again, we observe the striking correspondence between σ- and Z-index resp. ρ- and Wiener index. It seems to be a challenging graph-theoretical problem to explain this phenomenon.

n	$r(\sigma_n, Z_n)$	$r(\sigma_n, \rho_n)$	$r(Z_n, \rho_n)$	$r(\sigma_n, W_n)$	$r(Z_n, W_n)$	$r(\rho_n, W_n)$
4	-1.000000	1.000000	-1.000000	-1.000000	1.000000	-1.000000
5	-0.995871	0.986241	-0.997176	-0.960769	0.981981	-0.993399
6	-0.977051	0.969611	-0.982970	-0.901473	0.953231	-0.977255
7	-0.955329	0.959254	-0.943865	-0.863896	0.911843	-0.959471
8	-0.930868	0.947142	-0.918181	-0.819996	0.886845	-0.940935
9	-0.908594	0.932074	-0.869200	-0.778345	0.841803	-0.91815
10	-0.890714	0.920543	-0.836300	-0.748034	0.816189	-0.899454
11	-0.877343	0.903475	-0.797497	-0.714065	0.782806	-0.879018
12	-0.869047	0.889422	-0.767693	-0.689129	0.758290	-0.860836
13	-0.862946	0.872456	-0.739304	-0.663493	0.732342	-0.843721
14	-0.859211	0.857532	-0.715078	-0.642464	0.710476	-0.827013

Table 6.4: Correlation coefficients for trees, $n \leq 14$.

n	$\rho_S(\sigma_n, Z_n)$	$\rho_S(\sigma_n, \rho_n)$	$\rho_S(Z_n, \rho_n)$	$\rho_S(\sigma_n, W_n)$	$\rho_S(Z_n, W_n)$	$\rho_S(\rho_n, W_n)$
4	-1.000000	1.000000	-1.000000	-1.000000	1.000000	-1.000000
5	-1.000000	1.000000	-1.000000	-1.000000	1.000000	-1.000000
6	-1.000000	0.942857	-0.942857	-0.942857	0.942857	-1.000000
7	-1.000000	0.918182	-0.918182	-0.877273	0.886364	-0.986364
8	-0.994071	0.881670	-0.876729	-0.867836	0.870800	-0.996789
9	-0.996126	0.854591	-0.852798	-0.805273	0.809349	-0.990171
10	-0.997048	0.832577	-0.834320	-0.774514	0.777381	-0.992314
11	-0.997392	0.811737	-0.814267	-0.746093	0.749423	-0.990921
12	-0.997471	0.796388	-0.801514	-0.724382	0.729450	-0.990146
13	-0.997421	0.781437	-0.787808	-0.697123	0.703244	-0.987169
14	-0.997383	0.770002	-0.777472	-0.675956	0.682617	-0.984820

Table 6.5: Spearman's ρ for $n \leq 14$.

Chapter 7

Enumeration Problems for classes of self-similar graphs

7.1 Introduction

In the previous chapters, we studied the properties of various indices for trees; three of them were defined as the number of subsets of a certain type. Counting sets of different kinds in graphs – especially trees – ranges among the classical problems of combinatorics. However, the applications of these indices are certainly not restricted to trees. In this chapter, we are going to investigate self-similar graphs, which are typically related to fractals.

Fractal spaces, especially the Sierpiński gasket, were first considered as interesting state spaces in stochastics in physical literature, see for example [2, 95, 96]. This work was continued by the rigorous development of brownian motion on self-similar sets, see [4] and the references therein. In all this research the approximation of fractal sets by fractal-like graphs is of vital importance. Therefore graphs obeying some fractal law were studied in many respects: See for example [42, 56, 111] and the references therein for publications on spectra of fractal-like graphs, analysis and stochastics.

The notion of graphical substitution is the basic construction principle for fractal-like graphs; however, there is no unified theory. In the following we define a very general construction scheme, which can be applied to many classical examples, including self-similar graphs and trees with finitely many cone-types, see [84, 100]. The self-similar nature of graphs in this class translates to dynamical systems for combinatorial quantities like the number of independent vertex or edge subsets or connected subsets.

A special kind of self-similar graph that has been of interest is the complete t-ary tree [63]. It is constructed in the following way:

- start with a single vertex (the root) to obtain the level-zero-tree T_0,
- take t copies of T_{n-1} and connect their roots to a new common root to obtain T_n.

A natural reason to study complete t-ary trees is that they are usually extremal with respect to the cited graph invariants among all trees of bounded degree. The number of independent sets in these graphs has been investigated in [58], the number of subtrees in [103]. In this chapter, the stated way of construction is formalized and generalized.

Other examples of graphs with self-similar properties – even though they are not among the class generated by our construction principle – that appear in applications are the rectangular and hexagonal grid graphs. For example, the growth of the number of independent sets in a $m \times n$-grid is of interest in statistical physics (see [6]). It is known that the number of independent sets in a (n, m)-grid graph grows with α^{mn}, where $\alpha = 1.503048082\ldots$ is the so-called hard square entropy constant. The bound for this constant was successively improved by Weber [109], Engel [24] and Calkin and Wilf [13].

The calculation of asymptotic formulas of this type is the main aim of our investigations – usually, in our examples, we will observe a doubly exponential growth, where the implied constants can only

be calculated numerically. Recursively defined sequences with doubly exponential growth have been investigated, for instance, by Aho and Sloane [1] and Ioanescu and Stanica [52]. The formula for the sequence defined by $x_0 = 1$, $x_n = (x_{n-1} + 1)^2$ given in [1] ($x_n = \lfloor \alpha^{2^n} \rfloor - 1$, where $\alpha = 2.258518\ldots$) has been used by Székely and Wang to determine the number of subtrees in a complete binary tree [103].
In our final example connected subsets in finite Sierpiński graphs are counted. Besides the usual doubly exponential growth, an unusual exponential factor appears in the asymptotic formula. The base of this exponential factor is apparently the same as the resistance scaling factor of the infinite Sierpiński graph, see [4] for the definition of this constant. This indicates connections between the number of connected subsets in finite self-similar graphs and random walks on the associated infinite graphs.

7.2 Construction

In the following we describe a substitutional graph construction, which resembles the construction of graph-directed self-similar sets: Fix a number $m \in \mathbb{N}$ and let the following data be given:

(G1) Initial graphs $X_1, \ldots, X_m$.

(G2) Distinguished vertices on each initial graph. For $k \in \{1, \ldots, m\}$ the distinction is given as a map $\phi_k : \{1, 2, \ldots, \theta(k)\} \to V(X_k)$, where $\theta(k) \geq 1$ is the number of distinguished vertices on X_k.

(G3) Model graphs $G_1, \ldots, G_m$.

(G4) A map $\psi_k : \{1, 2, \ldots, \theta(k)\} \to V(G_k)$, which defines $\theta(k)$ distinguished vertices on G_k.

(G5) The number $s(k) \geq 1$ of substitutions associated to the model graph G_k for $k \in \{1, \ldots, m\}$ and a map $\tau_k : \{1, \ldots, s(k)\} \to \{1, \ldots, m\}$, which describes the type of substitution. Last but not least, injective maps $\sigma_{k,i} : \{1, \ldots, \theta(\tau_k(i))\} \to V(G_k)$ for $k \in \{1, \ldots, m\}$ and $i \in \{1, \ldots, s(k)\}$, which describe each substitution.

With this data we inductively construct m sequences $(X_{k,n})_{n \geq 0}$ of graphs and maps $\phi_{k,n} : \{1, \ldots, \theta(k)\} \to V(X_{k,n})$, which define distinguished vertices of the graph $X_{k,n}$: For $k \in \{1, \ldots, m\}$ and $n = 0$ set $X_{k,0} = X_k$ and $\phi_{k,0} = \phi_k$. Now fix $n > 0$ and $k \in \{1, \ldots, m\}$. For $i \in \{1, \ldots, s(k)\}$ let $Z_{k,n,i}$ be an isomorphic copy of the graph $X_{\tau_k(i),n-1}$, where the isomorphism is given by $\gamma_{k,n,i} : X_{\tau_k(i),n-1} \to Z_{k,n,i}$. Additionally, we require that the vertex sets $V(G_k)$ and $V(Z_{k,n,1}), \ldots, V(Z_{k,n,s(k)})$ are mutually disjoint. Now let $Y_{k,n}$ be the disjoint union of the graphs G_k and $Z_{k,n,1}, \ldots, Z_{k,n,s(k)}$ and define the relation $\sim$ on the vertex set $V(Y_{k,n})$ to be the reflexive, symmetric and transitive hull of

$$\bigcup_{i=0}^{s(k)} \Big\{ \{\sigma_{k,i}(j), \gamma_{n,k,i}(\phi_{k,n-1}(j))\} \,:\, j \in \{1, \ldots, \theta(\tau_k(i))\} \Big\} \subseteq V(Y_{k,n}) \times V(Y_{k,n}).$$

Then $X_{k,n} = Y_{k,n}/\!\sim$; i.e. vertices which are equivalent with respect to $\sim$ are identified. The condition that all $\sigma_{k,i}$ are injective is imposed to avoid multiple edges which might arise from the construction. The map $\phi_{k,n}$ is defined by $\phi_{k,n}(i) = \overline{\psi(i)} \in V(X_{k,n})$. Furthermore, we call the subgraph $\overline{Z_{k,n,i}}$ of $X_{k,n}$ (which is isomorphic to $X_{\tau_k(i),n-1}$) the i-th "part" of $X_{k,n}$.

Example 7.1 (Trees with finitely many cone types) Let $A = (a_{ij})$ be an $m \times m$ matrix with non-negative integer entries. For $k \in \{1, \ldots, m\}$ let $X_k = (\{x\}, \emptyset)$, $\theta(k) = 1$, and $\phi_k(1) = x$. Furthermore, let G_k be a star with root $o_k \in V(G_k)$ and $s(k) = a_{k1} + \cdots + a_{km}$ leaves $\{x_{k,1}, \ldots, x_{k,s(k)}\}$, and let $\psi_k(1) = o_k$. Finally, we set $\tau_k(j) = t$ if

$$\sum_{i=1}^{t-1} a_{ki} < j \leq \sum_{i=1}^{t} a_{ki}$$

and $\sigma_{k,i}(1) = x_{k,i}$. Then the graphs $X_{k,n}$ constructed as above describe finite analoga of infinite trees with finitely many cone types, see [84] and the references therein.

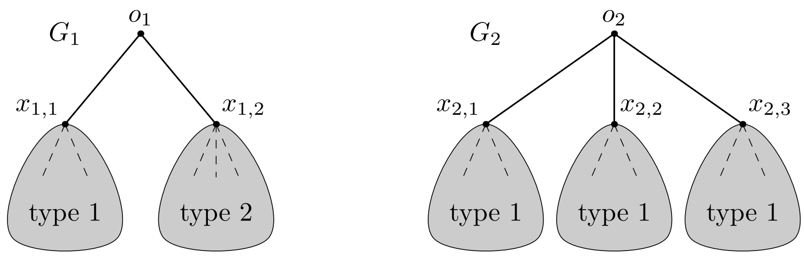

Figure 7.1: The model graphs G_1 and G_2.

Let $A = \left(\begin{smallmatrix} 1 & 1 \\ 3 & 0 \end{smallmatrix}\right)$, then Figure 7.1 shows a visualisation of the substitution procedure.

Example 7.2 (Sierpiński graphs, see [101]) Let $m = 1$ and fix some $d \in \mathbb{N}$. We define X_1 and G_1 by

$$V(X_1) = \left\{ \mathbf{x} = (x_1, \ldots, x_d) \in \mathbb{N}_0^d \,:\, \sum_{i=1}^{d} x_i = 1 \right\}, \qquad E(X_1) = \{\{\mathbf{x}, \mathbf{y}\} : \|\mathbf{x} - \mathbf{y}\|_1 = 2\}$$

and

$$V(G_1) = \left\{ \mathbf{x} = (x_1, \ldots, x_d) \in \mathbb{N}_0^d \,:\, \sum_{i=1}^{d} x_i = 2 \right\}, \qquad E(G_1) = \emptyset,$$

respectively. Let $\theta(1) = d$ and $\phi_1(i) = \mathbf{e}_i$, $\psi_1(i) = 2\mathbf{e}_i$, where $\mathbf{e}_i$ is the i-th canonical basis vector. In addition, let $s(1) = d$ and $\sigma_{1,i}(j) = \mathbf{e}_i + \mathbf{e}_j$. See Figure 7.2 for the case $d = 3$.

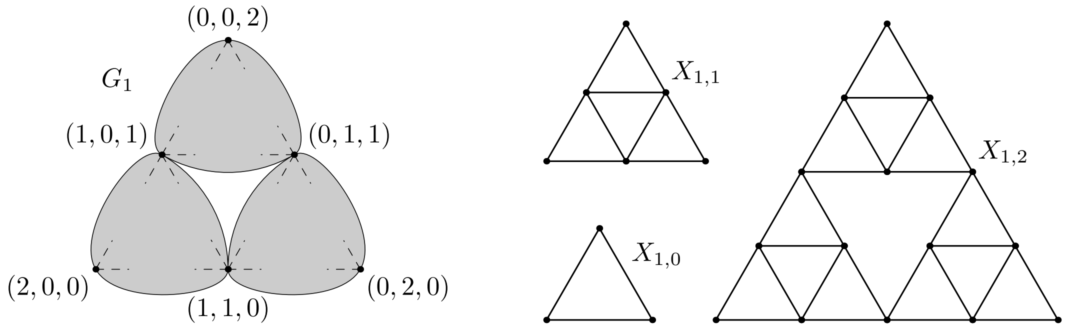

Figure 7.2: Model graph and finite Sierpiński graphs.

Example 7.3 Fix some integers $p, q \in \mathbb{N}$. Let $m = 1$, $\theta(1) = 2$ and $X_1 = K_p$. Let $x, y \in V(X_1)$ be two different vertices and set $\phi_1(1) = x$ and $\phi_1(2) = y$. Let G_1 be given by $V(G_1) = \{0, \ldots, q\}$ and $E(G_1) = \emptyset$, and define $\psi_1(1) = 1$ and $\psi_1(2) = 2$. Finaly, let $s(1) = q$ and $\sigma_{1,i}(1) = 0$, $\sigma_{1,i}(2) = i$ for $i \in \{1, \ldots, q\}$. See Figure 7.3 for the case $p = q = 4$. The associated infinite graphs were studied in [64, 65, 66] concerning growth, spectral properties and behaviour of random walk.

Example 7.4 Let $m = 1$ and let X_1 be any finite connected graph with at least two vertices x_1, x_2. We set $\theta(1) = 2$ and define $\phi_1(1) = x_1$ and $\phi_2(1) = x_2$. Let G_1 be any finite edge-less graph with at least two vertices v_1, v_2 and define $\psi_1(1) = v_1$ and $\psi_1(2) = v_2$. Furthermore, choose $s(1) = s$ mutually distinct pairs of vertices $(w_{1,1}, w_{1,2}), \ldots, (w_{s,1}, w_{s,2})$ in $V(G_1) \times V(G_1)$ and define $\sigma_{1,1}(j) = w_{j,1}$ and $\sigma_{1,2}(j) = w_{j,2}$ for $j \in \{1, \ldots, s\}$. We note that connectedness of the graphs $X_{1,1}, X_{1,2}, \ldots$ can be guaranteed if the pairs $(w_{1,1}, w_{1,2}), \ldots, (w_{s,1}, w_{s,2})$ induce a connected directed graph structure on G_1.

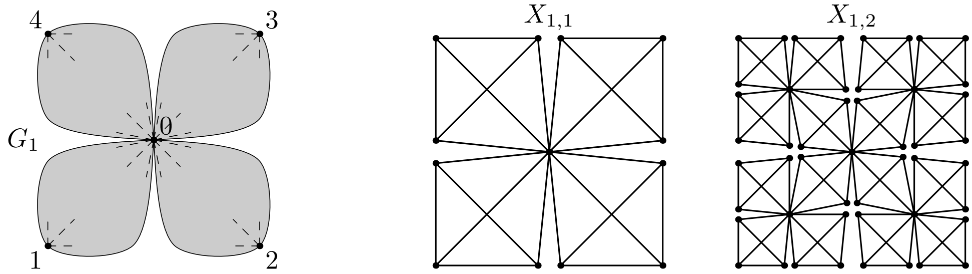

Figure 7.3: Model graph and $X_{1,1}$, $X_{1,2}$.

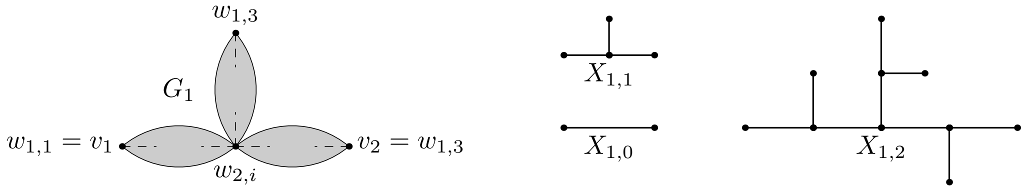

Figure 7.4: Model graph and $X_{1,0}$, $X_{1,1}$, $X_{1,2}$.

See Figure 7.4 for a simple example in this class. Spectral properties of the associated infinite graphs were investigated in [71].

Example 7.5 (The loop-erased Schreier graph of the Fabrykowski-Gupta group) First, let $m = 1$ and $X_1 = K_3$, where $V(X_1) = \{1, 2, 3\}$. Let $\theta(1) = 3$ and $\phi_1(i) = i$ for $i \in \{1, 2, 3\}$. Furthermore, define G_1 by

$$\begin{aligned} V(G_1) &= \{x_{11}, x_{12}, x_{13}, x_{21}, x_{22}, x_{23}, x_{31}, x_{32}, x_{33}\}, \\ E(G_1) &= \big\{\{x_{11}, x_{21}\}, \{x_{21}, x_{31}\}, \{x_{31}, x_{11}\}\big\}, \end{aligned}$$

and set $\psi_1(i) = x_{i2}$ for $i \in \{1, 2, 3\}$. Finally we set $s(1) = 3$ and $\sigma_{1,i}(j) = x_{ij}$.

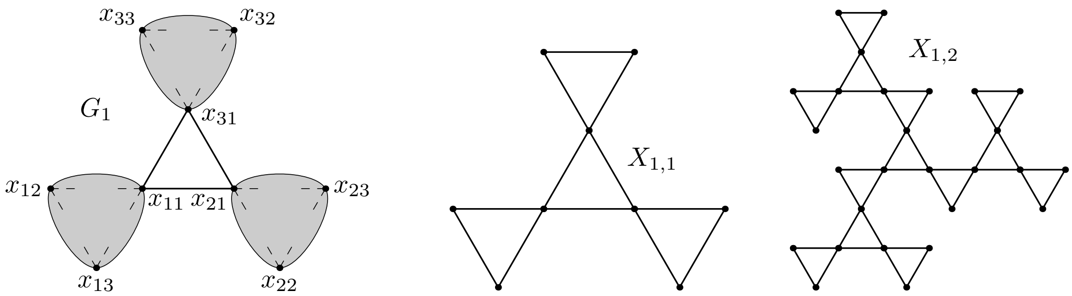

Figure 7.5: Model graph and $X_{1,1}$, $X_{1,2}$.

See Figure 7.5 for a visualization of the model graph G_1 and $X_{1,1}$, $X_{1,2}$. The Fabrykowski-Gupta group was introduced in [29], the corresponding Schreier graph was studied in [5]; see also [42].

7.3 Types of enumeration Problems

Our aim will be to solve enumeration problems in graphs of the type we defined in the previous section. We want to count the number of certain combinatorial objects (typically, sets of vertices or edges) satisfying a given property, such as independency or connectivity. Our method of solving these problems works for all properties satisfying some compatibility axioms which are presented in this section; these axioms guarantee us that we can establish recurrence equations reflecting the recursive construction of our graphs.
Let $\mathcal{C}(X)$ denote a family of combinatorial objects associated to a graph X. We want to count the number of elements $c \in \mathcal{C}(X_{k,n})$ (with the notation of the previous section) satisfying a certain property P. The set of all these elements is denoted by $\mathcal{C}(X_{k,n} \,|\, P)$. We suppose that for each $k \in \{1, \dots, m\}$ there are finitely many properties $P_{k,r}$, $r \in \{1, \dots, R_k\}$, of elements in $\mathcal{C}(X_{k,n})$ and subsets

$$B_{k,r} \subseteq \mathcal{C}(G_k) \times \prod_{i=1}^{s(k)} \{1, \dots, R_{\tau_k(i)}\},$$

so that P can be expressed in terms of $P_{k,r}$ and there exists a bijective correspondence between

$$\mathcal{C}(X_{k,n}|P_{k,r}) \qquad \text{and} \qquad \biguplus_{(b,r_1,\dots,r_{s(k)}) \in B_{k,r}} \{b\} \times \prod_{i=1}^{s(k)} \mathcal{C}(X_{\tau_k(i),n-1} \,|\, P_{\tau_k(i),r_i}). \tag{7.1}$$

Less formally spoken, the property $P_{k,r}$ can be reduced in some way to properties on the parts of $X_{k,n}$; given $(b, r_1, \dots, r_{s(k)}) \in B_{k,r}$ and objects $c_1, \dots, c_{s(k)}$ belonging to the parts of $X_{k,n}$, so that $c_i \in \mathcal{C}(X_{\tau_k(i),n-1} \,|\, P_{\tau_k(i),r_i})$, one can construct a unique object c with property $P_{k,r}$ from them, and the correspondence is bijective. Note that the same $s(k)$-tuple $(c_1, \dots, c_{s(k)})$ may appear more than once.

Example 7.6 We give a short example for illustration: let $\mathcal{C}(X_{k,n})$ be the family of vertex subsets of $X_{k,n}$, and let $P(c)$ be the property that the set c is an independent set, i.e. there is no pair of adjacent vertices in c. For the sake of notation set $\Theta(k) = \{1, \dots, \theta(k)\}$. Then we may define our properties in the following way: for all k and all subsets S of $\Theta(k)$, let a set $c \in \mathcal{C}(X_{k,n})$ with property $P_{k,S}$ be an independent set such that

$$c \cap \phi_{k,n}(\Theta(k)) = \phi_{k,n}(S).$$

Thus c contains exactly the distinguished vertices corresponding to elements of S. Clearly, P is the union of all of these properties. For $k \in \{1, \dots, m\}$, $i \in \{1, \dots, s(k)\}$ and $S \subseteq \Theta(k)$ set

$$\rho_{k,i}(S) = \{j \in \Theta(\tau_k(i)) : \sigma_{k,i}(j) \in \psi_k(S)\}.$$

So $\rho_{k,i}(S)$ corresponds to distinguished vertices of the i-th part of $X_{k,n}$, which are also distinguished vertices in $X_{k,n}$ itself. Then we define $B_{k,S}$ by

$$B_{k,S} = \mathcal{C}(G_k \,|\, Q_{k,S}) \times \prod_{i=1}^{s(k)} \{T \subseteq \Theta(\tau_k(i)) : T \cap \rho_{k,i}(\Theta(k)) = \rho_{k,i}(S)\}.$$

Here, a set b with property $Q_{k,S}$ in G_k is an independent subset such that

$$b \cap \psi_{k,n}(\Theta(k)) = \psi_{k,n}(S).$$

An independent set c in $X_{k,n}$ with property $P_{k,S}$ induces an independent set $b \in \mathcal{C}(G_k)$ and independent sets $c_1, \dots, c_{s(k)}$ in all parts of $X_{k,n}$. By the choice of S, it is fixed for the distinguished vertices of the i-th part whether they belong to c_i or not, so the c_i must satisfy properties of the form $P_{\tau_k(i),R}$. Conversely, given $b \in \mathcal{C}(G_k \,|\, Q_{k,S})$ and independent subsets in all parts of $X_{k,n}$ (with appropriately fixed distinguished vertices), one can construct a unique independent set with property $P_{k,S}$ from them.

A more intuitive description will be given in the examples of Section 7.5. The interested reader may check that each of the following properties can be handled in a similar way and thus meets with our requirements:

- matchings (independent edge subsets),
- connected subsets,
- subtrees or spanning subtrees,
- colorings,
- factors,
- vertex or edge coverings,
- maximal independent sets,
- maximal matchings.

The latter two need some additional care, but the reduction process works for them, too.

7.4 Polynomial recurrence equations

The benefit we take from the axioms of the preceding chapter is simple: it is easy now to derive recursive relations for the cardinalities of the sets $\mathcal{C}(X_{k,n} \mid P_{k,r})$. Let $c_n(k,r) := |\mathcal{C}(X_{k,n} \mid P_{k,r})|$. From the bijective correspondence (7.1) we immediately conclude that

$$c_n(k,r) = \sum_{(b,r_1,\ldots,r_{s(k)})\in B_{k,r}} \prod_{i=1}^{s(k)} c_{n-1}(\tau_k(i), r_i)$$

for $k \in \{1,\ldots,m\}$ and $r \in \{1,\ldots,R_k\}$. Now, all $c_n(k,r)$ can be obtained from the initial values $c_0(k,r)$ and this system of polynomial recurrence equations. In the following, we will show how to obtain asymptotic properties of the sequences $c_n(k,r)$ from such a system.

Proposition 7.1 Let $\mathbf{p} : \mathbb{R}^d \to \mathbb{R}^d$ be a non-linear polynomial function with non-negative coefficients and $\mathbf{c}_0 \in \mathbb{R}^d$, so that $c_{0,i} > 0$ for all $i \in \{1,\ldots,d\}$. Define the orbit sequence $(\mathbf{c}_n)_{n\geq 0}$ by $\mathbf{c}_{n+1} = \mathbf{p}(\mathbf{c}_n)$ for $n \in \mathbb{N}_0$. We assume that $c_{n,i}$ tends to ∞ as $n \to \infty$ for all $i \in \{1,\ldots,d\}$ and $c_{n,i} \asymp c_{n,j}$ as $n \to \infty$ holds for all $i,j \in \{1,\ldots,d\}$. Then $c_{n,i} = \exp(Kq^n + O(1))$ for all $i \in \{1,\ldots,d\}$, where $q > 1$ is the total degree of $\mathbf{p}$ and $K > 0$ is some constant.

Proof. Let $\mathbf{p} = (p_1,\ldots,p_d)$ and choose $k \in \{1,\ldots,d\}$, so that the total degree q of p_k is strictly larger than 1. By the conditions of the sequence $(\mathbf{c}_n)_{n\geq 0}$ there are $\mathbf{r}_n \in \mathbb{R}^d$, so that $c_{n,i} = r_{n,i}c_{n,k}$, and the set $\{r_{n,i} : n \in \mathbb{N}_0, i \in \{1,\ldots,d\}\}$ is bounded from below and above by positive constants. In the following we use multi-index notation: let

$$p_k(\mathbf{x}) = \sum_{\mathbf{i}} a_{\mathbf{i}} \mathbf{x}^{\mathbf{i}}.$$

This implies

$$c_{n+1,k} = p_k(\mathbf{c}_n) = \sum_{j=0}^{q} b_{n,j} c_{n,k}^j,$$

where the coefficients $b_{n,j}$ are defined by

$$b_{n,j} = \sum_{|\mathbf{i}|=j} a_{\mathbf{i}} \mathbf{r}_n^{\mathbf{i}}.$$

Notice that $\{b_{n,q} : n \in \mathbb{N}_0\}$ is bounded from below and above by positive constants and that $\{b_{n,j} : n \in \mathbb{N}_0\}$ is bounded above for all $j < q$. Write $x_n = \log(c_{n,k})$, then

$$x_{n+1} = qx_n + d_n, \tag{7.2}$$

where d_n is given by

$$d_n = \log\left(\sum_{j=0}^{q} b_{n,j} c_{n,k}^{j-q}\right).$$

Since $c_{n,k}$ tends to ∞, the numbers d_n are bounded. Now Equation (7.2) implies

$$x_n = q^n\left(x_0 + \sum_{\ell=0}^{n-1} \frac{d_\ell}{q^{\ell+1}}\right) = q^n\left(x_0 + \sum_{\ell=0}^{\infty} \frac{d_\ell}{q^{\ell+1}} + O(q^{-n})\right).$$

Define K by

$$K = x_0 + \sum_{\ell=0}^{\infty} \frac{d_\ell}{q^{\ell+1}},$$

then $c_{n,1} = \exp(Kq^n + O(1))$ follows. This implies the statement. Furthermore, we remark that the total degree of p_i must be q for any $i \in \{1, \ldots, d\}$. ■

Remark. With the notation of the previous proof we notice that the asymptotic behavior of the sequence $(\mathbf{c}_n)_n$ is mostly determined by those monomials of $\mathbf{p}$ of total degree q. By the previous result there are vectors $\mathbf{C}_n \in \mathbb{R}^d$ (bounded above and below) such that $\mathbf{c}_n = \mathbf{C}_n \exp(Kq^n)$. Now write $\mathbf{p} = \mathbf{h} + \mathbf{r}$, where all monomials of $\mathbf{h}$ have total degree q and the total degree of $\mathbf{r}$ is strictly smaller than q. So h is a homogeneous polynomial of degree q. Then

$$\begin{aligned}\mathbf{C}_{n+1} \exp(Kq^{n+1}) &= \mathbf{c}_{n+1} = \mathbf{p}(\mathbf{c}_n) = \mathbf{h}(\mathbf{c}_n) + \mathbf{r}(\mathbf{c}_n)\\ &= \mathbf{h}(\mathbf{C}_n \exp(Kq^n)) + \mathbf{r}(\mathbf{C}_n \exp(Kq^n))\\ &= \exp(Kq^{n+1})\mathbf{h}(\mathbf{C}_n) + O(\exp(K(q-1)q^n)).\end{aligned}$$

This implies $\mathbf{C}_{n+1} = \mathbf{h}(\mathbf{C}_n) + O(\exp(-Kq^n))$. In order to obtain information about $\mathbf{C}_n$ we have to study the dynamical system associated to the map $\mathbf{h}$. The case $\mathbf{r} \equiv \mathbf{0}$ is of special interest: on the one hand it occurs in the given examples, on the other hand the error term disappears leading to $\mathbf{C}_{n+1} = \mathbf{h}(\mathbf{C}_n)$. Thus, in this case we have to investigate the dynamical behavior of $\mathbf{h}$ in the projective space.

Proposition 7.2 Let $\mathbf{p} : \mathbb{R}^d \to \mathbb{R}^d$ be a homogeneous polynomial of degree $q > 1$ with an attracting fixed point $\mathbf{C} \neq \mathbf{0}$. Let $\mathbf{c}_0 \in \mathbb{R}^d$ and define $\mathbf{c}_{n+1} = \mathbf{p}(\mathbf{c}_n)$ for $n \in \mathbb{N}_0$. We assume that $(\mathbf{c}_n)_{n\geq 0}$ defines a sequence in the projective space $\mathbb{P}^{d-1}$ converging to $\mathbf{C}$ in $\mathbb{P}^{d-1}$. Then $\mathbf{c}_n = \mathbf{C}\exp(Kq^n + o(1))$ for some $K \in \mathbb{R}$.

Proof. As $\mathbf{c}_n \to \mathbf{C}$ in $\mathbb{P}^{d-1}$ there are $r_n \neq 0$ such that $r_n\mathbf{c}_n \to \mathbf{C}$ in $\mathbb{R}^d$. Thus the sequence $\boldsymbol{\varepsilon}_n = r_n\mathbf{c}_n - \mathbf{C}$ converges to $\mathbf{0}$. Define $\mathbf{u}_n$ by $\mathbf{u}_n = \mathbf{p}(\mathbf{C} + \boldsymbol{\varepsilon}_n) - \mathbf{C}$. As $\mathbf{C}$ is an attracting fixed point of $\mathbf{p}$, the sequence $(\mathbf{u}_n)_{n\geq 0}$ converges to $\mathbf{0}$, too. An easy computation yields

$$r_n^q(\mathbf{C} + \boldsymbol{\varepsilon}_{n+1}) = r_{n+1}(\mathbf{C} + \mathbf{u}_n).$$

There exists a $k \in \{1, \ldots, d\}$ with $C_k \neq 0$. Choose n_0 sufficiently large, so that

$$d_n = \frac{C_k + \varepsilon_{n+1,k}}{C_k + u_{n,k}}$$

satisfies $|d_n - 1| < \frac{1}{2}$ for all $n \geq n_0$. Notice that $d_n \to 1$. This implies

$$\log(r_n) = q\log(r_{n-1}) + \log(d_{n-1}) = q^n\left(q^{-n_0}\log(r_{n_0}) + \sum_{\ell=n_0}^{n-1} \frac{\log(d_\ell)}{q^{\ell+1}}\right) = -Kq^n + o(1),$$

where K is given by

$$K = -q^{-n_0}\log(r_{n_0}) - \sum_{\ell=n_0}^{\infty} \frac{\log(d_\ell)}{q^{\ell+1}}.$$

Therefore $r_n = \exp(-Kq^n + o(1))$. Since $r_n\mathbf{c}_n \to \mathbf{C}$, we obtain $\mathbf{c}_n = \mathbf{C}\exp(Kq^n + o(1))$. ■

Remark. The last proposition can be generalized to the case of an attracting cycle $\mathbf{C}_1, \ldots, \mathbf{C}_m$ of $\mathbf{p}$. If the sequence $(\mathbf{c}_n)$ is attracted by this cycle in $\mathbb{P}^{d-1}$, then an adapted version of the result above holds.

The preceding propositions give us the necessary tools to cope with a variety of set-counting problems for classes of self-similar graphs. Unfortunately, they are not applicable to all conceivable problems of that kind. In can be seen especially from the example of section 7.5.3 that there is a vast variety of possibilities for the asymptotical behavior of a polynomial recurrence system.

7.5 Examples

7.5.1 Matchings, maximal matchings and maximum matchings

We turn to Example 7.5 of Section 7.2 now. The sequence of graphs that was constructed in this example has some particularly nice properties in connection with matchings, therefore, we present the problem of enumerating the matchings on this graph here. First, we consider ordinary matchings.

Let $m_{0,n}$ be the total number of matchings in the level-n-graph $X_{1,n}$ of the construction described in Example 7.5 of Section 7.2. Furthermore, let $m_{1,n}$ be the number of matchings with the property that a fixed vertex from the set of distinguished vertices (i.e., one of the outermost vertices) is unmatched, and let $m_{2,n}$ be the number of matchings with the property that two fixed vertices from the set of distinguished vertices are unmatched. By symmetry, it is not relevant which of the distinguished vertices we choose.

It is easy to see that $m_{0,0} = 4$, $m_{1,0} = 2$ and $m_{2,0} = 1$, and that the following system of recurrence equations holds (we only have to consider four cases for the center triangle – either none of the edges of the center triangle belongs to the matchings or one of the three belongs to it):

$$\begin{aligned}
m_{0,n+1} &= m_{0,n}^3 + 3m_{0,n}m_{1,n}^2,\\
m_{1,n+1} &= m_{0,n}^2 m_{1,n} + m_{1,n}^3 + 2m_{0,n}m_{1,n}m_{2,n},\\
m_{2,n+1} &= m_{0,n}m_{1,n}^2 + m_{0,n}m_{2,n}^2 + 2m_{1,n}^2 m_{2,n}.
\end{aligned}$$

A straightforward induction shows us that $m_{0,n} = 2m_{1,n} = 4m_{2,n}$ holds for all n. This can also be seen by an easy combinatorial argument:

Let v be one of the distinguished vertices (or any of the outermost vertices in the graph $X_{1,n}$), let v' be its neighbor of degree 2, and let w be its neighbor of degree 4. Clearly, the number of matchings containing the edge vv' is the same as the number of matchings in which v and v' are not matched at all. By symmetry, the number of matchings which match v is the same as the number of matchings which match v'. Altogether, this shows that the number of matchings which match v is exactly half of the total number of matchings.

The fact that the number of matchings which contain edges incident to two fixed distinguished vertices is exactly $\frac{1}{4}$ of the total number of matchings reflects the fact that the distinguished vertices (and, generally, arbitrary pairs of non-adjacent vertices which belong to the same orbit as the distinguished vertices) are independent with respect to the number of matchings – whether one of the vertices is to be matched or not does not affect the fraction of matchings in which the other is matched. This is due to the described bijections between matchings containing the edge $v'v$ and those matching neither v nor v' resp. matchings containing vw and those containing $v'w$.

Thus, we only have to consider the simple recurrence equation

$$m_{0,n+1} = \frac{7}{4}m_{0,n}^3,$$

whose solution is given by $m_{0,n} = \frac{2}{\sqrt{7}}(2\sqrt{7})^{3^n}$. The first values of this sequence are $4, 112, 2458624$, $26008445689991790592, \ldots$ So if $E = \frac{3^{n+2}-3}{2}$ is the number of edges, $\left(\frac{16}{7}\right)^{1/3} 28^{E/9}$ of the 2^E edge subsets are independent. The constant $28^{1/9}$ is approximately 1.4480892743.
Now, let us consider maximal matchings, i.e. matchings which cannot be extended any more. A little more care is needed for them, and some more variables as well. Again, we only have to consider two distinguished vertices and four cases for the edges in the middle triangle, but we have to consider three types of matchings with respect to a distinguished vertex $v = \phi_{1,n}(i)$:

- maximal matchings which match v,
- maximal matchings which leave v unmatched,
- matchings (not necessarily maximal) which leave v unmatched, with the additional property that every edge that can be added to the mathing is incident to v.

Let us mark these properties by the numbers 0,1 and 2 respectively, and define sequences $M_{00,n}$, $M_{01,n}, \ldots, M_{22,n}$, where, for instance, $M_{02,n}$ denotes the number of matchings in $X_{1,n}$ with the property that they contain an edge incident to one fixed distinguished vertex $v = \phi_{1,n}(i)$ and leave another fixed distinguished vertex $w = \phi_{1,n}(j)$ unmatched and can at most be extended by an edge containing w. By thoroughly distinguishing cases for the edges of the middle triangle, we obtain the general recurrence equation

$$\begin{aligned} M_{ij,n+1} = {} & M_{i2,n}M_{j2,n}(M_{00,n} + 2M_{01,n} + M_{11,n}) + M_{i2,n}(M_{j0,n} + M_{j1,n})(M_{02,n} + M_{12,n}) \\ & + (M_{i0,n} + M_{i1,n})M_{j2,n}(M_{02,n} + M_{12,n}) + M_{i1,n}M_{j0,n}(M_{00,n} + M_{01,n}) \\ & + M_{i0,n}M_{j1,n}(M_{00,n} + M_{01,n}) + M_{i0,n}M_{j0,n}(M_{01,n} + M_{11,n}) \\ & + M_{i0,n}M_{j0,n}(M_{00,n} + M_{01,n}). \end{aligned}$$

together with the observation that, clearly, $M_{ij,n} = M_{ji,n}$. The initial values are given by $M_{00,0} = M_{01,0} = M_{02,0} = M_{22,0} = 1$ and $M_{11,0} = M_{12,0} = 0$. The total number of maximal matchings is given by $(M_{00,n} + 2M_{01,n} + M_{11,n})$. Now, if we regard the recursion for the $M_{ij,n}$ as a map in the projective space $\mathbb{P}^5$ of dimension 5, it is easy to check that every point of the algebraic surface

$$\left\{(x_{00}, x_{01}, x_{02}, x_{11}, x_{12}, x_{22}) = (a^2, ab, ac, b^2, bc, c^2)\right\} \tag{7.3}$$

is a superattractive fixed point of the dynamical system which is applied to the $M_{ij,n}$. In our case, the $M_{ij,n}$ tend (in projective space) to the following vector, which can be computed numerically:

$$(x_{00}, x_{01}, x_{02}, x_{11}, x_{12}, x_{22}) = (0.390764, 0.162426, 0.292467, 0.0675145, 0.121568, 0.218897).$$

These values are chosen in such a way that the vector is also a fixed point of the system in $\mathbb{R}^6$. Now, by the observations of Section 7.4, in particular Proposition 7.2, we know that

$$\begin{aligned} &(M_{00,n}, M_{01,n}, M_{02,n}, M_{11,n}, M_{12,n}, M_{22,n}) \\ &\qquad \sim (0.390764, 0.162426, 0.292467, 0.0675145, 0.121568, 0.218897) \cdot \beta^{3^n} \end{aligned}$$

for some constant β, whose numerical value is $\beta = 3.3200219636\ldots$ (we skip the calculational details). So, the total number of maximal matchings in the graph $X_{1,n}$ we are considering is asymptotically $1.1682830147 \cdot (1.3055968738)^E$, where E denotes the number of edges again. The first few values are $3, 29, 38375, 92180751403625, \ldots$ The parametrisation (7.3) shows us that

$$\frac{M_{01,n}}{M_{00,n}} \sim \frac{M_{11,n}}{M_{01,n}} \sim \frac{M_{12,n}}{M_{02,n}}$$

and

$$\frac{M_{02,n}}{M_{00,n}} \sim \frac{M_{12,n}}{M_{01,n}} \sim \frac{M_{22,n}}{M_{02,n}},$$

so pairs of distinguished vertices are at least "asymptotically independent" of each other in this case. Roughly speaking, as the distance grows, the vertices do not interfere any more.
Finally, we observe that the graphs we studied within this section cannot have perfect matchings, since the number of vertices of $X_{1,n}$ is 3^{n+1}, an odd number. However, the following remarkable fact holds:

Theorem 7.3 *For every vertex v in the level-n graph $X_{1,n}$ of our construction, there is exactly one perfect matching in the graph $X_{1,n} \setminus v$.*

Proof. By induction on n. For $n = 0$, the theorem is essentially trivial. For the induction step, let, for the sake of brevity, P_1, P_2 and P_3 denote the parts which are joined by the center triangle, and let w_1, w_2, w_3 be the corresponding vertices of the center triangle. Without loss of generality, suppose that v belongs to P_3. Since P_1 contains an odd number of vertices, not all of the vertices of P_1 can be matched within P_1. The only vertex of P_1 which has neighbors outside P_1 is w_1, so w_1 is matched to either w_2 or w_3. Since the same holds true for w_2, w_1 and w_2 must be matched to each other. Now, the graph decomposes into the three parts, each reduced by exactly one vertex. By the induction hypothesis, we are done. ■

Corollary 7.4 The level-n graph $X_{1,n}$ of our construction has exactly 3^{n+1} maximum matchings (i.e. matchings of largest possible size), which equals the number of vertices.

7.5.2 Independent subsets in tree-like graphs

Theorem 7.5 *Let $p, q \geq 2$ be fixed integers, and define $X_{1,n}$ as in Example 7.3 of Section 7.2. Denote by a_n the number of independent vertex subsets of $X_{1,n}$. Then we have*

$$a_n \sim c_{p,q} \alpha_{p,q}^{q^n}$$

for some constants $\alpha_{p,q}$ and $c_{p,q}$. $\alpha_{p,q}$ can be estimated in the following way:

$$\left(2p^{q^2-q} + 2(p^q - p^{q-1} + 1)^q\right)^{q^{-2}} \leq \alpha_{p,q} \leq \left(p^{q^2-q} + (p^q - p^{q-1} + 1)^q\right)^{q^{-2}}.$$

Furthermore, $\alpha_{p,q}$ has a Laurent expansion around $p = \infty$, whose first terms are

$$\alpha_{p,q} = p - \frac{1}{q-1} + \frac{2-q}{2(q-1)^2 p} + \dots$$

if $q > 2$.

Proof. We distinguish three cases for the number of independent vertex subsets, depending on the vertices $\phi_{1,n}(i)$ $(i = 1, 2)$:

- the number of independent vertex subsets containing none of these two vertices,
- the number of independent vertex subsets containing only $\phi_{1,n}(1)$ (by symmetry, this is the same as the number of independent vertex subsets containing only $\phi_{1,n}(2)$),
- the number of independent vertex subsets containing both of them.

We denote the first number by $a_{0,n}$, the second by $a_{1,n}$, and the third by $a_{2,n}$. Then, by distinguishing whether the center belongs to the independent subset or not, we obtain the following system of recurrence equations:

$$\begin{aligned}
a_{0,n+1} &= a_{0,n}^2 (a_{0,n} + a_{1,n})^{q-2} + a_{1,n}^2 (a_{1,n} + a_{2,n})^{q-2}, \\
a_{1,n+1} &= a_{0,n} a_{1,n} (a_{0,n} + a_{1,n})^{q-2} + a_{1,n} a_{2,n} (a_{1,n} + a_{2,n})^{q-2}, \\
a_{2,n+1} &= a_{1,n}^2 (a_{0,n} + a_{1,n})^{q-2} + a_{2,n}^2 (a_{1,n} + a_{2,n})^{q-2}.
\end{aligned}$$

We are interested in the total quantity

$$a_n = a_{0,n} + 2a_{1,n} + a_{2,n},$$

which, by the recurrence equations given above, satisfies

$$a_{n+1} = (a_{0,n} + a_{1,n})^q + (a_{1,n} + a_{2,n})^q.$$

Taking $x_n = \log a_n$, we obtain the recurrence

$$x_{n+1} = qx_n + \log\left(\left(\frac{a_{0,n} + a_{1,n}}{a_n}\right)^q + \left(\frac{a_{1,n} + a_{2,n}}{a_n}\right)^q\right).$$

We use d_n for the second summand, which can be estimated easily by using the fact that

$$\frac{a_{0,n} + a_{1,n}}{a_n} + \frac{a_{1,n} + a_{2,n}}{a_n} = 1$$

and $x \mapsto x^q$ is a convex function: we have

$$0 \geq d_n \geq \log 2^{1-q} = (1-q)\log 2.$$

Therefore, d_n is bounded. Now, the solution of

$$x_{n+1} = qx_n + d_n$$

is given by

$$x_n = q^n\left(x_0 + \frac{d_0}{q} + \frac{d_1}{q^2} + \cdots + \frac{d_{n-1}}{q^n}\right).$$

Since d_n is bounded, the sum

$$\sum_{k=0}^{\infty} \frac{d_k}{q^{k+1}}$$

converges, so x_n can be written as

$$x_n = q^n\left(x_0 + \sum_{k=0}^{\infty} \frac{d_k}{q^{k+1}} + R(n)\right),$$

and $R(n)$ satisfies

$$0 \leq R(n) \leq q^{-n}\log 2,$$

which means that

$$a_n = C(n)\alpha_{p,q}^{q^n},$$

where $C(n)$ is between 1 and 2 and $\alpha_{p,q}$ is given by

$$\alpha_{p,q} = \exp\left(x_0 + \sum_{k=0}^{\infty} \frac{d_k}{q^{k+1}}\right).$$

By calculating the first values of $a_{0,n}, a_{1,n}$ and $a_{2,n}$ explicitly (the starting values are $a_{0,0} = p-1, a_{1,0} = 1, a_{2,0} = 0$), we obtain an estimate for $\alpha_{p,q}$ – breaking up with d_1 gives the stated result. Furthermore, we see that

$$\alpha_{p,q} = \lim_{n\to\infty} a_n^{q^{-n}}$$

is uniformly convergent in p (since the error term can be bounded independently of p as above). Therefore, we can also obtain the Laurent expansion of $\alpha_{p,q}$ at $p = \infty$ by calculating the expansions of $a_K^{q^{-K}}$ (it is easy to see that the coefficients in the Laurent series of a_K must satisfy some linear recurrence equations) and passing to the limit. We obtain

$$\alpha_{p,q} = p - \frac{1}{q-1} + \frac{2-q}{2(q-1)^2 p} + O(p^{-2}),$$

if $q > 2$. In the simple special case of $q = 2$, the expansion is

$$p-1+p^{-1}+p^{-2}-2p^{-4}-3p^{-5}+p^{-6}+11p^{-7}+15p^{-8}-13p^{-9}-77p^{-10}-86p^{-11}+144p^{-12}+595p^{-13}+\cdots$$

which belongs to the function

$$\alpha(p,2) = \frac{1}{2}\left(-1+p+\sqrt{5-2p+p^2}\right).$$

In this special case, the corresponding graphs are chains of K_p's, and everything can be reduced to linear recurrence equations. It is not easy to tell whether $\alpha_{p,q}$ can be expressed by elementary functions in general. For $q = 3$, for instance, we obtain

$$p - \frac{1}{2} - \frac{1}{8}p^{-1} + \frac{7}{16}p^{-2} + \frac{91}{128}p^{-3} + \frac{827}{768}p^{-4} + \frac{2657}{3072}p^{-5} - \frac{3547}{6144}p^{-6} - \frac{138861}{32768}p^{-7} + \cdots$$

Last, we take a look at the term $C(n)$ and prove that it tends to a limit. We note first that $\frac{a_{0,n}}{a_{1,n}}$ and $\frac{a_{1,n}}{a_{2,n}}$ are bounded: trivially, $\frac{a_{0,n}}{a_{1,n}} \geq 1$. Moreover, for each independent subset that doesn't contain $\phi_{1,n}(1)$, we obtain an independent subset containing $\phi_{1,n}(1)$ by removing the neighbors of $\phi_{1,n}(1)$ (there is at most one of them within an independent set since they are pairwise adjacent) and adding $\phi_{1,n}(1)$. This shows that $\frac{a_{0,n}}{a_{1,n}} \leq p$ (as an a-priori estimate). Analogously, $1 \leq \frac{a_{1,n}}{a_{2,n}} \leq p$ holds as well. We introduce the notations $u_n = \frac{a_{0,n}}{a_{1,n}}$ and $v_n = \frac{a_{2,n}}{a_{1,n}}$. Then we observe that

$$\begin{aligned}
|u_{n+1}v_{n+1} - 1| &= \left| \frac{(1+u_n)^{q-2}(1+v_n)^{q-2}(u_n v_n - 1)^2}{(u_n(1+u_n)^{q-2} + v_n(1+v_n)^{q-2})^2} \right| \\
&\leq \left| \frac{(1+u_n)^{q-2}(1+v_n)^{q-2}(u_n v_n - 1)^2}{u_n^2(1+u_n)^{2(q-2)}} \right| \\
&= \left(\frac{1+v_n}{1+u_n} \right)^{q-2} \frac{(u_n v_n - 1)^2}{u_n^2} \\
&\leq |u_n v_n - 1| \cdot |\frac{u_n v_n - 1}{u_n^2}|
\end{aligned}$$

We note that $\frac{1}{p} - 1 \leq u_n v_n - 1 \leq u_n^2 - 1$ and $1 \leq u_n \leq p$ by our a-priori-estimates. Therefore, $\left|\frac{u_n v_n - 1}{u_n^2}\right| \leq 1 - \frac{1}{p^2}$ for all n, which shows that $u_n v_n$ tends to 1 as $n \to \infty$.
This means that the dynamical system

$$\begin{pmatrix} a_0 \\ a_1 \\ a_2 \end{pmatrix} \mapsto \begin{pmatrix} a_0^2(a_0+a_1)^{q-2} + a_1^2(a_1+a_2)^{q-2} \\ a_0 a_1 (a_0+a_1)^{q-2} + a_1 a_2 (a_1+a_2)^{q-2} \\ a_1^2(a_0+a_1)^{q-2} + a_2^2(a_1+a_2)^{q-2} \end{pmatrix},$$

regarded as a map in projective space, has a set of (superattractive, which is easy to verify) fixed points given by the algebraic curve $\{(z, 1, \frac{1}{z}) : z \in \mathbb{C}\}$, and the vector $(a_{0,n}, a_{1,n}, a_{2,n})$ has to tend to a fixed point from this set. The parametrisation of the curve shows that the percentage of independent subsets which contain one of the distinguished vertices is asymptotically independent of the other. Now, we can conclude that d_n tends to a limit d, which, in turn, means that

$$q^n R(n) = -q^n \sum_{k=n}^{\infty} \frac{d_k}{q^{k+1}}$$

tends to $-\frac{d}{q-1}$. This gives us the constant term in the asymptotics of a_n. ∎

7.5.3 Antichains in trees with finitely many cone types

In this section, we will regard a rooted tree of the type described in Example 7.1 of Section 7.2 as a partially ordered set and count the number of antichains in a tree of this type. In particular, we will prove the following theorem:

Theorem 7.6 *Let $A = (a_{ij})$ be an $m \times m$ matrix with non-negative integer entries, and define $X_{k,n}$ as in Example 7.1 of Section 7.2. Let $c_{k,n}$ be the number of antichains in $X_{k,n}$. Then we have*

$$c_{k,n} \sim \exp\left(\sum_{s=1}^{S} \lambda_s^n P_{s,k}(n) + Q_k(n)\log n + R_k(n)\right). \tag{7.4}$$

Here, the λ_s denote the eigenvalues of A of absolute value not less than 1 (except 1), and $P_{s,k}$, Q_k and R_k are computable polynomials. $Q_k \not\equiv 0$ can only happen if $\lambda = 1$ is an eigenvalue of A.

Proof. It is easy to see that

$$c_{k,n+1} = \prod_{j=1}^{s(k)} (1 + c_{\tau_k(j),n}) = \prod_{i=1}^{m} (1 + c_{i,n})^{a_{ki}}, \tag{7.5}$$

since an antichain in $X_{k,n}$ induces antichains (or empty sets) in the parts of $X_{k,n}$. If we substitute $x_{k,n} = \log c_{k,n}$, we obtain

$$x_{k,n+1} = \sum_{i=1}^{m} a_{ki} x_{i,n} + \sum_{i=1}^{m} a_{ki} \log(1 + c_{i,n}^{-1}).$$

Now we need an a-priori estimate for $c_{k,n}$. We prove that $c_{k,n}$ is either a non-constant polynomial in n for $n > n_0$ or grows at least exponentially. The former is only the case when the cones belonging to the vertices of $X_{k,n}$ are – with only finitely many exceptions – linear chains. We show this by considering the number of leaves of $X_{k,n}$. This number is given by a linear recursion (depending on A) and is non-decreasing. Thus it is either bounded (which means that almost all cones are linear chains) or grows at least linearly. Note that any collection of leaves forms an antichain, and that the number of antichains in a linear chain of length n is exactly n. Together with (7.5), this implies that $c_{k,n}$ is a polynomial in n for all $n > n_0$ if it does not grow at least exponentially.
We write $\mathbf{x}_n$ for the column vector $(x_{1,n}, \dots, x_{m,n})^{\mathrm{t}}$ and $\mathbf{d}_n = (d_{1,n}, \dots, d_{m,n})^{\mathrm{t}}$, where $d_{k,n} = \log(1 + c_{k,n}^{-1})$. Then the recursion transforms to

$$\mathbf{x}_{n+1} = A\mathbf{x}_n + A\mathbf{d}_n$$

or

$$\mathbf{x}_n = A^n \mathbf{x}_0 + A^n \mathbf{d}_0 + A^{n-1}\mathbf{d}_1 + \cdots + A\mathbf{d}_{n-1}.$$

Now, let $S^{-1}TS$ be the Jordan decomposition of A. Then this can be rewritten as

$$\mathbf{x}_n = S^{-1}(T^n S\mathbf{x}_0 + T^n S\mathbf{d}_0 + T^{n-1}S\mathbf{d}_1 + \cdots + TS\mathbf{d}_{n-1}).$$

For the inner sum, we may suppose that T is a single Jordan block. The total vector is then obtained from joining the vectors belonging to the single Jordan blocks. Let λ be the eigenvalue the Jordan block T belongs to and t the size of the block. We distinguish the following three cases:

(1) $|\lambda| < 1$: Then, since $A^j = O(\lambda^j j^{t-1})$ and $\mathbf{d}_j = O(j^{-1})$, we have

$$T^n S\mathbf{x}_0 + T^n S\mathbf{d}_0 + \cdots + TS\mathbf{d}_{n-1} = O\big(\tfrac{1}{n}\big).$$

(2) $|\lambda| > 1$: T is an invertible matrix, so we can write

$$\begin{aligned} T^n S\mathbf{x}_0 + T^n S\mathbf{d}_0 + \cdots + TS\mathbf{d}_{n-1} &= T^n \left(S\mathbf{x}_0 + \sum_{j=0}^{n-1} T^{-j} S\mathbf{d}_j \right) \\ &= T^n \left(S\mathbf{x}_0 + \sum_{j=0}^{\infty} T^{-j} S\mathbf{d}_j - \sum_{j=n}^{\infty} T^{-j} S\mathbf{d}_j \right). \end{aligned}$$

The infinite sums are convergent, since $T^{-j} = O(\lambda^{-j} j^{t-1})$. For $j > n_0$, we know that all $d_{k,j}$ are either of the form $\log\left(1 + p(j)^{-1}\right)$ for some polynomial p or exponentially decreasing in terms of j. By using the expansion around ∞, we obtain

$$S\mathbf{d}_j = (p_1(j^{-1}), \ldots, p_t(j^{-1}))^{\mathrm{t}} + O(j^{-t}),$$

where the p_i are polynomials of degree $\leq t-1$ with constant coefficient 0. It is well known that

$$\sum_{j=n}^{\infty} \lambda^{-j} j^{\ell} = \lambda^{-n} \left(\sum_{\nu=0}^{s-1} \binom{\ell}{\nu} \operatorname{Li}_{-\nu}(\lambda^{-1}) n^{\ell-\nu} + O(n^{\ell-s}) \right),$$

where $\operatorname{Li}_{\sigma}(z) = \sum_{j=0}^{\infty} j^{-\sigma} z^j$ is a *polylogarithm*, see [69]. Therefore, the sum $\sum_{j=n}^{\infty} T^{-j} S\mathbf{d}_j$ can be written in the form

$$T^{-n} \cdot \left((r_1(n), \ldots, r_t(n))^{\mathrm{t}} + O(n^{-1}) \right),$$

where the r_i are polynomials of degree $\leq t-1$. Altogether, this implies that

$$T^n \sum_{j=n}^{\infty} T^{-j} S\mathbf{d}_j = \mathbf{R}(n) + O(n^{-1}),$$

where $\mathbf{R}$ is a vector of polynomials of degree $\leq t-1$.

(3) $|\lambda| = 1$: this case is almost analogous to $|\lambda| > 1$. Again, we expand $\mathbf{d}_j$ around ∞; then, consider the sums

$$\sum_{j=1}^{n-1} \lambda^{-j} j^{\ell}.$$

For $\ell \leq -t$, these sums are convergent with an error term of $\sum_{j=n}^{\infty} \lambda^{-j} j^{\ell} = O(n^{-t})$. For all other ℓ, these sums can be written as

$$\sum_{j=1}^{n-1} \lambda^{-j} j^{\ell} = C_{\ell} + \lambda^{-n} L(n) + O(n^{-r}),$$

where r can be made arbitrary and $L(n)$ is an expansion around $n = \infty$. This yields terms of the form

$$T^n \sum_{j=0}^{n} T^{-j} S\mathbf{d}_j = \lambda^n \mathbf{P}(n) + \mathbf{R}(n) + O(n^{-1})$$

for some polynomials $\mathbf{P}, \mathbf{Q}$ of degree $\leq t-1$. The only exception is $\lambda = 1$ – here, logarithmic terms may appear in view of $\sum_{j=1}^{n} j^{-1} \sim \log n$.

Altogether, we obtain a formula of the type (7.4), which finishes the proof. ∎

Remark. Note that the same way of reasoning can be used for maximal antichains, whose recursion is given by

$$c_{k,n+1} = 1 + \prod_{j=1}^{s(k)} c_{\tau_k(j),n} = 1 + \prod_{i=1}^{m} c_{i,n}^{a_{ki}},$$

which transforms into the recursion for antichains after performing the simple substitution $c_{k,n} = 1 + \tilde{c}_{k,n}$.

Remark. The number of antichains is also the number of subtrees containing the root – the leaves of such a subtree always define an antichain and vice versa.
We give two particularly nice examples for our theorem:

Example 7.1 Consider the complete binary tree belonging to the 1×1-matrix with a single entry of 2. Then the number c_n of antichains is given by $c_0 = 1$ and $c_{n+1} = (c_n + 1)^2$. The solution of this recursion has already been given by Aho and Sloane [1]; this was also noted by Székely and Wang [103] who considered the number of subtrees in a complete binary tree. In fact, we have

$$c_n = \left\lfloor \alpha^{2^n} \right\rfloor - 1,$$

where

$$\alpha = \exp\left(\sum_{i=0}^{\infty} 2^{-i} \log(1 + c_i^{-1}) \right) = 2.258518\ldots$$

The sequence $(c_n) = (1, 4, 25, 676, 458329, \ldots)$ is number A004019 in Sloane's "On-Line Encyclopedia of Integer Sequences" [102].

Example 7.2 Let $A = \left(\begin{smallmatrix} 1 & 1 \\ 0 & 1 \end{smallmatrix}\right)$. Then we obtain a comb-like tree. The corresponding recursion is given by $c_0 = 1$ and

$$c_n = (n + 1)(c_{n-1} + 1).$$

This sequence is known for more than 300 years, counting the number of permutations of nonempty subsets of $\{0, 1, \ldots, n\}$. The solution of the recursion is seen to be $\lfloor e(n + 1)! \rfloor - 1$ (Sloane's A007526 [102]; the first terms of the sequence are $1, 4, 15, 64, 325, 1956, 13699, \ldots$).

7.5.4 Connected subsets in a Sierpiński graph

The construction of Sierpiński graphs was described in Example 7.2 of Section 7.2. We will consider the case $d = 2$ only and calculate the number of connected subsets in the level-n Sierpiński graph.
This example shows us that it may be necessary to consider several auxiliary properties as well. In fact, we need seven different sequences: we consider sets of vertices with the property that every connected component of the induced subgraphs contains at least one of the corner vertices. Our auxiliary sequences are distinguished by the number of corner vertices contained in the subsets and the partition of these corner vertices induced by the connected components.

- $a_{1,n}$ counts the number of subsets with three connected components, each of which contains one corner vertex.
- $a_{2,n}$ counts the number of subsets with two connected components, one of them containing two corner vertices, the other component one,
- $a_{3,n}$ counts the number of subsets with two connected components, each of which contains one corner vertex.
- $a_{4,n}$ counts the number of connected subsets containing all corner vertices,
- $a_{5,n}$ counts the number of connected subsets containing two corner vertices.
- $a_{6,n}$ counts the number of connected subsets containing one corner vertex.
- Eventually, $a_{7,n}$ counts the number of connected subsets containing no corner vertex (excluding the empty set).

It takes some time and patience to work through all possibilities and thus determine the correct recurrence equations, but this task can be simplified by means of a computer. As an example, we derive the equation for $a_{4,n+1}$. Let the three vertices which connect the parts of a Sierpiński graph be called the *links*. At least two of them have to belong to a connected set containing all corner vertices – otherwise, it is impossible to connect the corners.

- If all links are contained in a connected subset, either all the induced subsets in all three parts are connected or two of them are connected and one of them has two connected components, each containing one of the links. The corner can be contained in either of these components. This yields a summand of $a_{4,n}^3 + 6a_{2,n}a_{4,n}^2$.
- Suppose that only two of the links are contained in a connected subset. Then the induced subsets in all the parts have to be connected, which leads to a summand of $3a_{4,n}a_{5,n}^2$.

So we arrive at the recursive relation

$$a_{4,n+1} = a_{4,n}^3 + 6a_{2,n}a_{4,n}^2 + 3a_{4,n}a_{5,n}^2.$$

In a similar way, recurrence equations can be determined in all other cases as well by accurately distinguishing cases. This leads us to the following system (note that the polynomials on the right are not homogeneous; however, we could achieve this by introducing the trivial sequence which counts the empty set only):

$$\begin{aligned}
a_{1,n+1} &= 12a_{1,n}a_{2,n}a_{4,n} + 3a_{1,n}a_{5,n}^2 + 14a_{2,n}^3 + 12a_{2,n}a_{3,n}a_{5,n}\\
&\quad + 3a_{2,n}^2a_{4,n} + 3a_{3,n}^2a_{4,n} + 6a_{3,n}a_{5,n}a_{6,n} + a_{6,n}^3,\\
a_{2,n+1} &= a_{1,n}a_{4,n}^2 + 7a_{2,n}^2a_{4,n} + a_{2,n}a_{4,n}^2 + 3a_{2,n}a_{5,n}^2 + 2a_{3,n}a_{4,n}a_{5,n} + a_{5,n}^2a_{6,n},\\
a_{3,n+1} &= 2a_{1,n}a_{4,n}a_{5,n} + 4a_{2,n}a_{3,n}a_{4,n} + 2a_{2,n}a_{4,n}a_{5,n} + 6a_{2,n}^2a_{5,n} + 4a_{2,n}a_{5,n}a_{6,n}\\
&\quad + 2a_{3,n}a_{4,n}a_{6,n} + 3a_{3,n}a_{5,n}^2 + 2a_{3,n}a_{5,n} + 2a_{5,n}a_{6,n}^2 + a_{6,n}^2,\\
a_{4,n+1} &= 6a_{2,n}a_{4,n}^2 + a_{4,n}^3 + 3a_{4,n}a_{5,n}^2,\\
a_{5,n+1} &= 4a_{2,n}a_{4,n}a_{5,n} + a_{3,n}a_{4,n}^2 + a_{4,n}^2a_{5,n} + 2a_{4,n}a_{5,n}a_{6,n} + a_{5,n}^3 + a_{5,n}^2,\\
a_{6,n+1} &= 2a_{2,n}a_{5,n}^2 + 2a_{3,n}a_{4,n}a_{5,n} + a_{4,n}a_{5,n}^2 + a_{4,n}a_{6,n}^2\\
&\quad + 2a_{5,n}^2a_{6,n} + 2a_{5,n}a_{6,n} + a_{6,n},\\
a_{7,n+1} &= 3a_{3,n}a_{5,n}^2 + a_{5,n}^3 + 3a_{5,n}a_{6,n}^2 + 3a_{6,n}^2 + 3a_{7,n}.
\end{aligned} \tag{7.6}$$

The initial values are $(a_{1,0}, a_{2,0}, a_{3,0}, a_{4,0}, a_{5,0}, a_{6,0}, a_{7,0}) = (0, 0, 0, 1, 1, 1, 0)$, and the total number of connected subsets (including the empty set) at level n is given by $a_{4,n} + 3a_{5,n} + 3a_{6,n} + a_{7,n} + 1$. Asymptotically, the terms of total degree 3 in our system of recurrences are much larger than the others, so we have to study the dynamical system generated by these terms:

$$\begin{pmatrix} a_1\\ a_2\\ a_3\\ a_4\\ a_5\\ a_6\\ a_7 \end{pmatrix} \mapsto \begin{pmatrix} 12a_1a_2a_4 + 3a_1a_5^2 + 14a_2^3 + 12a_2a_3a_5 + 3a_2^2a_4 + 3a_3^2a_4 + 6a_3a_5a_6 + a_6^3\\ a_1a_4^2 + 7a_2^2a_4 + a_2a_4^2 + 3a_2a_5^2 + 2a_3a_4a_5 + a_5^2a_6\\ 2a_1a_4a_5 + 4a_2a_3a_4 + 2a_2a_4a_5 + 6a_2^2a_5 + 4a_2a_5a_6 + 2a_3a_4a_6 + 3a_3a_5^2 + 2a_5a_6^2\\ 6a_2a_4^2 + a_4^3 + 3a_4a_5^2\\ 4a_2a_4a_5 + a_3a_4^2 + a_4^2a_5 + 2a_4a_5a_6 + a_5^3\\ 2a_2a_5^2 + 2a_3a_4a_5 + a_4a_5^2 + a_4a_6^2 + 2a_5^2a_6\\ 3a_3a_5^2 + a_5^3 + 3a_5a_6^2 \end{pmatrix}$$

Unfortunately, it has no positive fixed points in projective space. So we have to apply a little trick: set $\gamma = \frac{5}{3}$ and

$$a_{i,n} = \begin{cases} \gamma^{3n/2}A_{i,n} & \text{for } i = 1,\\ \gamma^{n/2}A_{i,n} & \text{for } i = 2, 3,\\ \gamma^{-n/2}A_{i,n} & \text{for } i = 4, 5, 6, 7. \end{cases}$$

In addition, we denote by $\mathbf{A}_n$ the vector $(A_{1,n}, \ldots, A_{7,n})$. Then, our recurrence equations transform to

$$\mathbf{A}_{n+1} = \mathbf{P}(\mathbf{A}_n) + \gamma^{-n}\mathbf{Q}_1(\mathbf{A}_n) + \gamma^{-2n}\mathbf{Q}_2(\mathbf{A}_n) + \gamma^{-3n}\mathbf{Q}_3(\mathbf{A}_n) + \mathbf{R}(\mathbf{A}_n),$$

where $\mathbf{P}$, $\mathbf{Q}_1$, $\mathbf{Q}_2$, and $\mathbf{Q}_3$ are homogeneous polynomials of degree three and $\mathbf{R}$ contains the remaining terms of lower degree. The polynomial $\mathbf{P}$ is given by

$$\mathbf{P} : \begin{pmatrix} A_1 \\ A_2 \\ A_3 \\ A_4 \\ A_5 \\ A_6 \\ A_7 \end{pmatrix} \mapsto \begin{pmatrix} \gamma^{-3/2}(14A_2^3 + 12A_1A_2A_4) \\ \gamma^{-1/2}(7A_2^2A_4 + A_1A_4^2) \\ \gamma^{-1/2}(4A_2A_3A_4 + 6A_2^2A_5 + 2A_1A_4A_5) \\ \gamma^{1/2}(6A_2A_4^2) \\ \gamma^{1/2}(A_3A_4^2 + 4A_2A_4A_5) \\ \gamma^{1/2}(2A_2A_5^2 + 2A_3A_4A_5) \\ \gamma^{1/2}(3A_3A_5^2) \end{pmatrix}.$$

When we study the dynamical system generated by $\mathbf{P}$ we observe that the algebraic surface defined by

$$\left\{(A_1, A_2, A_3, A_4, A_5, A_6, A_7) = \left(\frac{1}{10\mu^3}, \frac{1}{2\sqrt{15}\mu}, \frac{\lambda}{\sqrt{15}\mu}, \mu, \lambda\mu, \lambda^2\mu, \lambda^3\mu\right)\right\}$$

is the set of attractive fixed points. Indeed, one can check that, as a vector in projective space, $\mathbf{A}_n$ tends to a fixed point $\mathbf{C}$, whose numerical value is

$$(0.573118, 0.291082, 0.817477, 0.443515, 0.622786, 0.874517, 1.228000).$$

A rigorous proof of this fact would involve the following steps:

- Check that $\mathbf{A}_n$ lies within a suitable neighborhood of the fixed point for a sufficiently large value of n,
- prove inductively that it will stay within these boundaries for all larger n (since the fixed point is attractive, the first term is a contraction within a suitable neighborhood; the remaining terms are easily estimated since they are very small for sufficiently large n).

Again, we notice an "independency phenomenon" for the corners of the triangle.
So, finally, we obtain the asymptotics $\mathbf{A}_n \sim \mathbf{C} \cdot \beta^{3^n}$, where the numerical value of β is 2.3032106556. Altogether, we find the asymptotic number of connected subsets in the level n-Sierpiński graph to be

$$6.163424 \cdot \gamma^{-\frac{n}{2}} \cdot \beta^{3^n} \sim 2.940541 \cdot V^{\frac{1}{2}\left(1-\frac{\log 5}{\log 3}\right)} \cdot \beta^{\frac{2V}{3}}.$$

Here $V = \frac{3}{2}(3^n + 1)$ denotes the number of vertices in this formula. The numerical value of $\beta^{2/3}$ is 1.7440373203... The first terms of the sequence are

$$8, 48, 6307, 16719440488, 48419029140762918489723896893\,1, \ldots$$

Remark. We observe that there are more sets of the "half-connected" (two connected components) or "one-third-connected" (three connected components) type – by an exponential factor – than connected sets. Furthermore, when we take a closer look at the recurrence relations, we see that the summands which contribute most always correspond to the case that all three "links" are contained in the set. This means that almost all (in some sense) connected subsets contain all three links.

Remark. The Sierpiński triangle is easily generalized by varying the number of subdivisions per triangle side (and thus varying the number of subtriangles) or generalizing the construction to higher dimensions. By computer experiments, we observed that similar results hold for these generalizations, where the constant $\gamma = \frac{5}{3}$ is replaced by other rational numbers. For the 3- and 4-dimensional analogues, the constants are $\frac{3}{2}$ and $\frac{7}{5}$ respectively, leading us to the conjectured formula $\frac{d+3}{d+1}$, where d is the dimension. On the other hand, by increasing the number of subdivisions, we obtain the sequence

$$\frac{5}{3}, \frac{15}{7}, \frac{103}{41}, \frac{1663}{591}, \frac{21559}{7025}, \ldots$$

which is rather difficult to explain. We did not find any hints on its origin in Sloane's encyclopedia [102]. It is a remarkable fact, however, that all these constants are indeed rational numbers, since they are given by rather complicated algebraic systems of equations only. It seems to be a highly challenging problem to find a proof for this.
Surprisingly, these rational numbers exactly match the resistance scaling factors of the generalized Sierpiński gaskets, see [4] for a definition of this constant: Consider the level-n graph $X_{1,n}$ as electrical network with constant resistant on its edges and denote by $\mathcal{E}_n$ the associated energy form. Then there is a restriction of $\mathcal{E}_{n+1}$ to $X_{1,n}$, which is called the trace of $\mathcal{E}_{n+1}$. It turns out that the trace of $\mathcal{E}_{n+1}$ and $\mathcal{E}_n$ are the same up to a constant, which is called the resistance scaling factor.

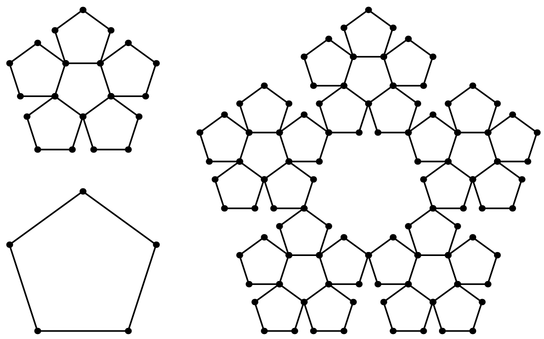

Figure 7.6: The Pentagasket: A pentagonal analogue of the Sierpiński gasket.

Interestingly, when we consider the pentagonal analogue of the Sierpiński gasket, see Figure 7.6, the basis of the exponential factor is not rational any more; however, it still equals the resistance scaling factor, which is $\frac{1}{10}(9+\sqrt{161})$ in this case, see for example [42].

Part II

Properties of the sum of digits and general q-additive functions

Chapter 8

Waring's problem with restrictions on q-additive functions

8.1 Introduction and statement of results

A set $A \subseteq \mathbb{N}$ is said to be a *basis* (*asymptotic basis*) of order s if every positive integer (sufficiently large positive integer) n can be represented as

$$n = x_1 + \ldots + x_s \text{ with } x_1, \ldots, x_s \in A.$$

The classical problem of Waring corresponds to the question whether the set A_k of k-th powers is a basis (resp. asymptotic basis). There is a vast amount of literature on this topic, compare [85, 106] for instance; [107] gives a comprehensive survey on Waring's problem. In a paper of Thuswaldner and Tichy [104], the authors discuss a generalization of Waring's problem with restrictions on the sum of digits. In particular, they show that the set

$$A_{k,h,m} := \{n^k | s_q(n) \equiv h \mod m\}$$

forms an asymptotic basis of order $2^k + 1$, where $s_q(n)$ denotes the q-adic sum of digits. The sum of digits is the classical example of a q-*additive* function, i.e.

$$s_q(aq^h + b) = s_q(aq^h) + s_q(b)$$

whenever $b < q^h$. In fact, it is even *completely* q-*additive*, which means that

$$s_q(aq^h + b) = s_q(a) + s_q(b)$$

whenever $b < q^h$. Thus it is natural to consider the analogous problem for general (completely) q-additive functions. This chapter is devoted to such a generalization. Let w be some integer-valued weight function on the set $\{0, \ldots, q-1\}$ of q-adic digits, and define $v(n)$ by

$$v(n) = \sum_{j=0}^{l} w(d_j), \text{ where } n = \sum_{j=0}^{l} d_j q^j. \tag{8.1}$$

All integer-valued completely q-additive functions are of this form with $w(0) = 0$. The sum of digits corresponds to $w(d) = d$, the q-adic length to $w(d) = 1$. We are going to prove that a completely q-additive function, under some conditions, still satisfies the theorem of Thuswaldner and Tichy:

Theorem 8.1 *Let $s, k \in \mathbb{N}$, $s > k^2(\log k + \log\log k + O(1))$, $h_i, m_i, q_i \in \mathbb{N}$ $(1 \le i \le s)$ with $m_i, q_i \ge 2$, and let $v_i(n)$ be defined by some weight function $w_i(d)$ on the q_i-adic digits for all i. Suppose that for all i the following holds true:*

There is no prime $P|m_i$ such that $w_i(0), \ldots, w_i(q_i - 1)$ is an arithmetic progression modulo P and $w_i(0) \equiv w_i(q_i - 1) \mod P$.

Then if $r(N)$ is the number of representations of N of the form

$$N = x_1^k + \ldots + x_s^k \qquad (v_i(x_i) \equiv h_i \mod m_i),$$

there is a positive constant δ such that

$$r(N) = \frac{1}{m_1 \ldots m_s} \mathfrak{S}(N) \Gamma\Big(1 + \frac{1}{k}\Big)^s \Gamma\Big(\frac{s}{k}\Big)^{-1} N^{s/k-1} + O(N^{s/k-1-\delta}). \tag{8.2}$$

The implied constant depends only on s, k and m_i. $\mathfrak{S}(N)$ is the singular series for the classical Waring problem – it is an arithmetic function for which there exist positive constants $0 < c_1 < c_2$ depending only on k and s such that $c_1 < \mathfrak{S}(N) < c_2$.

The proof will be essentially the same as in the paper of Thuswaldner and Tichy, apart from some minor changes. It is based on the following correlational result generalizing Theorem 3.3 of [104]:

Theorem 8.2 *Let k, m, h, q and N be positive integers with $m \geq 2$, $q \geq 2$, and let $v(n)$ be a function defined by (8.1) for some weight w. Suppose that there is a prime P in the factorization of the denominator of $\frac{h}{m}$ (in its lowest terms) such that either*

- $P \nmid (w(q-1) - w(0))$

or

- *$w(0), \ldots, w(q-1)$ is not an arithmetic progression modulo P (which is equivalent to the fact that s is a linear combination of the q-adic digit sum and the q-adic length modulo P).*

Now let $I_1, \ldots, I_k, J$ be intervals of integers with $\sqrt{N} \leq |I_j|, |J| \leq N$ $(1 \leq j \leq k)$. Set

$$Y(I_1, \ldots, I_k, J) := \sum_{h_1 \in I_1} \cdots \sum_{h_k \in I_k} \left| \sum_{n \in J} e\Big(\frac{h}{m} \Delta_{h_k, \ldots, h_1}(v)(n)\Big) \right|^2.$$

Then

$$Y(I_1, \ldots, I_k, J) \ll |I_1| \ldots |I_k| |J|^2 N^{-\eta} \tag{8.3}$$

holds with $\eta > 0$ depending on m, k and q.

The proof will be given in the following section. Having proved this theorem, one can obtain the following result in litterally the same way as in [104] and finally prove Theorem 8.1 by means of the circle method. The original version of the proof given in [104] was modified by Pfeiffer and Thuswaldner in [91] – they used the results of Ford [32] to improve the bound for s from 2^k to $k^2(\log k + \log \log k + O(1))$. Their proof can easily be adapted to the current problem. Note also that the results of this chapter can be generalized to systems of congruences in just the same way as in the paper of Pfeiffer and Thuswaldner.

Theorem 8.3 *Let k, m, h, q, N be positive integers with the same properties as in Theorem 8.2 and let $v(n)$ be defined as before. Then the estimate*

$$\Big| \sum_{n=1}^{N} e\Big(\theta n^k + \frac{h}{m} v(n)\Big) \Big| \ll N^{1-\gamma} \tag{8.4}$$

holds uniformly in $\theta \in [0, 1)$ with $\gamma := \eta 2^{-(k+1)}$ (η as in Theorem 8.2).

8.2 Proof of the main theorem

First, let's repeat the basic definitions and lemmas of [104]:

Definition 8.1 Let $\mathcal{M} := \{1, 2, \ldots, k\}$ and $\mathcal{M}' := \{0, 1, \ldots, k+1\}$, and define the class of functions $\mathcal{F} := \{f : 2^{\mathcal{M}} \to \mathcal{M}'\}$. By F_0 and F_1, we denote the special functions

$$F_0(S) := 0 \text{ for all } S \subseteq \mathcal{M}$$

$$F_1(S) := \begin{cases} 1 & S = \mathcal{M} \\ 0 & \text{otherwise.} \end{cases}$$

Furthermore, the operator Ξ is defined by

$$\Xi_{\mathbf{r},i}(f)(S) := \left\lfloor \frac{i + \sum_{j \in S} r_j + f(S)}{q} \right\rfloor$$

for each vector $\mathbf{r} = (r_1, \ldots, r_k) \in \{0, \ldots, q-1\}^k$ and each $0 \le i < q$.

The following result is easy to show:

Lemma 8.4 For each pair $\mathbf{r}, i$ we have $\Xi_{\mathbf{r},i}(\mathcal{F}) \subseteq \mathcal{F}$. Furthermore, let

$$\Xi_{\{\mathbf{r}_l, i_l\}_{1 \le l \le L}} := \Xi_{\mathbf{r}_L, i_L} \circ \ldots \circ \Xi_{\mathbf{r}_1, i_1}$$

denote the iterates of Ξ. Then for arbitrary $f \in \mathcal{F}$,

$$\Xi_{\{\mathbf{0},0\}_{1 \le l \le L'}}(f) = F_0$$

if $L' := \left\lfloor \frac{\log(k+1)}{\log q} \right\rfloor + 1$, and with $L'' := \left\lfloor \frac{k-1}{q-1} \right\rfloor + 1$,

$$\Xi_{\{\mathbf{r}_l^*, i_l^*\}_{1 \le l \le L''}}(F_0) = F_1$$

for certain special values $\{\mathbf{r}_l^*, i_l^*\}$ depending on k and q.

Definition 8.2 Let $I_1, \ldots, I_k, J$ be intervals of integers and $f, f_1, f_2 \in \mathcal{F}$. Define

$$\Phi(h_1, \ldots, h_k; J; f) := \sum_{n \in J} e\left(\frac{h}{m} \sum_{S \subseteq \mathcal{M}} (-1)^{k-|S|} v\Big(n + \sum_{t \in S} h_t + f(S)\Big) \right),$$

$$\Psi(h_1, \ldots, h_{k-1}; I_k, J; f_1, f_2) := \sum_{h_k \in I_k} \Phi(h_1, \ldots, h_k; J; f_1) \overline{\Phi(h_1, \ldots, h_k; J; f_2)},$$

$$X(I_1, \ldots, I_k, J; f_1, f_2) := \sum_{h_1 \in I_1} \cdots \sum_{h_{k-1} \in I_{k-1}} \Psi(h_1, \ldots, h_{k-1}; I_k, J; f_1, f_2).$$

Then $Y(I_1, \ldots, I_k, J) = X(I_1, \ldots, I_k, J, F_0, F_0)$.

Proposition 8.5 Let $f_1, f_2 \in \mathcal{F}$ and let $I_1, \ldots, I_k, J$ be intervals of integers. Then

$$\begin{aligned} X(qI_1, \ldots, qI_k, qJ; f_1, f_2) = &\sum_{r_1=0}^{q-1} \cdots \sum_{r_k=0}^{q-1} \sum_{i_1=0}^{q-1} \sum_{i_2=0}^{q-1} \alpha(f_1, f_2, \mathbf{r}, i_1, i_2) \\ &\cdot X(I_1, \ldots, I_k, J; \Xi_{\mathbf{r},i_1}(f_1), \Xi_{\mathbf{r},i_2}(f_2)) + O\left(|I_1| \ldots |I_k||J|\right). \end{aligned} \tag{8.5}$$

The implied constant depends only on q and k. Here,

$$\alpha(f_1, f_2, \mathbf{r}, i_1, i_2) := e\left(\frac{h}{m} \sum_{S \subseteq \mathcal{M}} (-1)^{k-|S|} \Big(w(b(f_1, S, \mathbf{r}, i_1)) - w(b(f_2, S, \mathbf{r}, i_2)) \Big) \right),$$

and $b(f, S, \mathbf{r}, i) \in \{0, \ldots, q-1\}$ is defined as the remainder of $i + \sum_{t \in S} r_t + f(S)$ modulo q.

Proof. We exploit the fact that $v(qa+b) = v(a) + w(b)$ for $a > 0$, $b < q$, to derive from

$$i + \sum_{t \in S} r_t + f(S) = q\Xi_{\mathbf{r},i}(f)(S) + b(f, S, \mathbf{r}, i)$$

(which follows from the definition of Ξ) the identity

$$\begin{aligned} v\Big(qn + \sum_{t \in S} qh_t + i + \sum_{t \in S} r_t + f(S)\Big) &= v\Big(qn + \sum_{t \in S} qh_t + q\Xi_{\mathbf{r},i}(f)(S) + b(f, S, \mathbf{r}, i)\Big) \\ &= v\Big(n + \sum_{t \in S} h_t + \Xi_{\mathbf{r},i}(f)(S)\Big) + w(b(f, S, \mathbf{r}, i)) \end{aligned}$$

whenever $n > 0$. This yields

$$\Phi(q\mathbf{h} + \mathbf{r}; qJ; f) = \sum_{i=0}^{q-1} e\Big(\frac{h}{m} \sum_{S \in \mathcal{M}} (-1)^{k-|S|} w(b(f, S, \mathbf{r}, i))\Big) \Phi(\mathbf{h}; J; \Xi_{\mathbf{r},i}(f)) + O(q).$$

Applying this to Ψ and X in turn gives us the desired result. ■

Next, we need some special values of α:

Lemma 8.6 For $0 \le i < q-1$, we have

$$\alpha(F_0, F_0, \mathbf{0}, 0, 0) = e(0) = 1, \tag{8.6}$$

$$\alpha(F_1, F_0, \mathbf{0}, i, 0) = e\Big(\frac{h}{m}(w(i+1) - w(i))\Big), \tag{8.7}$$

$$\alpha(F_1, F_0, \mathbf{0}, q-1, 0) = e\Big(\frac{h}{m}(w(0) - w(q-1))\Big). \tag{8.8}$$

The proof is the same as in [104, Lemma 5.1]. Now, iterating Proposition 8.5 gives us (using the notation $\mathcal{Q}_l := \{0, \dots, q-1\}^l$)

$$\begin{aligned} &X(q^L I_1, \dots, q^L I_k, q^L J; f_1, f_2) = \\ &\quad \sum_{r_1, \dots, r_L \in \mathcal{Q}_k} \sum_{i_1, \dots, i_L \in \mathcal{Q}_2} \Big(\prod_{l=1}^{L} \alpha(\Xi_{(\mathbf{r}_j, i_{j1})_{1 \le j \le l-1}}(f_1), \Xi_{(\mathbf{r}_j, i_{j2})_{1 \le j \le l-1}}(f_2), \mathbf{r}_l, i_{l1}, i_{l2})\Big) \\ &\quad \cdot X(I_1, \dots, I_k, J; \Xi_{(\mathbf{r}_l, i_{l1})_{1 \le l \le L}}(f_1), \Xi_{(\mathbf{r}_l, i_{l2})_{1 \le l \le L}}(f_2)) + O\left(|I_1| \dots |I_k||J|\right), \end{aligned}$$

where the implied constant depends on q, k and L. We select $L := L' + L'' + 3$ (L', L'' as in Lemma 8.4) and extract two summands from the above sum in analogy to [104]. Let P be a prime satisfying the conditions of Theorem 1. If $w(0), \dots, w(q-1)$ is not an arithmetic progression modulo P, then the sequence $w(1) - w(0), \dots, w(q-1) - w(q-2)$ is not constant, so we may choose $0 \le i_1, i_2 < q-1$ in such a way that $w(i_1+1) - w(i_1) \not\equiv w(i_2+1) - w(i_2) \mod P$. If on the other hand $w(0), \dots, w(q-1)$ is an arithmetic progression modulo P, then $w(0) \not\equiv w(q-1) \mod P$.

In the first case, we let the first summand V_1 correspond to the selection

$$\begin{array}{lll} \mathbf{r}_l = (0, \dots, 0), & \mathbf{i}_l = (0, 0) & (1 \le l \le L'), \\ \mathbf{r}_l = \mathbf{r}^*_{l-L'}, & \mathbf{i}_l = \mathbf{i}^*_{l-L'} & (L'+1 \le l \le L-3), \\ \mathbf{r}_l = (0, \dots, 0), & \mathbf{i}_l = (q-1, 0) & (l = L-2), \\ \mathbf{r}_l = (0, \dots, 0), & \mathbf{i}_l = (i_1, 0) & (l = L-1), \\ \mathbf{r}_l = (0, \dots, 0), & \mathbf{i}_l = (0, 0) & (l = L), \end{array}$$

and let the second summand V_2 correspond to the same selection with $\mathbf{i}_{L-1} = (i_2, 0)$. Then, using the abbreviation

$$A(f_1, f_2) := \prod_{l=1}^{L-2} \alpha(\Xi_{(\mathbf{r}_j, i_{j1})_{1\le j\le l-1}}(f_1), \Xi_{(\mathbf{r}_j, i_{j2})_{1\le j\le l-1}}(f_2), \mathbf{r}_l, i_{l1}, i_{l2}),$$

we arrive at

$$V_1 = A(f_1, f_2)\,\alpha(F_1, F_0, \mathbf{0}, i_1, 0)\,\alpha(F_0, F_0, \mathbf{0}, 0, 0)\,X(I_1, \ldots, I_k, J; F_0, F_0)$$

and

$$V_2 = A(f_1, f_2)\,\alpha(F_1, F_0, \mathbf{0}, i_2, 0)\,\alpha(F_0, F_0, \mathbf{0}, 0, 0)\,X(I_1, \ldots, I_k, J; F_0, F_0).$$

Now, by Lemma 8.6,

$$V_1 = A(f_1, f_2) e\Big(\frac{h}{m}(w(i_1+1) - w(i_1))\Big) X(I_1, \ldots, I_k, J; F_0, F_0)$$

and

$$V_2 = A(f_1, f_2) e\Big(\frac{h}{m}(w(i_2+1) - w(i_2))\Big) X(I_1, \ldots, I_k, J; F_0, F_0).$$

Therefore,

$$\begin{aligned} V_1 + V_2 =& A(f_1, f_2) \left(e\Big(\frac{h}{m}(w(i_1+1) - w(i_1))\Big) + e\Big(\frac{h}{m}(w(i_2+1) - w(i_2))\Big) \right) \\ & X(I_1, \ldots, I_k, J; F_0, F_0). \end{aligned}$$

Since $P \nmid \Big((w(i_1+1) - w(i_1)) - (w(i_2+1) - w(i_2))\Big)$, we are now able to apply the same argument as in [104], namely that

$$e\Big(\frac{h}{m}(w(i_1+1) - w(i_1))\Big) + e\Big(\frac{h}{m}(w(i_2+1) - w(i_2))\Big) \le \left|1 + e\left(\frac{1}{m}\right)\right| \le 2 - \Big(\frac{\pi}{2m}\Big)^2,$$

to prove a matrix inequality of the form

$$\begin{aligned} (|X(q^L I_1, \ldots, q^L I_k, q^L J; f_1, f_2)|)_{(f_1,f_2)\in\mathcal{F}^2} \le& B \cdot (|X(I_1, \ldots, I_k, J; g_1, g_2)|)_{(g_1,g_2)\in\mathcal{F}^2} \\ &+ O\left(|I_1| \ldots |I_k||J|\right), \end{aligned} \tag{8.9}$$

where B is a matrix whose row sums are $\le q^{L(k+2)}(1-\varepsilon)$ for a certain $\varepsilon > 0$ depending on q, k and m. In the second case (i.e., $P \nmid w(0) - w(q-1)$), we may use almost the same parameters with $\mathbf{i}_{L-1} = (q-1, 0)$ for V_1 and $\mathbf{i}_{L-1} = (0,0)$ for V_2; these are exactly the parameters used in [104], and the argument stays the same. Iterating this matrix inequality and specializing $f_1 = f_2 = F_0$ then gives the estimate of Theorem 8.2. The O-term in (8.9) is of no harm since it can be included in the estimate (note also that it appears only if $w(0) \ne 0$).

Remark. The crucial tool in the proof of Thuswaldner and Tichy is the fact that the application of inequality (8.9) saves a factor of $(1-\varepsilon)$ from the trivial estimate. Now, let us consider arbitrary (not completely) q-additive functions, which can be written as

$$v(n) = \sum_{j=0}^{l} w^{(j)}(d_j), \text{ where } n = \sum_{j=0}^{l} d_j q^j, \tag{8.10}$$

i.e. the weight depends on the position of a digit, too. Then, it is necessary that a "positive percentage" of the weights satisfies the condidion of Theorem 8.2 so that the argument can still be applied. Formally, if $\omega(l)$ denotes the number of weights $w^{(i)}$ with $i \le l$ which satisfy the condition, the proof should still work (with some technical and notational inconveniences) if

$$\liminf_{l\to\infty} \frac{\omega(l)}{l} > 0.$$

8.3 Final remarks and conclusion

Remark. First, we are going to explain why the condition posed on m_i is also necessary. Suppose there is a $P|m_i$ such that $w_i(0), \dots, w_i(q_i-1)$ is an arithmetic progression modulo P and $w_i(0) \equiv w_i(q_i-1) \mod P$. Then either $w_i(0), \dots, w_i(q-1)$ is constant modulo P, which means that the congruence condition for v_i is in fact a condition on the length of the q_i-adic expansion, or $w_i(d) \equiv A \cdot d + B \mod P$ for some $A \not\equiv 0 \mod P$.
In that case, the condition $w_i(0) \equiv w_i(q_i-1) \mod P$ turns into $P|(q_i-1)$, so $v_i(n)$ is a linear combination of the digit sum and length of n modulo P, and since also $s_{q_i}(n) \equiv n \mod P$ for all $P|(q_i-1)$, it is in fact a linear combination of n and its length, so the restriction is actually equivalent to congruence restrictions on intervals of the form $[q_i^r, q_i^{r+1})$. In both cases, the asymptotics cannot hold any longer.

Remark. Second, we discuss the size of the asymptotic order in the case $k = 1$ shortly. Theorem 8.1 (with the weaker estimate $s > 2^k$) tells us that it must be either 2 or 3 in the case that the conditions of the theorem are satisfied. It seems to be a nontrivial problem to determine whether it is 2 or 3 given some function v. Note, however, that it must be 3 for the q-adic sum of digits in view of the integers of the form

$$n_K := q^K - 1 = \sum_{i=0}^{K-1} (q-1)q^i.$$

If we write n_K as the sum of two integers n_1, n_2 with $s_q(n_1) \equiv s_q(n_2) \equiv h \mod m$, there cannot be any carry, so we would have $s_q(n_K) = K(q-1) \equiv 2h \mod m$, which is impossible for infinitely many values of K.
Note also that the set defined by $v(n) \equiv h \mod m$ can still be an asymptotic basis of $\mathbb{N}$ even if the conditions are violated. However, if we consider the q-adic length modulo m for instance, the order as an asymptotic basis might be as large as q^m.

Remark. It is very difficult to give information about the order of the set $A = \{n^k | v(n) \equiv h \mod m\} \cup \{0, 1\}$ as a basis of $\mathbb{N}$ (0 and 1 have to be added to the set so that it is really a basis). In fact, the order depends highly on the parameters even in the very special case that $k = 1$ and $a = s_q$ is the q-adic sum of digits:

- If we take $q = 2$ and $h = 0$, $2^m - 1 = \sum_{i=0}^{m-1} 2^i$ is the smallest positive integer whose sum of digits is $\geq m$. Therefore, it is also the smallest element of the set $\{n | v(n) \equiv h \mod m\}$. All smaller integers can only be represented as the sum of 0's and 1's, thus at least $2^m - 2$ summands are needed.
- On the other hand, let $r \geq 2$ be arbitrary, $h = r$ and q sufficiently large, e.g. $q = 3m + r$. Then the distance between two subsequent elements of the set $\{n | v(n) \equiv h \mod m\}$ is at most $2m - 1$ (which is easy to verify). Such a gap can be filled with $\leq \lfloor \frac{m}{r} \rfloor + r - 1$ summands from the set $\{1, r, m + r\}$; so a total of $\lfloor \frac{m}{r} \rfloor + r$ summands is sufficient. Taking $r = \lfloor \sqrt{m} \rfloor$ thus gives an order $\leq 2\sqrt{m} + O(1)$.

These two examples show that the order of the studied set as a basis of $\mathbb{N}$ may grow exponentially in terms of the modulus as well as sublinearly. So there is probably not much hope that one can give any precise information on the order in general.

Chapter 9

Numbers with fixed sum of digits in linear recurrent number systems

9.1 Previous results

Linear recurrent digit systems are a generalization of the usual radix representations; they have been studied, for example, in [10, 36, 40, 41, 90]. We start with a definition of these systems: let $G = (G_n)$ $(n = 0, 1, \ldots)$ be a linear recurring sequence of order $d \geq 1$, i.e.

$$G_{n+d} = a_1 G_{n+d-1} + a_2 G_{n+d-2} + \ldots + a_d G_n \tag{9.1}$$

with integral coefficients and integral initial values. We assume that the coefficients $a_1 \geq a_2 \geq \ldots \geq a_d > 0$ are non-increasing ($a_1 > 1$ if $d = 1$) and that $G_0 = 1$ and

$$G_n > a_1(G_0 + \ldots + G_{n-1}),\ n = 1, \ldots, d-1.$$

For an arbitrary positive integer N, we define $L = L(N)$ by $G_L \leq N < G_{L+1}$ (and set $L(0) = 0$). Furthermore, set $N_L = N$,

$$\epsilon_j = \left\lfloor \frac{N_j}{G_j} \right\rfloor,\ N_{j-1} = N_j - G_j \epsilon_j\ (1 \leq j \leq L),$$

and finally $\epsilon_0 = N_0$, yielding a unique representation of N of the form

$$N = \sum_{j=0}^{L(N)} \epsilon_j G_j, \tag{9.2}$$

the G-ary representation of N with digits ϵ_j. If $d = 1$ and $a_1 = g$, we obtain the well-known base-g representation of N.
Now, the sum of digits is naturally defined as

$$s_G(N) = \sum_{j=0}^{L(N)} \epsilon_j.$$

The best-known instance of such a digit system is probably the Zeckendorf expansion [112], belonging to the Fibonacci sequence $G_0 = 1$, $G_1 = 2$, $G_{n+2} = G_{n+1} + G_n$.
In [90], Pethő and Tichy generalized a well-known result of Delange [17] on the mean value of the sum of digits to linear recurring sequences. For usual base-g expansions, numbers with fixed sum of digits were studied by Mauduit and Sárközy in [76]. Their first main result states that the number of

integers with $\leq \nu$ digits and sum of digits $k \leq \frac{g-1}{2}\nu$ (for reasons of symmetry, this case is obviously sufficient) is, uniformly for $k \to \infty$,

$$r^{-k}(1+r+\dots r^{g-1})^{\nu}\pi^{1/2}(D\nu)^{-1/2}(1+O(D\nu)^{-1/2}), \tag{9.3}$$

where the implied constant depends only on the base g; r is defined as the unique positive zero of

$$Q(x) = -k(1+x+\dots+x^{g-1}) + \nu x(1+2x+\dots+(g-1)x^{g-2}),$$

and $D = 2\pi^2(B-A^2)$, where

$$A = \left(\sum_{j=1}^{g-1} jr^j\right)\left(\sum_{j=0}^{g-1} r^j\right)^{-1} = \frac{k}{\nu} \quad \text{and} \quad B = \left(\sum_{j=1}^{g-1} j^2 r^j\right)\left(\sum_{j=0}^{g-1} r^j\right)^{-1}.$$

Secondly, they showed that the integers with fixed sum of digits are uniformly distributed in residue classes if the modulus is not too large and relatively prime to $(g-1)g$ – this theorem was further generalized in a very recent paper of Mauduit, Pomerance and Sárközy [74], relaxing the condition that the modulus is relatively prime to $(g-1)g$. Furthermore, they were able to prove an Erdős-Kac-type theorem for integers with fixed sum of digits.
Similar results for other kinds of digitally restricted sets are due to Erdős, Mauduit and Sárközy ([27, 28], integers with missing digits), Fouvry and Mauduit resp. Mauduit and Sárközy ([33, 34, 75], integers with congruence conditions for the sum of digits).
In this chapter, we are going to prove a generalization of formula (9.3) to linear recurrent digit systems and study the distribution in residue classes. It turns out that we have uniform distribution if there is no prime divisor P of the modulus such that (G_n) is constant modulo P for all but finitely many values of n.
We will make use of the following notational convention: we use $c_1(G), c_2(G), \dots$ for constants which depend only on the basis G of our digital system, and we write $f(N) = O_G(g(N))$, if there is a constant $C(G)$ depending only on G such that, for sufficiently large N, $f(N) \leq C(G)g(N)$ holds.

9.2 Asymptotic enumeration

We start with a characterization of admissible digital expansions given by Pethő and Tichy in [90]:

Lemma 9.1 The $(t+1)$-tuple $(\epsilon_0, \dots, \epsilon_t) \in \mathbb{N}_0^{t+1}$ is the sequence of G-ary digits of an integer if and only if

$$\sum_{j=0}^{n} \epsilon_j G_j < G_{n+1} \tag{9.4}$$

for all $0 \leq n < d-1$ and

$$(\epsilon_n, \dots, \epsilon_{n-d+1}) < (a_1, \dots, a_d) \tag{9.5}$$

lexicographically (i.e. there is an i such that $\epsilon_{n+1-j} = a_j$ for $j < i$ and $\epsilon_{n+1-i} < a_i$) for all $d-1 \leq n \leq t$.

This lemma enables us to establish a generating function for the integers with fixed sum of digits:

Proposition 9.2 Let $F(k,\nu)$ be the set of integers with $\leq \nu$ base-G digits and sum of digits k. Then we have

$$|F(k,\nu)| = [x^\nu y^k]\,\frac{p(x,y)}{q(x,y)},$$

where $p(x,y)$ and $q(x,y)$ are polynomials and $q(x,y)$ is given by

$$q(x,y) = 1 - \sum_{i=1}^{d}\left(\sum_{j=0}^{a_i-1} y^j\right)\left(\prod_{l=1}^{i-1} y^{a_l}\right)x^i. \tag{9.6}$$

Proof. By the preceding lemma, we have to consider sequences satisfying the two conditions (9.4) and (9.5). We call such sequences *good.* Let a good sequence $(\epsilon_0, \ldots, \epsilon_t)$ be given. By (9.5), there is an i such that $\epsilon_{t+1-j} = a_j$ for $j < i$ and $\epsilon_{t+1-i} < a_i$. The remaining digits $(\epsilon_0, \ldots, \epsilon_{t-i})$ obviously form a good sequence. Conversely, a sequence $(b, a_{i-1}, \ldots, a_1)$ with $b < a_i$ may be appended to any good sequence of length $\geq d$ to form another good sequence. Thus, if

$$g(t) = \sum_{\epsilon} y^{s(\epsilon)},$$

where the sum is over all good sequences $\epsilon = (\epsilon_0, \ldots, \epsilon_t)$ and $s(\epsilon) = \epsilon_0 + \ldots + \epsilon_t$, we have

$$g(t) = \sum_{i=1}^{d} \left(\sum_{j=0}^{a_i - 1} y^j \right) \left(\prod_{l=1}^{i-1} y^{a_l} \right) g(t-i)$$

if t is large enough. This shows that the generating function for our problem is given by a rational function of the form $\frac{p(x,y)}{q(x,y)}$, with $q(x,y)$ as in (9.6). ■

Lemma 9.3 Let $q(x,y)$ be given by (9.6), and define $\lambda = \lambda(y)$ for positive y as the unique positive solution to $q(\lambda, y) = 0$. Furthermore, define

$$\mu(y) = -\frac{y\lambda'(y)}{\lambda(y)} = \frac{yq_y(\lambda(y), y)}{\lambda(y)q_x(\lambda(y), y)}. \tag{9.7}$$

Then $\mu(y)$ is a continuous, strictly increasing function with $\lim_{y\to 0} \mu(y) = 0$ and $\lim_{y\to\infty} \mu(y) = A = \max_i \frac{a_1 + \ldots + a_i - 1}{i}$. Furthermore, there exists a constant $c_1(G) > 0$ depending on G such that $\mu'(y) \geq c_1(G)$ for all $y \in [0, 1]$.

Proof. Obviously, $q(x,y)$ is strictly decreasing in x and y, and $q(0,y) = 1$, whereas $q(x,y) \to -\infty$ as $x \to \infty$. Therefore, $\lambda(y)$ is well-defined, and so is $\mu(y)$. Clearly, $\lambda(y)$ and $\mu(y)$ are continuous. As $q(x,0) = 1 - x$, we know that $\lambda(0) = 1$. Furthermore, $q_x(x,0) = -1$, which means that $\mu(0) = 0$.
Since $\lambda(y)$ is an algebraic function with no branch points on $[0,\infty)$ (note that the derivative $q_x(\lambda(y), y)$ is strictly negative on this interval), $\lambda(y)$ has a holomorphic continuation and is thus infinitely often differentiable. Since $\lambda(y) \neq 0$ for all y, this also holds for $\mu(y)$.
$r(x,y) = 1 - q(x,y)$ is a polynomial in x, y with positive coefficients and constant coefficient 0. We write $r(x,y) = \sum_{k,l} r_{kl} x^k y^l$. Implicit differentiation yields

$$\mu(y) = \frac{yq_y(\lambda(y), y)}{\lambda(y)q_x(\lambda(y), y)} = \frac{yr_y(\lambda(y), y)}{\lambda(y)r_x(\lambda(y), y)}$$

and

$$\begin{aligned} \mu'(y) \;&=\; \frac{1}{x^3 y r_x(x,y)^3} \Big(y^2 r_y(x,y)^2 (x r_x(x,y) + x^2 r_{xx}(x,y)) + x^2 r_x(x,y)^2 (y r_y(x,y) + y^2 r_{yy}(x,y)^2) \\ &\quad - 2x^2 y^2 r_x(x,y) r_y(x,y) r_{xy}(x,y) \Big) \Big|_{x=\lambda(y)}. \end{aligned}$$

The denominator is positive for $y > 0$. The numerator can be written as

$$\begin{aligned} &\left(\sum_{k,l} l r_{kl} x^k y^l \right)^2 \left(\sum_{k,l} k^2 r_{kl} x^k y^l \right) + \left(\sum_{k,l} k r_{kl} x^k y^l \right)^2 \left(\sum_{k,l} l^2 r_{kl} x^k y^l \right) \\ &- 2 \left(\sum_{k,l} k r_{kl} x^k y^l \right) \left(\sum_{k,l} l r_{kl} x^k y^l \right) \left(\sum_{k,l} k l r_{kl} x^k y^l \right). \end{aligned}$$

We set $u_{kl} = \sqrt{r_{kl}x^k y^l}$, $v_{kl} = k\sqrt{r_{kl}x^k y^l}$ and $w_{kl} = l\sqrt{r_{kl}x^k y^l}$. Then this equals

$$\left(\sum_{k,l} u_{kl}w_{kl}\right)^2 \left(\sum_{k,l} v_{kl}^2\right) + \left(\sum_{k,l} u_{kl}v_{kl}\right)^2 \left(\sum_{k,l} w_{kl}^2\right) - 2\left(\sum_{k,l} u_{kl}v_{kl}\right)\left(\sum_{k,l} u_{kl}w_{kl}\right)\left(\sum_{k,l} v_{kl}w_{kl}\right)$$
$$= \langle \mathbf{u},\mathbf{w}\rangle^2\langle \mathbf{v},\mathbf{v}\rangle + \langle \mathbf{u},\mathbf{v}\rangle^2\langle \mathbf{w},\mathbf{w}\rangle - 2\langle \mathbf{u},\mathbf{v}\rangle\langle \mathbf{u},\mathbf{w}\rangle\langle \mathbf{v},\mathbf{w}\rangle,$$

where $\langle .,.\rangle$ denotes the scalar product. Combining the inequality between the arithmetic and geometric mean and the Cauchy-Schwarz inequality yields

$$\begin{aligned}\langle \mathbf{u},\mathbf{w}\rangle^2\langle \mathbf{v},\mathbf{v}\rangle + &\langle \mathbf{u},\mathbf{v}\rangle^2\langle \mathbf{w},\mathbf{w}\rangle - 2\langle \mathbf{u},\mathbf{v}\rangle\langle \mathbf{u},\mathbf{w}\rangle\langle \mathbf{v},\mathbf{w}\rangle \\ &\geq 2\sqrt{\langle \mathbf{u},\mathbf{w}\rangle^2\langle \mathbf{v},\mathbf{v}\rangle\langle \mathbf{u},\mathbf{v}\rangle^2\langle \mathbf{w},\mathbf{w}\rangle} - 2\langle \mathbf{u},\mathbf{v}\rangle\langle \mathbf{u},\mathbf{w}\rangle\langle \mathbf{v},\mathbf{w}\rangle \\ &\geq 2\sqrt{\langle \mathbf{u},\mathbf{w}\rangle^2\langle \mathbf{u},\mathbf{v}\rangle^2\langle \mathbf{v},\mathbf{w}\rangle^2} - 2\langle \mathbf{u},\mathbf{v}\rangle\langle \mathbf{u},\mathbf{w}\rangle\langle \mathbf{v},\mathbf{w}\rangle \\ &= 0\end{aligned}$$

with equality if and only if $\mathbf{v},\mathbf{w}$ are linearly dependent. In our case, this can only be if $r_{kl} \neq 0$ happens only for one value of $\frac{k}{l}$. By our conditions on the a_i, this is impossible. Therefore, $\mu'(y) > 0$ for all $y \in (0,\infty)$, which implies that $\mu(y)$ is strictly increasing. Direct calculation shows that $\mu'(0) = 1$. So $\mu'(y)$ is continuous and positive on the compact interval $[0,1]$ and has thus a minimum $c_1(G) > 0$. Finally, we note that $r(x,y)$ behaves like

$$\sum_i y^{\sum_{l=1}^i a_l - 1} x^i$$

for $y \to \infty$. Now it is easy to see that

$$q_y(\lambda(y),y) \sim \sum_i \frac{iA}{y} \text{ and } q_x(\lambda(y),y) \sim \sum_i \frac{i}{\lambda(y)},$$

where the sum is over all i (there might be more than one) for which $\frac{a_1+\ldots+a_i-1}{i} = A$. It follows immediately that $\lim_{y\to\infty} \mu(y) = A$. ■

Remark. It is easily proved that $A = a_1 - \frac{1}{M} \geq \frac{1}{2}$, where M is the largest index such that $a_1 = a_M$.

Lemma 9.4 Let $\lambda_1(y)$ be the solution of smallest modulus of $q(x,y) = 0$ for arbitrary complex y, and let $\lambda_2(y)$ be one of the solutions of second-smallest modulus. Then there exist positive constants $\phi(G), c_2(G), c_3(G), \kappa_1(G)$ depending only on the sequence G such that $c_2(G) < 1$ and

$$\left|\frac{\lambda_1(y)}{\lambda_2(y)}\right| \leq \min(c_2(G), c_3(G)|y|^{\kappa_1(G)}) \tag{9.8}$$

for all $y \in B = \{z \in \mathbb{C} : |z| \leq 1, |\arg z| \leq \phi(G)\}$ and λ_1 coincides with the branch λ on B.

Proof. $\lambda_1(y)$ coincides with $\lambda(y)$ on the compact interval $[0,1]$, since we already know that $\lambda(y)$ is the unique solution of minimal modulus on this interval. Note that all branches of the equation $q(x,y) = 0$ except λ tend to ∞ with some negative power of y as $y \to 0$. Therefore, there exists some $\delta > 0$ such that $\lambda_1(y) = \lambda(y)$ and

$$\left|\frac{\lambda_1(y)}{\lambda_2(y)}\right| \leq c_4(G)|y|^{\kappa_1(G)} \tag{9.9}$$

for all y with $|y| \leq \delta$, where $c_4(G), \kappa_1(G)$ are constants depending on G.
The absolute distance to the second-smallest solution is a continuous function on $(0,1]$, and it tends to ∞ as $y \to 0$, so it has a minimum on $[0,1]$.
Furthermore, if we choose ϵ_1 small enough to avoid all the (finitely many) branch points of the equation $q(x,y) = 0$ – there are none on $[\delta/2,1]$ –, all branches are holomorphic on $[\delta/2,1] \times [-\epsilon_1,\epsilon_1]$, so they

satisfy a Lipschitz condition. This means that we can find $\epsilon_2 > 0$ such that λ is the unique branch of smallest modulus on $[\delta/2, 1] \times [-\epsilon_2, \epsilon_2]$.
Choose $\phi(G)$ small enough such that B is contained in

$$\{y \in \mathbb{C} : |y| \leq \delta\} \cup [\delta/2, 1] \times [-\epsilon_2, \epsilon_2].$$

B is a compact set, and the function $f(y) = \left|\frac{\lambda_1(y)}{\lambda_2(y)}\right|$ is continuous on this set, if we take $f(0) = 0$. Thus it has a maximum, which must be < 1. Take this as the constant $c_2(G)$. Then, (9.9) holds for some constant $c_3(G)$. ■

Corollary 9.5

$$f(x, y) = \frac{p(x, y)}{q(x, y)} - \frac{p(\lambda_1(y), y)}{q_x(\lambda_1(y), y)(x - \lambda_1(y))}$$

is a holomorphic function on $\{x \in \mathbb{C} : |x| < |\lambda_2(y)|\}$ for all $y \in B$, and there exist constants $c_5(G), \kappa_2(G)$ depending only on G such that

$$|f(x, y)| \leq c_5(G) y^{-\kappa_2(G)} \tag{9.10}$$

holds on $\{x \in \mathbb{C} : |x| \leq \sqrt{|\lambda_1(y)||\lambda_2(y)|}\}$. As a consequence,

$$[x^\nu]\frac{p(x, y)}{q(x, y)} = -\frac{p(\lambda_1(y), y)}{q_x(\lambda_1(y), y)}\lambda_1(y)^{-\nu-1}(1 + O_G(\eta_G^{-\nu})), \tag{9.11}$$

where $\eta_G > 1$ depends only on G.

Proof. Note that $\frac{p(\lambda_1(y),y)}{q_x(\lambda_1(y),y)(x-\lambda_1(y))}$ is the principal part of $\frac{p(x,y)}{q(x,y)}$ at $x = \lambda_1(y)$, so $f(x, y)$ is indeed holomorphic, since $\frac{p(x,y)}{q(x,y)}$ has a single pole at $\lambda_1(y)$ and no other singularity for $|x| < |\lambda_2(y)|$. Now, we write

$$q(x, y) = r(y)(x - \lambda_1(y))(x - \lambda_2(y)) \ldots (x - \lambda_d(y))$$

for $y \in B \setminus \{0\}$ and note that

$$q_x(\lambda_1(y), y) = r(y)(x - \lambda_2(y)) \ldots (x - \lambda_d(y)),$$

yielding

$$f(x, y) = \frac{p(x, y)}{r(y)(x - \lambda_1(y))} \left(\frac{1}{(x - \lambda_2(y)) \ldots (x - \lambda_d(y))} - \frac{1}{(\lambda_1(y) - \lambda_2(y)) \ldots (\lambda_1(y) - \lambda_d(y))}\right).$$

y is bounded on B, and $|x| < |\lambda_2(y)|$ can be bounded by a power of y. Furthermore, the factors $(x - \lambda_i(y))$ are bounded below by $|\lambda_2(y)|\left|1 - \sqrt{\left|\frac{\lambda_1(y)}{\lambda_2(y)}\right|}\right|$ for $x \leq \sqrt{|\lambda_1(y)||\lambda_2(y)|}$, and the factors $(\lambda_1(y) - \lambda_i(y))$ by $|\lambda_2(y)|\left|1 - \left|\frac{\lambda_1(y)}{\lambda_2(y)}\right|\right|$.
Altogether, we see that (9.10) holds for some constant $c_5(G)$ if $y \in B \setminus \{0\}$ and $|x| \leq \sqrt{|\lambda_1(y)||\lambda_2(y)|}$. For $y = 0$, however, the claim is essentially trivial. Now, we have

$$[x^\nu]\frac{p(x, y)}{q(x, y)} = [x^\nu]\frac{p(x, y)}{q_x(\lambda_1(y), y)(x - \lambda_1(y))} + [x^\nu]f(x, y)$$

and

$$[x^\nu]f(x, y) = \oint_{\mathcal{C}} x^{-\nu-1} f(x, y)\, dx \leq 2\pi c_5(G) y^{-\kappa_2(G)} \sqrt{|\lambda_1(y)||\lambda_2(y)|}^{-\nu},$$

where $\mathcal{C}$ is the circle of radius $\sqrt{|\lambda_1(y)||\lambda_2(y)|}$ around 0. Finally,

$$[x^\nu]\frac{p(x, y)}{q_x(\lambda_1(y), y)(x - \lambda_1(y))} = -\frac{p(\lambda_1(y), y)}{q_x(\lambda_1(y), y)}\lambda_1(y)^{-\nu-1}$$

for $\nu > \deg_x p(x, y)$. The claim now follows from the preceding lemma. ■

Next, we need a lemma from [76]:

Lemma 9.6 (Mauduit/Sárközy [76]) For $g > 1$, $0 < r \le 1$ and all $\alpha \in \mathbb{R}$ we have

$$\left|\frac{1 + re(\alpha) + re(2\alpha) + \ldots + r^{g-1}e((g-1)\alpha)}{1 + r + r^2 + \ldots + r^{g-1}}\right| \le 1 - \frac{2r}{g}\|\alpha\|^2. \tag{9.12}$$

Lemma 9.7 There exist constants $c_6(G), c_7(G)$ depending only on G such that

$$\left|[x^\nu]\frac{p(x, re(\alpha))}{q(x, re(\alpha))}\right| \le c_6(G)\exp(-c_7(G)r\nu\|\alpha\|^2)[x^\nu]\frac{p(x,r)}{q(x,r)} \tag{9.13}$$

for all $0 < r \le 1$ and all $\alpha \in \mathbb{R}$.

Proof. Note that $z_\nu(y) := [x^\nu]\frac{p(x,y)}{q(x,y)}$ is a polynomial with positive coefficients in y. So, obviously, $|z_\nu(re(\alpha))| \le z_\nu(r)$ for all ν. Furthermore, $z_\nu(y)$ satisfies a recurrence relation of the form

$$z_\nu(y) = \sum_{i=1}^{d}\left(\sum_{j=0}^{a_i-1} y^j\right)\left(\prod_{l=1}^{i-1} y^{a_l}\right) z_{\nu-i}(y).$$

It follows that

$$|z_\nu(y)| \le \sum_{i=1}^{d}\left|\sum_{j=0}^{a_i-1} y^j \prod_{l=1}^{i-1} y^{a_l}\right| |z_{\nu-i}(y)|.$$

First, we assume that $a_1 > 1$. Then, by the preceding lemma,

$$\left|\sum_{j=0}^{a_1-1}(re(\alpha))^j\right| \le \left(1 - \frac{2r}{a_1}\|\alpha\|^2\right)\sum_{j=0}^{a_1-1} r^j.$$

Trivially,

$$\left|\sum_{j=0}^{a_i-1}(re(\alpha))^j\left(\prod_{l=1}^{i-1}(re(\alpha))^{a_l}\right)\right| \le \sum_{j=0}^{a_i-1} r^j \prod_{l=1}^{i-1} r^{a_l}$$

for all $i > 1$. Now, if we define $Z_\nu(r,\alpha)$ by $Z_\nu(r,\alpha) = z_\nu(r)$ for $\nu < d$ and

$$Z_\nu(r,\alpha) = \left(1 - \frac{2r}{a_1}\|\alpha\|^2\right)\sum_{j=0}^{a_1-1} r^j Z_{\nu-1}(r,\alpha) + \sum_{i=2}^{d}\sum_{j=0}^{a_i-1} r^j \prod_{l=1}^{i-1} r^{a_l} Z_{\nu-i}(r,\alpha),$$

we know that $Z_\nu(r,\alpha) \ge |z_\nu(re(\alpha))|$ for all ν. Since

$$\left(1 - \frac{2r}{a_1}\|\alpha\|^2\right)\sum_{j=0}^{a_1-1} r^j \ge \left(1 - \frac{r}{4}\right)(1+r) = 1 + \frac{r(3-r)}{4} \ge 1,$$

$Z_\nu(r,\alpha)$ is an increasing sequence. Furthermore,

$$\sum_{j=0}^{a_1-1} r^j \ge \sum_{j=0}^{a_i-1} r^j \prod_{l=1}^{i-1} r^{a_l}$$

for all $i \ge 2$, since $r \le 1$ and the a_i are nonincreasing. It follows that

$$\begin{aligned}
Z_\nu(r,\alpha) &\le \left(1 - \frac{2r}{a_1 d}\|\alpha\|^2\right)\sum_{i=1}^{d}\sum_{j=0}^{a_i-1} r^j \prod_{l=1}^{i-1} r^{a_l} Z_{\nu-i}(r,\alpha) \\
&\le \exp\left(-\frac{2r}{a_1 d}\|\alpha\|^2\right)\sum_{i=1}^{d}\sum_{j=0}^{a_i-1} r^j \prod_{l=1}^{i-1} r^{a_l} Z_{\nu-i}(r,\alpha) \\
&\le \sum_{i=1}^{d}\exp\left(-\frac{2ri}{a_1 d^2}\|\alpha\|^2\right)\sum_{j=0}^{a_i-1} r^j \prod_{l=1}^{i-1} r^{a_l} Z_{\nu-i}(r,\alpha)
\end{aligned}$$

and thus

$$Z_\nu(r,\alpha) \le c_6(G)\exp(-c_7(G)r\nu\|\alpha\|^2)z_\nu(r)$$

for constants $c_6(G), c_7(G) = \frac{2}{a_1 d^2}$ by simple induction on ν. This proves the claim in the case of $a_1 > 1$. If $a_1 = a_2 = \ldots = a_d = 1$, iterate the recurrence equation for z_ν once to obtain

$$z_\nu(y) = \sum_{i=2}^{d} y^{i-2}(1+y)z_{\nu-i}(y) + y^{d-1}z_{\nu-d-1}$$

and apply the same method to this equation (note that we have at least one term of the form $(1+y)$, as $d \ge 2$ in this case). ■

Now, we are ready to prove our first main theorem following the same line of proof as Mauduit and Sárközy:

Theorem 9.8 *Let $F(k,\nu)$ be defined as in Proposition 9.2 and take A as in Lemma 9.3. Then, uniformly for $l = \min(k, A\nu - k) \to \infty$, we have*

$$|F(k,\nu)| = \frac{p(\lambda(r),r)}{-\lambda(r)q_x(\lambda(r),r)}\pi^{1/2}(D\nu)^{-1/2}r^{-k}\lambda(r)^{-\nu}(1 + O_G((D\nu)^{-1/2})), \tag{9.14}$$

where r is defined by $\mu(r) = \frac{k}{\nu}$ and $D = 2\pi^2 r\mu'(r)$.

Proof. From Proposition 9.2, we know that

$$|F(k,\nu)| = [x^\nu y^k]\,\frac{p(x,y)}{q(x,y)}.$$

First, let $\frac{k}{\nu} \le \mu(1)$. Choose $0 < r \le 1$ in such a way that $\mu(r) = \frac{k}{\nu}$ – this is possible by Lemma 9.3. Now, we have

$$|F(k,\nu)| = r^{-k}\int_{-1/2}^{1/2}[x^\nu]\frac{p(x,re(\alpha))}{q(x,re(\alpha))}e(-k\alpha)\,d\alpha.$$

We split the integral in two parts: define

$$J_1 = \int_{-\delta}^{\delta}[x^\nu]\frac{p(x,re(\alpha))}{q(x,re(\alpha))}e(-k\alpha)\,d\alpha$$

and

$$J_2 = \int_{\delta<|\alpha|\le 1/2}[x^\nu]\frac{p(x,re(\alpha))}{q(x,re(\alpha))}e(-k\alpha)\,d\alpha,$$

where $\delta = k^{-1/2}\log k$. We will deal with J_1 first. If k is large enough, we have $\delta < \phi(G)$, so we may apply Corollary 9.5. This means that

$$J_1 = \left(\int_{-\delta}^{\delta}\frac{p(\lambda_1(re(\alpha)),re(\alpha))}{-q_x(\lambda_1(re(\alpha)),re(\alpha))}\lambda_1(re(\alpha))^{-\nu-1}e(-k\alpha)\,d\alpha\right)(1 + O_G(\eta_G^{-\nu})).$$

We expand $\frac{p(\lambda_1(y),y)}{-q_x(\lambda_1(y),y)}$ in a Taylor series around $y = r$; $p(x,y)$ and $-q_x(x,y)$ are polynomials with positive coefficients, and we have $-q_x(1,0) = 1$ and $p(1,0) = 1$ (note that $\frac{p(x,0)}{q(x,0)}$ is the counting series for integers with sum of digits 0). This means that $p(\lambda(y),y)$ and $-q_x(\lambda(y),y)$ can be bounded above and below for $y \le 1$ (the bounds depending only on G), and their derivatives are also bounded. The derivatives of λ are thus bounded as well. Therefore, we have

$$\frac{p(\lambda_1(re(\alpha)),re(\alpha))}{-q_x(\lambda_1(re(\alpha)),re(\alpha))\lambda_1(re(\alpha))} = \frac{p(\lambda(r)),r)}{-q_x(\lambda(r),r)\lambda(r)}\left(1 + b(r)\alpha + O_G(\alpha^2)\right).$$

Likewise, we obtain

$$\lambda_1(re(\alpha)) = \lambda(r) + 2\pi i\alpha r\lambda'(r) - 2\pi^2\alpha^2 r(\lambda'(r) + r\lambda''(r)) + O_G(r\alpha^3).$$

Inserting yields

$$J_1 = \lambda(r)^{-\nu-1}(1 + O_G(\eta_G^{-\nu}))\int_{-\delta}^{\delta}\frac{p(\lambda(r)),r)}{-q_x(\lambda(r),r)}\left(1 + b(r)\alpha + O_G(\alpha^2)\right)$$
$$\exp\left(-\frac{2\pi i\alpha\nu r\lambda'(r)}{\lambda(r)} + \frac{2\pi^2 r\alpha^2\nu(\lambda(r)\lambda'(r) + r\lambda(r)\lambda''(r) - r\lambda'(r)^2)}{\lambda(r)^2} + O_G(r\alpha^3\nu) - 2\pi i k\alpha\right)d\alpha.$$

r was chosen in such a way that $\mu(r) = -\frac{r\lambda'(r)}{\lambda(r)} = \frac{k}{\nu}$. Thus, the coefficients of α in the exponent cancel out. Furthermore, note that

$$\frac{2\pi^2 r\nu(\lambda(r)\lambda'(r) + r\lambda(r)\lambda''(r) - r\lambda'(r)^2)}{\lambda(r)^2} = -2\pi^2 r\nu\mu'(r) \le -2\pi^2 r\nu c_1(G) < 0$$

by Lemma 9.3. We write $D = 2\pi^2 r\mu'(r)$ and use the standard estimates

$$\begin{aligned}
&\int_{-\delta}^{\delta}(b(r)\alpha + O_G(\alpha)^2)\exp(-D\nu\alpha^2 + O_G(r\alpha^3\nu))\,d\alpha\\
&\quad= \int_{-\delta}^{\delta}(b(r)\alpha + O_G(\alpha^2) + O_G(r\alpha^4\nu))\exp(-D\nu\alpha^2)\,d\alpha\\
&\quad= O_G\left(\int_0^{\delta}\alpha^2\exp(-D\nu\alpha^2)\,d\alpha\right) + O_G\left(r\nu\int_0^{\delta}\alpha^4\exp(-D\nu\alpha^2)\,d\alpha\right),
\end{aligned}$$

$$\begin{aligned}
\int_{-\delta}^{\delta}\exp(-D\nu\alpha^2 + O_G(r\nu\alpha^3))\,d\alpha &= \int_{-\delta}^{\delta}\exp(-D\nu\alpha^2)\,d\alpha + O_G\left(r\nu\int_0^{\delta}\alpha^3\exp(-D\nu\alpha^2)\right)\\
&= \frac{1}{\sqrt{D\nu}} - 2\int_{\delta}^{\infty}\exp(-D\nu\alpha^2)\,d\alpha + O_G\left(r\nu\int_0^{\delta}\alpha^3\exp(-D\nu\alpha^2)\right),
\end{aligned}$$

$$\begin{aligned}
\int_0^{\delta}\alpha^p\exp(-D\nu\alpha^2)\,d\alpha &= (D\nu)^{-(p+1)/2}\int_0^{\sqrt{D\nu}\delta}x^p\exp(-x^2)\,dx\\
&\le (D\nu)^{-(p+1)/2}\int_0^{\infty}x^p\exp(-x^2)\,dx\\
&= O\left((D\nu)^{-(p+1)/2}\right)
\end{aligned}$$

and

$$\begin{aligned}
\int_{\delta}^{\infty}\exp(-D\nu\alpha^2)\,d\alpha &= \frac{1}{2\sqrt{D\nu}}\int_{D\nu\delta^2}^{\infty}x^{-1/2}\exp(-x)\,dx\\
&\le \frac{1}{2D\nu\delta}\exp(-D\nu\delta^2).
\end{aligned}$$

Since $\mu'(y)$ is bounded on $[0,1]$ by Lemma 9.3, there are constants $c_8(G)$ and $c_9(G)$ such that

$$c_8(G)\frac{k}{\nu} \le r \le c_9(G)\frac{k}{\nu}.$$

Therefore, these estimates imply that

$$J_1 = \frac{p(\lambda(r),r)}{-\lambda(r)q_x(\lambda(r),r)}(2\pi r\nu\mu'(r))^{-1/2}\lambda(r)^{-\nu}(1 + O_G((D\nu)^{-1/2})).$$

Finally, we estimate J_2: by Lemma 9.7,

$$\begin{aligned}|J_2| &= \left| \int_{\delta \le |\alpha| \le 1/2} [x^\nu] \frac{p(x, re(\alpha))}{q(x, re(\alpha))} e(-k\alpha)\, d\alpha \right| \\ &\le 2c_6(G)[x^\nu] \frac{p(x,r)}{q(x,r)} \int_\delta^{1/2} \exp(-c_7(G) r\nu \|\alpha\|^2)\, d\alpha \\ &= O_G(\lambda(r)^{-\nu} \exp(-c_7(G) r\nu\delta^2)).\end{aligned}$$

Altogether, we have established formula (9.14) for $\frac{k}{\nu} \le \mu(1)$. We indicate how to extend it to the case $\frac{k}{\nu} \ge \mu(1)$: if A is taken as in Lemma 9.3 and $l = A\nu - k$, we have

$$|F(k,\nu)| = [x^\nu y^l] \frac{p(xy^A, y^{-1})}{q(xy^A, y^{-1})}.$$

The proof now goes along the same lines, with $\mu(y)$ replaced by $A - \mu(y^{-1})$ and the roles of y and y^{-1} interchanged. ■

Corollary 9.9 There is a constant $c_{10}(G)$ depending only on G such that the number of integers $\le N$ with sum of digits k is bounded below by

$$c_{10}(G) \cdot \frac{p(\lambda(r), r)}{-\lambda(r) q_x(\lambda(r), r)} r^{-k} \lambda(r)^{-\nu} k^{-1/2} \tag{9.15}$$

uniformly for $k \le \mu(1)\nu$, $k \to \infty$, where $\nu + 1$ is the number of digits of N.

Theorem 9.8 is a consequence of general theorems of Bender and Richmond [7, 9] (see also Drmota [21]) in the case when r is bounded above and below by positive constants. Equivalenty, $\frac{k}{\nu} \in [a,b]$ for constants $0 < a < b < A$. It is easy to see that the sum of digits asymptotically follows a normal distribution with mean $\mu(1)\nu$ and variance $\mu'(1)\nu$: note first that $r^{-k}\lambda(r)^{-\nu} = \left(r^{\mu(r)}\lambda(r)\right)^{-\nu}$. The maximal value of $-\log\left(r^{\mu(r)}\lambda(r)\right)$ is achieved when the derivative is 0, i.e.

$$\frac{\mu(r)}{r} + \mu'(r)\log(r) + \frac{\lambda'(r)}{\lambda(r)} = \mu'(r)\log(r) = 0,$$

which happens if $r = 1$. The following corollary of Theorem 9.8 gives precise information:

Corollary 9.10 When k is near the mean value, i.e. $\Delta = \mu(1)\nu - k = o(\nu)$, we have

$$|F(k,\nu)| = \frac{p(\lambda(1), 1)}{-\lambda(1) q_x(\lambda(1), 1)} \lambda(1)^{-\nu} \cdot (2\pi\nu\mu'(1))^{-1/2} \exp\left(-\frac{\Delta^2}{2\nu\mu'(1)}\right)\left(1 + O_G\left(\frac{\Delta}{\nu} + \nu^{-1/2}\right)\right). \tag{9.16}$$

Proof. We set $\eta = 1 - r$ and use the Taylor expansion of μ around 1 to find that

$$\eta = \frac{\Delta}{\nu\mu'(1)} + O_G\left(\frac{\Delta^2}{\nu^2}\right).$$

Then,

$$r^{-k} = \exp(-k\log(1-\eta)) = \exp\left(k\eta + \frac{1}{2}k\eta^2 + O(k\eta^3)\right)$$

and

$$\lambda(r)^{-\nu} = \lambda(1)^{-\nu} \exp\left(\nu\left(\frac{\lambda'(1)}{\lambda(1)}\eta + \frac{\lambda'(1)^2 - \lambda(1)\lambda''(1)}{2\lambda(1)^2}\eta^2 + O_G(\eta^3)\right)\right).$$

Furthermore,

$$\frac{p(\lambda(r),r)}{-\lambda(r)q_x(\lambda(r),r)}(2\pi r\nu\mu'(r))^{-1/2} = \frac{p(\lambda(1),1)}{-\lambda(1)q_x(\lambda(1),1)}(2\pi\nu\mu'(1))^{-1/2}\left(1+O_G\left(\frac{\Delta}{\nu}\right)\right).$$

We insert $k = \mu(1)\nu - \Delta$ and use the formula

$$\mu'(y) = \frac{y\lambda'(y)^2 - y\lambda(y)\lambda''(y) - \lambda(y)\lambda'(y)}{\lambda(y)^2}$$

to obtain the stated result. ■

Remark. Note that $\frac{p(\lambda(1),1)}{-\lambda(1)q_x(\lambda(1),1)}\lambda(1)^{-\nu}$ is (asymptotically) the number of all integers with an expansion of $\leq \nu$ digits.

Corollary 9.11 If k is small, i.e. $k = o(\nu)$, we have

$$|F(k,\nu)| = (2\pi k)^{-1/2}\exp\left(-k\log\frac{k}{\nu} + k + \frac{1-\lambda''(0)}{2}\cdot\frac{k^2}{\nu} + O_G\left(\frac{k^3}{\nu^2}+\frac{1}{\sqrt{k}}\right)\right). \tag{9.17}$$

Remark. It is easy to check that

$$\lambda''(0) = \begin{cases} 4 & d=2,\ a_1=a_2=1, \\ 2 & d=1,\ a_1=2 \text{ or } d>2,\ a_1=a_2=\ldots=a_d=1, \\ 0 & \text{otherwise.}\end{cases}$$

Proof. We see that

$$r = \frac{k}{\nu} - \frac{\mu''(0)}{2}\left(\frac{k}{\nu}\right)^2 + O_G\left(\left(\frac{k}{\nu}\right)^3\right),$$

since $\mu'(0) = 1$. This gives us

$$r\mu'(r) = \frac{k}{\nu} + \frac{\mu''(0)}{2}\left(\frac{k}{\nu}\right)^2 + O_G\left(\left(\frac{k}{\nu}\right)^3\right)$$

and

$$\lambda(r) = 1 - r + \frac{\lambda''(0)}{2}r^2 + O_G(r^3) = 1 - \frac{k}{\nu} + \frac{\lambda''(0)+\mu''(0)}{2}\left(\frac{k}{\nu}\right)^2 + O_G\left(\left(\frac{k}{\nu}\right)^3\right).$$

Therefore,

$$\frac{p(\lambda(r),r)}{-\lambda(r)q_x(\lambda(r),r)} = \frac{p(\lambda(0),0)}{-\lambda(0)q_x(\lambda(0),0)}\left(1+O_G\left(\frac{k}{\nu}\right)\right) = 1 + O_G\left(\frac{k}{\nu}\right),$$

$$2\pi r\mu'(r)\nu = 2\pi k\left(1+O_G\left(\frac{k}{\nu}\right)\right),$$

$$-k\log r = -k\log\frac{k}{\nu} + \frac{\mu''(0)}{2}\cdot\frac{k^2}{\nu} + O_G\left(\frac{k^3}{\nu^2}\right),$$

and

$$-\nu\log\lambda(r) = k - \frac{\lambda''(0)+\mu''(0)-1}{2}\cdot\frac{k^2}{\nu} + O_G\left(\frac{k^3}{\nu^2}\right).$$

Inserting in (9.14) yields the stated result. ■

Example 9.1 It is not difficult to check that our result agrees with (9.3) in the case $d = 1$, $a_1 = g$. We will consider the classical Zeckendorf expansion ($d = 2$, $a_1 = a_2 = 1$, $G_0 = 1$, $G_1 = 2$) as another example. In this case, we have

$$p(x, y) = 1 + xy,\ q(x, y) = 1 - x - yx^2,$$

yielding

$$\lambda(y) = \frac{1}{2y}\left(\sqrt{1+4y} - 1\right),\ \mu(y) = \frac{1}{2}\left(1 - \frac{1}{\sqrt{1+4y}}\right).$$

If we set $\frac{k}{n} = \gamma$, we obtain

$$|F(k,\nu)| \sim \sqrt{\frac{(1-\gamma)^3}{2\pi\gamma(1-2\gamma)^3\nu}} \cdot \left(\frac{(1-\gamma)^{1-\gamma}}{\gamma^\gamma(1-2\gamma)^{1-2\gamma}}\right)^\nu. \tag{9.18}$$

The mean value is given by $\mu\nu = \mu(1)\nu = \frac{1}{2}\left(1 - \frac{1}{\sqrt{5}}\right)\nu$, the variance by $\sigma^2\nu = \mu'(1)\nu = 5^{-3/2}\nu$.

9.3 Distribution in residue classes

The aim of this section is to prove that $F(k, \nu)$ is well-distributed in residue classes modulo m provided that m is not too large and there is no prime divisor P of m such that G_n is constant modulo P for all but finitely many values of n.

Theorem 9.12 *Let $V(k, N)$ be the set of integers $\le N$ with G-ary sum of digits k. There exist positive constants $k_0(G)$, $c_{11}(G)$, $c_{12}(G)$, $c_{13}(G)$ (depending on G only) such that for all $l = \max(k, A\nu - k) \ge k_0(G)$ (ν denoting the number of G-ary digits of N), $2 \le m < \exp(c_{11}(G)l^{1/2})$, $h \in \mathbb{Z}$, for which there is no prime divisor P of m such that (G_n) is constant modulo P for all but finitely many values of n, we have*

$$\left| |\{n \in V(k,N) : n \equiv h \mod m\}| - \frac{1}{m}|V(k,N)| \right| < \frac{c_{11}(G)}{m}|V(k,N)| \exp\left(-c_{12}(G)\frac{k}{\log m}\right). \tag{9.19}$$

Remark. The condition on the prime factors of m is a necessary one. If (G_n) was constant modulo P for all but finitely many values of n, the restriction on the sum of digits would imply a condition on the residues modulo P. Note that $(g^n)_{n\ge 0}$ is constant modulo P for all but finitely many values of n if and only if $P|g(g-1)$.

Proof. We follow the lines of [76] again. Again, we consider the case $k \le \mu(1)\nu$ only. if

$$D(z, \gamma) = \sum_{n=1}^{N} z^{s_G(n)} e(n\gamma),$$

where $z \in \mathbb{C}$, $\gamma \in \mathbb{R}$, we have

$$\frac{1}{m}\sum_{p=1}^{m} e\left(-\frac{hp}{m}\right) D\left(z, \frac{p}{m}\right) = \sum_{\substack{1\le n\le N \\ n\equiv h \mod m}} z^{s_G(n)}.$$

Now we take r as in the proof of Theorem 9.8 and obtain

$$\begin{aligned}|\{n \le N : s_G(n) = k, n \equiv h \mod m\}| &= r^{-k}\int_0^1 e(-k\beta) \sum_{\substack{1\le n\le N \\ n\equiv h \mod m}} (re(\beta))^{s_G(n)}\, d\beta \\ &= \frac{1}{m}r^{-k}\sum_{p=1}^{m}\int_0^1 e\left(-k\beta - \frac{hp}{m}\right) D\left(re(\beta), \frac{p}{m}\right)\, d\beta.\end{aligned}$$

Obviously, the summand corresponding to $p = m$ equals $\frac{1}{m}|V(k,N)|$. Thus we have to estimate

$$\frac{1}{m} r^{-k} \sum_{p=1}^{m-1} \int_0^1 \left| D\left(re(\beta), \frac{p}{m}\right)\right| \, d\beta.$$

We write N in base-G representation:

$$N = \sum_{j=0}^{L(N)} \epsilon_j G_j = \sum_{i=1}^{t} \epsilon_{\nu_i} G_{\nu_i},$$

where $\nu_1 > \nu_2 > \ldots > \nu_t$ and all ϵ_{ν_i} are positive (i.e., we neglect all digits 0 in the base-G representation). Then, the set $\{0, \ldots, N\}$ can be partitioned into sets A_l, where A_l is the set of integers representable as

$$\sum_{i=1}^{l-1} \epsilon_{\nu_i} G_{\nu_i} + aG_{\nu_l} + b,$$

where $0 \le a \le \epsilon_{\nu_l} - 1$ and b is an arbitrary integer with $\le \nu_l$ G-ary digits. Let the set of all such integers be denoted by B_{ν_l}. Additionally, we set $A_{t+1} = \{N\}$. Then we have

$$\begin{aligned} 1 + D(re(\beta), \gamma) &= \sum_{n=0}^{N} (re(\beta))^{s_G(n)} e(n\gamma) \\ &= \sum_{l=1}^{t+1} \sum_{n \in A_l} (re(\beta))^{s_G(n)} e(n\gamma) \\ &= (re(\beta))^{s_G(N)} e(N\gamma) + \sum_{l=1}^{t} \sum_{a=0}^{\epsilon_{\nu_l}-1} \sum_{b \in B_{\nu_l}} (re(\beta))^{\epsilon_{\nu_1} + \ldots + \epsilon_{\nu_{l-1}} + a + s_G(b)} \\ &\quad e\left(\left(\sum_{i=1}^{l-1} \epsilon_{\nu_i} G_{\nu_i} + aG_{\nu_l} + b\right)\gamma\right), \end{aligned}$$

from which it follows that

$$\begin{aligned} |D(re(\beta), \gamma)| &\le 2 + \sum_{l=1}^{t} r^{\epsilon_{\nu_1} + \ldots + \epsilon_{\nu_{l-1}}} \left| \sum_{a=0}^{\epsilon_{\nu_l}-1} (re(\beta + G_{\nu_l}\gamma))^a \right| \left| \sum_{b \in B_{\nu_l}} (re(\beta))^{s_G(b)} e(b\gamma) \right| \\ &\le 2 + \sum_{l=1}^{t} r^{l-1} \epsilon_{\nu_l} \left| \sum_{b \in B_{\nu_l}} (re(\beta))^{s_G(b)} e(b\gamma) \right|. \end{aligned}$$

We write

$$u_\nu(\beta, \gamma) := \sum_{b \in B_\nu} (re(\beta))^{s_G(b)} e(b\gamma).$$

Then we see that u_ν satisfies a recursive relation:

Lemma 9.13 For $\nu \ge 2d$, we have

$$u_\nu(\beta, \gamma) = \sum_{i=1}^{d} \left(\sum_{j=0}^{a_i - 1} (re(\beta + G_{\nu-i}\gamma))^j \right) \left(\prod_{l=1}^{i-1} (re(\beta + G_{\nu-l}\gamma))^{a_l} \right) u_{\nu-i}(\beta, \gamma). \tag{9.20}$$

Proof. This is proved in the same way as Proposition 9.2: note that appending a sequence of the form $(\epsilon, a_{i-1}, \ldots, a_1)$ with $\epsilon < a_i$ to a good sequence of length $\nu - i$ gives a factor of

$$(re(\beta))^{a_1 + \ldots + a_{i-1} + \epsilon} e((G_{\nu-1}a_1 + \ldots + G_{\nu-i+1}a_{i-1} + G_{\nu-i}\epsilon)\gamma).$$

∎

The recurrence can be used to prove an analogue of Lemma 9.7:

Lemma 9.14 There exist constants $c_{14}(G), c_{15}(G)$ depending only on G such that

$$u_\nu(\beta,\gamma) \le c_{14}(G) \exp\left(-c_{15}(G) r \sum_{n=0}^{\nu-1} \|\beta + G_n\gamma\|^2\right) u_\nu(0,0) \tag{9.21}$$

for all $0 < r \le 1$ and all $\beta, \gamma \in \mathbb{R}$.

Proof. This is done almost analogously to the proof of Lemma 9.7. For $a_1 > 1$ (the other case is similar), we have

$$|u_\nu(\beta,\gamma)| \le \left(1 - \frac{2r}{a_1}\|\beta + G_{\nu-1}\gamma\|^2\right) \sum_{j=0}^{a_1-1} r^j |u_{\nu-1}(\beta,\gamma)| + \sum_{i=2}^{d} \sum_{j=0}^{a_i-1} r^j \prod_{l=1}^{i-1} r^{a_l} |u_{\nu-i}(\beta,\gamma)|$$

by the same argument as in Lemma 9.7. If we define $U_\nu(\beta,\gamma)$ by $U_\nu(\beta,\gamma) = u_\nu(0,0)$ for $\nu < d$ and

$$U_\nu(\beta,\gamma) = \left(1 - \frac{2r}{a_1}\|\beta + G_{\nu-1}\gamma\|^2\right) \sum_{j=0}^{a_1-1} r^j U_{\nu-1}(\beta,\gamma) + \sum_{i=2}^{d} \sum_{j=0}^{a_i-1} r^j \prod_{l=1}^{i-1} r^{a_l} U_{\nu-i}(\beta,\gamma),$$

we know that $|u_\nu(\beta,\gamma)| \le U_\nu(\beta,\gamma)$ for all ν, and the argument of Lemma 9.7 shows that

$$U_\nu(\beta,\gamma) \le \left(1 - \frac{2r}{a_1 d}\|\beta + G_{\nu-1}\gamma\|^2\right) \sum_{i=1}^{d} \sum_{j=0}^{a_i-1} r^j \prod_{l=1}^{i-1} r^{a_l} U_{\nu-i}(\beta,\gamma).$$

Write $C_i := \sum_{j=0}^{a_i-1} r^j \prod_{l=1}^{i-1} r^{a_l}$. For a sequence $\mathbf{x} = (x_n)_{n\ge 0}$ with $1 \ge x_n \ge 1 - \frac{r}{2}$, define $W_\nu(\mathbf{x})$ by $W_\nu(\mathbf{x}) = u_\nu(0,0)$ for $\nu < d$ and

$$W_\nu(\mathbf{x}) = x_\nu \sum_{i=1}^{d} C_i W_{\nu-i}(\mathbf{x}).$$

Since $x_\nu C_1 \ge \left(1 - \frac{r}{2}\right)(1+r) = 1 + \frac{r(1-r)}{2} \ge 1$, we know that $W_\nu(\mathbf{x})$ is increasing, and we also know that the C_i are decreasing, so $C_i W_{\nu-i}(\mathbf{x})$ is always decreasing. Let $\mathbf{x}^{(n)}$ be the sequence $\mathbf{x}$ with 1 at the place of x_n. We claim that

$$W_\nu(\mathbf{x}) \le \left(1 - \frac{1-x_n}{d}\right) W_\nu(\mathbf{x}^{(n)})$$

holds for $\nu \ge n$. This is trivial for $\nu = n$, since we have

$$W_n(\mathbf{x}) = x_n W_n(\mathbf{x}^{(n)})$$

and $\left(1 - \frac{1-x_n}{d}\right) \ge x_n$. We proceed by induction: for $1 \le j \le d-1$, we have

$$\begin{aligned}
W_{n+j}(\mathbf{x}) &= \sum_{i=1}^{j-1} C_i W_{n+j-i}(\mathbf{x}) + C_j W_n(\mathbf{x}) + \sum_{i=j+1}^{d} C_i W_{n+j-i}(\mathbf{x}) \\
&\le \left(1 - \frac{1-x_n}{d}\right) \sum_{i=1}^{j-1} C_i W_{n+j-i}(\mathbf{x}^{(n)}) + x_n C_j W_n(\mathbf{x}^{(n)}) + \sum_{i=j+1}^{d} C_i W_{n+j-i}(\mathbf{x}^{(n)}) \\
&\le \left(1 - \frac{1-x_n}{d}\right) \sum_{i=1}^{j-1} C_i W_{n+j-i}(\mathbf{x}^{(n)}) + \frac{d-j+x_n}{d-j+1} \sum_{i=j}^{d} C_i W_{n+j-i}(\mathbf{x}^{(n)}) \\
&\le \left(1 - \frac{1-x_n}{d}\right) \sum_{i=1}^{d} C_i W_{n+j-i}(\mathbf{x}^{(n)}) \\
&= \left(1 - \frac{1-x_n}{d}\right) W_{n+j}(\mathbf{x}^{(n)}).
\end{aligned}$$

For $j \geq d$, the induction is even simpler. Another straightforward induction shows that

$$W_\nu(\mathbf{x}) \leq \prod_{j=d}^{\nu} \left(1 - \frac{1-x_j}{d}\right) W_\nu(\mathbf{1}),$$

where $\mathbf{1}$ is the sequence consisting only of 1's. In our special case, we take $x_n = 1 - \frac{2r}{a_1 d}\|\beta + G_{n-1}\gamma\|^2$ to show that

$$\begin{aligned} U_\nu(\beta,\gamma) &\leq \prod_{n=d}^{\nu} \left(1 - \frac{2r}{a_1 d^2}\|\beta + G_{n-1}\gamma\|^2\right) u_\nu(0,0) \\ &\leq \left(1 - \frac{1}{2a_1 d^2}\right)^{1-d} \prod_{n=1}^{\nu} \left(1 - \frac{2r}{a_1 d^2}\|\beta + G_{n-1}\gamma\|^2\right) u_\nu(0,0) \\ &\leq \left(1 - \frac{1}{2a_1 d^2}\right)^{1-d} \exp\left(-\frac{2r}{a_1 d^2}\sum_{n=0}^{\nu-1}\|\beta + G_n\gamma\|^2\right) u_\nu(0,0), \end{aligned}$$

which finally proves the claim. ■

Lemma 9.15 Let $m, \rho \in \mathbb{N}$ and $1 \leq p \leq m-1$. If there is no prime divisor P of m such that the sequence G_n is constant modulo P for all but finitely many values of n, we have

$$\sum_{n=0}^{\rho-1} \left\|\beta + G_n \frac{p}{m}\right\|^2 \geq c_{16}(G)\frac{\rho}{\log m} + O_G(1). \tag{9.22}$$

Proof. Without loss of generality, we may assume that $(p,m) = 1$ (cancellation of common factors only improves the bound, and the conditions keep true). First, we show that there exist constants $c_{17}(G)$ and $c_{18}(G)$ such that, among any set of $c_{17}(G) + c_{18}(G)\log m$ consequent integers, there is an integer n such that

$$\left\|(G_{n+1} - G_n)\frac{p}{m}\right\| \geq \frac{1}{2(a_1 + \ldots + a_d)}.$$

For this purpose, we define a sequence $(A_n)_{n\geq 0}$ by $A_n \equiv (G_{n+1} - G_n)p \mod m$ and $-\frac{m}{2} < A_n \leq \frac{m}{2}$. We want to show that there are constants $c_{17}(G)$ and $c_{18}(G)$ such that for all $I \geq 0$, there is an $n < c_{17}(G) + c_{18}(G)\log m$ with

$$\left\|\frac{A_{I+n}}{m}\right\| \geq \frac{1}{2(a_1 + \ldots + a_d)}.$$

First, of all, we will take $c_{17}(G) \geq d$. Consider the values $A_I, A_{I+1}, \ldots, A_{I+d-1}$. If one of them has absolute value $\geq \frac{m}{2(a_1+\ldots+a_d)}$, we are done. Otherwise, define the sequence $(B_n)_{n\geq 0}$ by $B_n = A_{I+n}$ ($n = 0, \ldots, d-1$) and

$$B_{n+d} = a_1 B_{n+d-1} + a_2 B_{n+d-2} + \ldots + a_d B_n.$$

Note that $B_n \equiv A_{I+n}$ for all values of n. Now we use a result of Brauer [12] that was also applied in [90]: The characteristic polynomial

$$x^d - a_1 x^{d-1} - \ldots - a_d$$

has a dominating root $\theta \in [a_1, a_1+1)$ that is a Pisot number, i.e., all conjugates $\theta_2, \ldots, \theta_d$ (if $d > 1$) have modulus < 1. Thus, we can express B_n by an explicit formula:

$$B_n = \beta\theta^n + \sum_{i=2}^{d} \beta_i n^{\delta(i)}\theta_i^n,$$

where the β_i are linear combinations of the initial values $B_0, B_1, \ldots, B_{d-1}$ (with algebraic coefficients depending only on the characteristic polynomial). Therefore, there exist constants $c_{19}(G)$ and $\kappa_3(G)$ such that

$$|B_n - \beta\theta^n| \leq c_{19}(G) m n^{\kappa_3(G)} |\theta_2|^n.$$

The coefficient β is also a linear combination of the initial values, i.e. it is of the form

$$x_0B_0 + \ldots + x_{d-1}B_{d-1},$$

where the x_i are algebraic numbers depending on the characteristic polynomial. By a result of Schmidt (cf. [23, Theorem 2.1]), the inequality

$$0 < |x_0B_0 + \ldots + x_{d-1}B_{d-1}| < M^{-d+1-\epsilon}$$

with $|B_n| \leq M$ has only finitely many solutions for every $\epsilon > 0$; therefore, there are constants $c_{20}(G) > 0$ and $\kappa_4(G)$ such that either

$$\beta = x_0B_0 + \ldots + x_{d-1}B_{d-1} = 0$$

or

$$|\beta| = |x_0B_0 + \ldots + x_{d-1}B_{d-1}| \geq c_{20}(G)M^{-\kappa_4(G)}$$

whenever $|B_0|, \ldots, |B_{d-1}| \leq M$. We know that β cannot be 0, since then we would have $\lim_{n\to\infty} B_n = 0$, i.e. $A_n \equiv 0 \mod m$ for all but finitely many values of n. This contradicts the assumptions on G: as $(p, m) = 1$, G_n would be constant modulo m for all but finitely many values of n. Therefore, since $|B_n| \leq \frac{m}{2(a_1+\ldots+a_d)}$ for $0 \leq n \leq d-1$, $|\beta| \geq c_{21}(G)m^{-\kappa_4}$, where $c_{21} > 0$ depends only on G. It follows that

$$|B_n| \geq c_{21}(G)m^{-\kappa_4}\theta^n - c_{19}(G)mn^{\kappa_3(G)}|\theta_2|^n$$

for all n; there are constants $c_{22}(G)$ and $c_{23}(G)$ such that

$$c_{21}(G)m^{-\kappa_4(G)}\theta^n - c_{19}(G)mn^{\kappa_3(G)}|\theta_2|^n > \frac{m}{2(a_1+\ldots+a_d)}$$

for all $n \geq c_{22}(G)\log m + c_{23}(G)$. Thus, $B_n \geq \frac{m}{2(a_1+\ldots+a_d)}$ for some $n \leq c_{22}(G)\log m + c_{23}(G)$; for the smallest index n for which this is true, we must also have $B_n \leq \frac{m}{2}$, so

$$\left\|\frac{A_{I+n}}{m}\right\| = \left\|\frac{B_n}{m}\right\| \geq \frac{1}{2(a_1+\ldots+a_d)}.$$

This proves the claim, and the lemma is a simple consequence if we make use of the inequality

$$\left\|\beta + G_{n+1}\frac{p}{m}\right\|^2 + \left\|\beta + G_n\frac{p}{m}\right\|^2 \geq \frac{1}{2}\left\|G_{n+1}\frac{p}{m} - G_n\frac{p}{m}\right\|^2.$$

■

We turn back to the proof of Theorem 9.12. By the preceding lemmas, there are constants $c_{24}(G)$ and $c_{25}(G)$ such that

$$u_\nu\left(\beta, \frac{p}{m}\right) \leq c_{24}(G)\exp\left(-c_{25}(G)\frac{r\nu}{\log m}\right)u_\nu(0,0).$$

Therefore, since $u_{\nu_l}(0,0) = \sum_{b\in B_{\nu_l}} r^{s_G(b)}$, we have

$$\left|D\left(re(\beta), \frac{p}{m}\right)\right| \leq c_{24}(G)\left(\sum_{l=1}^{t} r^{l-1}\epsilon_{\nu_l}\exp\left(-c_{25}(G)\frac{r\nu_l}{\log m}\right)\sum_{b\in B_{\nu_l}} r^{s_G(b)}\right) + O_G(1).$$

We divide the sum on the right side into two parts by defining the integer q for which $\nu_q \geq \nu/2 > \nu_{q+1}$ (set $\nu_{t+1} = 0$): the first part is defined by

$$S_1 := \sum_{l=1}^{q} r^{l-1}\epsilon_{\nu_l}\exp\left(-c_{25}(G)\frac{r\nu_l}{\log m}\right)\sum_{b\in B_{\nu_l}} r^{s_G(b)} \leq c_{26}(G)\exp\left(-c_{25}(G)\frac{r\nu/2}{\log m}\right)\sum_{l=1}^{q} r^{l-1}\sum_{b\in B_{\nu_l}} r^{s_G(b)},$$

where $c_{26}(G)$ is the largest possible digit that can appear in a G-ary expansion. Next, we observe that

$$\sum_{b\in B_{\nu_l}} r^{s_G(b)} = [x^{\nu_l}]\frac{p(x,r)}{q(x,r)}.$$

By Corollary 9.5, this equals

$$\sum_{b\in B_{\nu_l}} r^{s_G(b)} = -\frac{p(\lambda(r),r)}{q_x(\lambda(r),r)}\lambda(r)^{-\nu_l-1}(1+O_G(\eta_G^{-\nu_l})),$$

so that we obtain

$$\begin{aligned}
S_1 &\le c_{26}(G)\exp\left(-c_{25}(G)\frac{r\nu/2}{\log m}\right)\sum_{l=1}^{q} r^{l-1}\cdot\left(-\frac{p(\lambda(r),r)}{q_x(\lambda(r),r)}\right)\lambda(r)^{-\nu_l-1}\left(1+O_G\left(\eta_G^{-\nu_l}\right)\right)\\
&= c_{26}(G)\exp\left(-c_{25}(G)\frac{r\nu/2}{\log m}\right)\left(1+O_G\left(\eta_G^{-\nu/2}\right)\right)\cdot\left(-\frac{p(\lambda(r),r)}{\lambda(r)q_x(\lambda(r),r)}\right)\lambda(r)^{-\nu}\cdot\sum_{l=1}^{q} r^{l-1}\lambda(r)^{\nu-\nu_l}\\
&\le c_{26}(G)\exp\left(-c_{25}(G)\frac{r\nu/2}{\log m}\right)\left(1+O_G\left(\eta_G^{-\nu/2}\right)\right)\cdot\left(-\frac{p(\lambda(r),r)}{\lambda(r)q_x(\lambda(r),r)}\right)\lambda(r)^{-\nu}\cdot\sum_{j=0}^{\infty}(r\lambda(r))^{j}.
\end{aligned}$$

If $a_1 \ge 2$, we have $q((1+r+\ldots+r^{a_1-1})^{-1},r) < 0$ and thus $\lambda(r) \le (1+r+\ldots+r^{a_1-1})^{-1} \le (1+r)^{-1}$, which in turn means that $r\lambda(r) \le \frac{r}{1+r} \le \frac{1}{2}$. If $a_1 = 1$, we also have $a_2 = 1$ and thus $q(\frac{\sqrt{1+4r}-1}{2r}, r) \le 0$, so we obtain $r\lambda(r) \le \frac{\sqrt{1+4r}-1}{2} \le \frac{\sqrt{5}-1}{2}$. This means that the infinite sum converges and is bounded by $\frac{3+\sqrt{5}}{2}$. Together with Corollary 9.9, we obtain

$$S_1 = O_G\left(|V(k,N)|r^k k^{1/2}\exp\left(-c_{25}(G)\frac{r\nu/2}{\log m}\right)\right).$$

The other part of the sum,

$$S_2 := \sum_{l=q+1}^{t} r^{l-1}\epsilon_{\nu_l}\exp\left(-c_{25}(G)\frac{r\nu_l}{\log m}\right)\sum_{b\in B_{\nu_l}} r^{s_G(b)},$$

can be estimated as follows:

$$\begin{aligned}
S_2 &\le c_{26}(G)\sum_{l=q+1}^{t} r^{l-1}\sum_{b\in B_{\nu_l}} r^{s_G(b)}\\
&= c_{26}(G)\sum_{l=q+1}^{t} r^{l-1}\cdot\left(-\frac{p(\lambda(r),r)}{q_x(\lambda(r),r)}\right)\lambda(r)^{-\nu_l-1}\left(1+O_G\left(\eta_G^{-\nu_l}\right)\right)\\
&\le c_{26}(G)\cdot\left(-\frac{p(\lambda(r),r)}{\lambda(r)q_x(\lambda(r),r)}\right)\sum_{j=1}^{t-q} r^{j-1}\lambda(r)^{-\nu/2+(j-1)}(1+O_G(1))\\
&\le c_{26}(G)\cdot\left(-\frac{p(\lambda(r),r)}{\lambda(r)q_x(\lambda(r),r)}\right)\lambda(r)^{-\nu/2}\sum_{j=0}^{\infty}(r\lambda(r))^{j}(1+O_G(1))
\end{aligned}$$

and thus

$$S_2 = O_G\left(|V(k,N)|r^k k^{1/2}\lambda(r)^{\nu/2}\right).$$

It is known that $\mu'(y)$ is bounded above and below by positive constants depending only on G, which means that there are constants c_8, c_9 such that

$$c_8(G)\frac{k}{\nu} \le r \le c_9(G)\frac{k}{\nu}.$$

Furthermore, $\lambda'(y) = -\frac{\lambda(y)\mu(y)}{y}$ is strictly negative on $(0,1]$ with $\lim_{y\to 0+}\lambda'(y) = -1$, so it is bounded above and below by negative constants. So there are constants $c_{27}(G)$ and $c_{28}(G)$ such that

$$c_{27}(G)\frac{k}{\nu} \leq \lambda(0) - \lambda(r) = 1 - \lambda(r) \leq c_{28}(G)\frac{k}{\nu},$$

and thus

$$\lambda(r)^{\nu/2} \leq \left(1 - c_{27}(G)\frac{k}{\nu}\right)^{\nu/2} \leq \exp\left(-\frac{c_{27}(G)}{2}k\right).$$

Altogether, we obtain

$$S_1 + S_2 = O_G\left(|V(k,N)|r^k k^{1/2}\left(\exp\left(-c_{29}(G)\frac{k}{\log m}\right) + \exp\left(-\frac{c_{27}(G)}{2}k\right)\right)\right),$$

which proves Theorem 9.12. ■

Remark. As an example, we note that, since the Fibonacci numbers clearly satisfy the condition for any modulus, the set of integers with a fixed number of 1's in the Zeckendorf representation is well-distributed modulo any integer modulus.

As in [76], Theorem 9.12 can also be used to prove the following:

Corollary 9.16 If $z \in \mathbb{N}$, $z \geq 2$, then there are constants $N_0(G), c_{30}(G), c_{31}(G)$ (depending on G and z) such that for all $N \geq N_0(G)$ and all k with

$$|\mu(1)\nu - k| < c_{30}(G)(\log N)^{3/4},$$

where $\nu + 1$ is the number of G-ary digits of N, the number of integers in $V(k,N)$ which are not divisible by the z-th power of a prime P in the set

$$\mathcal{P} := \{P : P \text{ prime}, P \text{ satisfies the condition of Theorem 9.12}\}$$

is given by

$$\left(\zeta(z)\prod_{P\in\mathcal{P}}\left(1 - \frac{1}{p^z}\right)\right)^{-1}|V(k,N)|\left(1 + O\left(\exp(-c_{31}(G)(\log N)^{1/2})\right)\right). \tag{9.23}$$

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