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Applications of the Kernel Method

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Abstract

Recursions occur frequently throughout various areas of mathematics. To obtain a solution, that is a closed formula for the numbers defined by the recursive equation, one may apply the generating function approach. This involves encoding these numbers as coefficients of a formal power series F. A functional equation which implicitly defines this function may be derived from the recursion, however, it might be difficult to find an explicit expression for the solution of the resulting equation. For certain cases, namely if the functional equation consists of a linear combination of F and a number of functions closely related to it, the Kernel method provides a simple way to actually compute it. One finds couplings of variables such that the numerator of the generating function, called the Kernel, vanishes. Considering the combinatorial context and hence that F must have a formal power series expansion, this yields additional equations for the involved entities, which are essentially the generating function evaluated with special arguments. From this, an expression for the generating function in general and subsequently the solution of the recursion may be obtained.

The Kernel method, gaining popularity in the recent years, belongs to mathematical folklore since the 1970's and was most likely discovered several times by different authors. In this thesis, inspired by Prodinger's "A collection of examples" (2004), we will present one of those instances as given by Knuth (1968). Furthermore, we will demonstrate the usefulness of the method in more sophisticated examples. We will study these in full detail, discuss the necessary theorems and notions to understand the theoretical depth behind the Kernel method and encounter some of its limitations.

Zusammenfassung

Rekursive Gleichungen finden oftmals Anwendung in vielen verschiedenen Gebieten der Mathematik. Eine Lösung solcher Gleichungen, das heißt eine geschlossene Formel zur Berechnung der durch die Rekursion definierten Zahlen, kann mithilfe einer erzeugenden Funktion gefunden werden. Hierbei werden die Zahlen als Koeffizienten einer formalen Potenzreihe F kodiert. Eine Funktionalgleichung, welche diese implizit definiert, kann aus der Rekursion gewonnen werden. Es ist jedoch häufig sehr schwierig, daraus eine explizite Darstellung der Funktion zu finden. Im speziellen Fall, dass die Gleichung eine Linearkombination von F und einiger sehr ähnlichen Funktionen darstellt, bietet die Kernelmethode ein einfaches Mittel, die erzeugende Funktion zu berechnen. Es werden dabei Kombinationen von Variablen gefunden, sodass der Nenner, der sogenannte Kernel, der erzeugenden Funktion verschwindet. Aufgrund des kombinatorischen Kontextes folgt, dass F eine formale Potenzreihenentwicklung besitzen muss. Daher ergeben sich zusätzliche Gleichungen für die betrachteten Objekte, welche im Wesentlichen der erzeugenden Funktion, ausgewertet mit speziellen Argumenten, entsprechen. Aus diesen kann eine allgemeine Formel für die Funktion und damit die Lösung der Rekursion erhalten werden.

Die Kernelmethode, welche in den letzten Jahren zunehmend Popularität gewann, gehört seit den 1970er Jahren zur mathematischen Folklore und wurde vermutlich von verschiedenen Autoren immer wieder neu entdeckt. In dieser Diplomarbeit, inspiriert von Prodingers „A collection of examples" (2004), werden wir eine dieser Arbeiten von Knuth (1968) präsentieren, sowie die Nützlichkeit der Methode in komplexeren Beispielen aufzeigen. Wir werden diese in allen Details vorstellen, die nötigen Theoreme und Begriffe für das Verständnis der Theorie hinter der Kernelmethode besprechen und die Grenzen der Methode kennen lernen.

Contents

1 Introduction

The Kernel method in combinatorics is an approach to solve certain kinds of functional equations, which are not solvable using classical algebraic methods. It is not to be confused with the so-called Kernel trick or Kernel methods in the field of machine learning. Prodinger, whose collection of examples [Pro04] inspired this thesis, and Banderier and Flajolet [BF02] state that it belongs to mathematical folklore for quite some time (probably the 1970's) and has seen a revival in the last few years. Most likely it has been "rediscovered" independently multiple times. Both of the aforementioned works cite a book by Knuth as one of the more prominent and well documented instances (we will discuss it in Chapter 2).

The argument has been turned into a real method, especially due to the works by authors like Bousquet-Mélou and Petkovšek [BMP00] or the techniques presented in [BBMD$^+$02]. It proved to be very useful for many kinds of counting problems and found applications in various fields of combinatorics, such as path or tree enumeration. Despite the different contexts, there is a unifying theme connecting those problems, which also describes the workflow when using the Kernel method.

Our goal in this thesis is to give interested mathematicians (whether professional, student or self-proclaimed) an insight into the workings of this technique - to this end, we will state the required notions and theorems and proceed to carefully examine four examples in the following chapters, where the the method is the key to solving the task: aside from Knuth's exercise mentioned before, we take a look at the enumeration of parking functions 3, vexillary involutions 4 and partially directed paths confined to a symmetric wedge 5. Along the way we will try to point out the important concepts and arguments, as well as compare the application of the Kernel method in these demonstrations. We hope to convince the reader that most of the technical issues which arise can be taken care of and convey the elegance of the underlying idea. To begin with, let us state the basics briefly and in a very general form here.

1.1 The Kernel method

Given a counting task, it is often possible to find a recursive description for the involved combinatorial objects. Sometimes it is also quite easy, or natural, to do so, for example by using symbolic methods. Then one can introduce formal power series as generating functions of the coefficients of the recurrence relation, which leads to a functional equation. This equation, if equivalent to the recursion, uniquely defines the generating function as a power series. Thus, if one can find a series which satisfies the equation, one obtains an (more or less) explicit expression for the function. Note that there might be other kinds of solutions, like rational functions, which we are not interested in. From this it might be possible to find a power series expansion, yielding the solution of the recursion as the coefficients of the series. Or if this is too complicated or does not give legible results, an asymptotic analysis may be performed to determine the asymptotic behaviour of the numbers defined by the recursion.
Clearly, it is not always that simple. While obtaining a functional equation might not be the problem, solving it can prove to be very hard. One difficulty is that it might contain too many variables. In special cases, the relation might be a linear combination of formal series (usually ordinary power series), one of them being the unknown main generating function F we are looking for, and the others some of its specializations, which do not depend on all variables simultaneously. If we denote $\vec{x} = (x_1, x_2, \dots, x_m)$ (analogously for $\vec{y}$), this situation looks like

$$K(\vec{x})F(\vec{x}) = \sum_{i=1}^{n} Q_i(\vec{x})F(\vec{y_i}) + R(\vec{x}). \tag{1.1}$$

Here, the series K, Q and R are given by the recursion defining this equation. The so-called Kernel K is given as the coefficient of F (or rather its denominator) and will be the key to solving the problem. For all $(i,j) \in \{1, 2, \dots, n\} \times \{1, 2, \dots, m\}$, the $y_{i,j}$ are such that not all of the x_j occur in the argument vector $\vec{y_i}$. Usually, some of these components are set to zero or one and the remaining involve couplings of some, but not all, of the x_j. Zeilberger [Zei00] calls variables, which are merely introduced as aid during computations, catalytic. Like Bousquet-Mélou, we will adopt this name for the $y_{i,j}$ which "vanish" from the equation at some point. Classes of equations with one catalytic variable always yield algebraic solutions and have been well studied (see Section 1.2), while more catalytic variables also mean more work to find a solution (in general).

Looking at the fundamental functional equation, one notices that it contains multiple unknown entities - not only the generating function itself, but also its specializations. Thus, solving it by simple algebraic manipulations is not possible. One then proceeds by studying the Kernel and finding its roots, that is, couplings of variables such that K is set to zero. Essentially, one expresses some of the catalytic variables as branches of (algebraic) functions of the other arguments. Clearly these steps depend strongly on the form of the Kernel. From this, one obtains new relations (by simply plugging in the roots of the Kernel) for the unknown entities in the fundamental equation, as long as the substitution of these branches into the generating function is analytically valid. Eventually, if enough information can be obtained this way, one can find all of the unknown functions on the right hand side of equation (1.1). Subsequently the main generating function may be obtained

by division by the Kernel. This is a valid algebraic manipulation, even if the Kernel is zero at the origin and therefore seems to yield singularities there, which implies that the generating function is not a formal power series. However, it is already known a-priori that the generating function admits a power series expansion, given the combinatorial context. Thus, the Kernel has to be a factor of the right hand side and can be canceled from the equation. This yields the solution to the functional equation and not only that, it often provides a reasonable compact expression, too. Thus, even if the coefficients can not be read off easily, the results for the generating function can be used for an asymptotic analysis.
For our purposes this informal description shall be enough. A similar basic introduction can be found in a summary for a seminar held by Bousquet-Mélou [BM01a]. Concrete examples for equations will follow, and should provide enough insight to understand which types of equations are likely to be successfully attacked with the Kernel method.

One key aspect of the Kernel method is the ”mechanic” nature of the proofs it is applied in. In every field of mathematics, often multiple proofs for the same statement can be found, sometimes differing radically from each other in their main ideas. This is not different for combinatorics. Indeed, there are several techniques which provide a backbone of techniques to try for a given combinatorial problem, including e.g. the bijective proof, double counting, recursion and/or the generating function approach. Sometimes all of these and more can be used to show that a certain theorem holds.
The Kernel method certainly belongs to the class of techniques which carry an implicit outline of the proof they are applied in. In short, given a combinatorial problem, the recipe is to define an appropriate generating function (by e.g. finding a recursive description first) and derive a functional equation for it. If it can not be solved directly and is of the form (1.1) we have specified above, the Kernel method in one of its flavors might be applied. Afterwards, one hopefully proceeds by simplifying the result to obtain an expression for the generating function and extracting its coefficients, if necessary. Multiple other steps might be necessary to accomplish that, as shown, for example, in Chapter 4. But in general the way to go on is clear, albeit not easy to follow sometimes.
This also demonstrates one of the reasons for the usefulness of the Kernel method - it works on the level of generating functions and hence, not directly in the language of the combinatorial problem itself. Speaking about functional equations remains the same, regardless where that equation is coming from. Therefore, it is possible to understand results with little knowledge of the actual problem's background - (essentially) all one needs to know is how to derive a recursion.
Now, that is certainly not to everyone's liking. There is a saying by Wilf, that ”bijective proofs give one a certain satisfying feeling that one really understands why a theorem is true” (this does not mean that he does not approve of the use of generating functions, though, since he wrote this in his book about them [Wil94]). Or, as in [Yan01]: ”Whenever a result is found by generating function analysis, a combinatorial explanation is expected.” But on the other hand, as Bousquet-Mélou states [BM01b] ”finding proofs from the other end of the spectrum, of a more mechanic fabrication, is interesting in its own right”. Others, like Zeilberger, would surely applaud to this - his sometimes controversial idea is to teach computers do mathematics and he has written numerous programs to this end [Zei]. The author himself believes, too, that it is certainly useful to have an approach which can be

applied to many problems in the same way, with only small alterations, in strong contrast to, e.g., bijective proofs which require a lot of adaption to the current task.
Moreover, the Kernel method might provide a starting point for problems which could not be tackled otherwise yet or make finding a result easier. Identities derived in such a way could show underlying combinatorial interpretations and connected entities more clearly and point a direction in which to look for, when trying to fully "understand" the problem (by e.g. finding a bijective proof). Examples for such situations can be found in [BM05], where a result is rederived in a systematic manner using the Kernel method (the earlier solutions were partially guessed), in Chapter 4, where the already known bijection had an even more complicated proof, or in Chapter 5, where certain generating functions have combinatorial interpretations, but whose form could not be derived from that using other techniques (at least not at the time of writing).
Clearly, what is considered to be an elegant or "combinatorial" proof might be open for discussion, but the Kernel method proves to be well suited for producing results and solving problems and can thus be deemed successful.

Despite its mechanistic nature, many insightful steps are necessary to successfully apply the Kernel method in a proof. Modern day helpers, that is, computer algebra systems such as the well known Maple or Mathematica, are big timesavers when manipulating long algebraic expressions and working with generating functions (see e.g. the GFun [SZ94] or Zeilberger's packages for Maple). In fact, Maple was used sometimes for deriving equations in this paper, although the author also tried to recapture the results manually, too. And it proved to be possible, as outlined in this thesis. Also, while the number crunching abilities of the computer systems are much more sophisticated than a human's, and often less error prone, they do need a guiding hand to be able to work with some expressions efficiently (e.g. that involves choosing the right square root of a quadratic expression, so that terms can be canceled). Nevertheless, the Kernel method, involving generating functions and many equations, is well suited to put the calculation power of modern computers and symbolic math software to good use.

1.2 Further generalizations and references

In this section we want to give a brief and very incomplete overview of how the Kernel method is used nowadays and provide some references to continue, if the reader's appetite is whet after the lecture of the examples presented here. Clearly, there is a vast amount of literature using the notion of the Kernel method, but since it is more of a computational aid, it is rarely the main topic of the specific paper. Thus, let us only mention a few more specialized ones, which are not mentioned prominently elsewhere in this thesis.

First off, the inspiration for this thesis was mainly Prodinger's collection of examples, where some more demonstrations of the technique can be found. However, he does not really mention the various flavors the Kernel method comes in. Besides the ordinary version, we will get to know the so-called obstinate and iterated versions (in Chapters 4 and 5 respectively). Furthermore, there is also an algebraic variant, which is somewhat different. It is mentioned in papers by Bousquet-Mélou (e.g. [BMM08, BM05]) and in contrast to the usual Kernel approach, it does not require that the Kernel is set to zero. It suffices to find couplings of the variables such that the Kernel remains constant. This can be easier than finding its roots, but on the other hand, the resulting equations obtained by plugging in said couplings can be more complex. Compared to the ordinary Kernel method, all of its variants (especially the iterated and algebraic) have not found as many applications yet.

It is not a coincidence that Bousquet-Mélou is mentioned so often in this thesis - many of her publications use the Kernel method in one of its forms. Besides the papers already cited in this thesis, there are too many to reference here (the author counted over a dozen at her homepage and he surely missed a few). She has also contributed to the development of the method (e.g. in [BBMD$^+$02]), its variants and to frameworks of solving certain problems, in which the Kernel method plays a central role.
As an example, in [BMM08] she shows together with Mishna how the approach can be used to systematically solve enumeration problems for certain kinds of lattice walks.
In [BMJ06] polynomial equations of the form $p(F(t,x), F_1(x), F_2(x), \ldots, F_k(x)) = 0$ are studied, where $F(t,x)$ and $F_i(x), i \in \{1, 2, \ldots, k\}$ are formal power series. From this, using a generalization of the Kernel method, new relations for all of the occurring series are computed, which leads, among others, to applications in solving certain enumeration problems.
Together with Petkovsek [BMP00] she also determined the nature of generating functions stemming from multivariate, linear recursions with constant coefficients. They used the essential ideas of the Kernel method to solve the algebraic case. This is an especially nice application of the method and provides much background on how to apply it in a very general context.

There are also some recent works by Mansour (who also has some papers using the Kernel method, e.g. [Man06, Man07]) and Song [MS09] and Hou [HM08, HM11] in which they study a generalization of the Kernel method to solve equation systems in which the number of unknowns exceeds the number of equations, whereas one usually only deals with one equation. They also include some applications for their method.

Another very similar method, in the sense that it provides a way to solve certain cases of functional equations coming from combinatorial problems, appears to be the so-called quadratic method, introduced by Tutte [Tut63] for the study of rooted maps. Such maps are a special case of planar maps, which consist of a connected planar graph and an embedding in the plane, such that one vertex and one incident edge are distinguished as a root. The key difference is that the fundamental functional equation is quadratic in the main generating function, unlike the equations considered here, which are linear in this function. This approach is also briefly discussed in [BM01a, BM02].

1.3 Notations, a little background and Theorems

Let us briefly make some remarks about the notation and recall some of the necessary theorems we are going to use repeatedly. All of these tools will be rather basic and well known in the field of combinatorics, so any introductory or intermediate text should provide more background for the interested reader (good examples are [Sta99a, Sta99b, FS09].
We will make heavy use of generating functions of sequences, which are essentially "a clothesline on which our sequence is hanging out to dry", as Wilf describes them in [Wil94]. His book is also an excellent resource to get a nice overview of the generating function approach. Note that for brevity as well as clarity, we will often omit certain arguments of generating functions, if the context allows it without (too much) ambiguity.

To begin with, let $\mathrm{R} = (\mathrm{R}, +, \cdot, -, 0, 1)$ be a unit ring.
Denote by $\mathrm{R}[x] := \{\sum_{i=0}^{n} r_i x^i : n \in \mathbb{N}, r_i \in \mathrm{R}\}$ the ring of polynomials in the variable x with coefficients in R. If one allows infinite sums, one obtains the ring of formal power series $\mathrm{R}[[x]] := \left\{\sum_{i\geq 0} r_i x^i : r_i \in \mathrm{R}\right\}$. Furthermore, we denote polynomials in x and $\overline{x} := 1/x$ as $\mathrm{R}[x, \overline{x}]$, the ring of Laurent polynomials. The field of Laurent series in a variable x include a finite number of negative powers and are given by $\mathrm{R}((x)) := \left\{\sum_{i\geq -n} r_i x^i : n \in \mathbb{N}, r_i \in \mathrm{R}\right\}$. The positive part of a Laurent series is the formal power series obtained by omitting all negative powers x^i with $i < 0$, i.e. starting the summation at $i = 0$.

The elementary operation addition and subtraction of formal series (and thus, by replacing infinite with finite sums, on polynomials) are defined coefficientwise,

$$\sum_{i\geq 0} f_i x^i + \sum_{i\geq 0} g_i x^i := \sum_{i\geq 0} (f_i + g_i) x^i,$$

whereas the multiplication is given by the so-called Cauchy product:

$$\sum_{i\geq 0} f_i x^i \cdot \sum_{i\geq 0} g_i x^i := \sum_{i\geq 0} \left(\sum_{j=0}^{i} a_j b_{i-j} \right) x^i.$$

A formal power series $F(x) \in \mathrm{R}[[x]]$ is called invertible if $1/F(x)$ is also in $\mathrm{R}[[x]]$. This is the case if and only if the constant term $\left[x^0\right] F(x)$ has a multiplicative inverse in the ring R.
The composition of two series $F(x) = \sum_{i\geq 0} f_i x^i$ and $G(x) = \sum_{i\geq 0} g_i x^i$ is defined by

$$F(G(x)) := \sum_{i\geq 0} f_i G(x)^i.$$

Note that this requires $g_0 = 0$, otherwise the coefficients $\left[x^i\right] F(G(X))$ may depend on infinitely many coefficients of $F(x)$ and $G(x)$. A formal power series $F(x)$ with no constant term has a composition inverse $F^{-1}(x) \in \mathrm{R}[[x]]$, for which $F(F^{-1})(x) = F^{-1}(F(x)) = x$ holds, if and only if $\left[x^1\right] F(x)$ is invertible in R.
This summarizes the essential facts about power series we will need. All of these notions, as well as the following, can be generalized to a finite number of variables in a straightforward manner.

To introduce some further notions concerning formal power series, let K be a field of characteristic zero.
We say that a series $F \in \mathrm{K}[[x]]$ is rational, if there exist polynomials $p(x)$ and $q(x) \neq 0$ in $\mathrm{K}[x]$ such that $F(x) = p(x)/q(x)$. The series F is algebraic if there exists a polynomial $p(x, y) \neq 0$ in $\mathrm{K}[x, y]$ such that $p(x, F(x)) = 0$. It is algebraic of degree m if $p(x, y)$ has degree m in y and there is no polynomial of strictly lower degree for which the same relation holds. If F is not algebraic, it is said to be transcendental. Lastly, if F satisfies a nontrivial linear differential equation with polynomial coefficients, i.e., $p_0(x)F(x) + p_1(x)F'(x) + \ldots + p_k(x)F^{(k)}(x) = 0$ with $p_i(x) \in \mathrm{K}[x], \forall i \in \{1, 2, \ldots, k\}$, then F is called D-finite or holonomic.

A result based on the formal residual calculus, which we will use regularly is the Lagrange inversion formula. We state it as a theorem:

Theorem 1.1 (Lagrange inversion formula)**.** *Let $F(x)$ and $\varphi(x)$ be in* $\mathrm{K}[[x]]$*, such that $\left[x^0\right] \varphi(x) \neq 0$, i.e. $\varphi(x)$ is invertible. Let $z = x/\varphi(x)$. Then it holds that*

$$\begin{aligned}
[z^n]\, F(x) &= \frac{1}{n} \left[x^{n-1}\right] F'(x)(\varphi(x))^n, \quad n \geq 1, \\
\left[z^0\right] F(x) &= \left[x^0\right] F(x).
\end{aligned}$$

There are many proofs for this statement and the same holds for another helpful result, which we will borrow from complex analysis. It can often be applied in the combinatorial setting of generating functions.

Theorem 1.2 (Cauchy's Coefficient Formula)**.** *Let $F(x)$ be a complex function and assume it is analytic in a region (i.e. an open set) around the origin. Then the coefficients of the power series representation of $F(x)$ are given by*

$$[x^n]\, F(x) = \frac{1}{2\pi i} \oint \frac{F(x)}{x^{n+1}}\, dx, \quad \forall n \in \mathbb{N},$$

where the integral is evaluated along any simple loop around 0 within the region of analyticity.

Many further statements from mathematical (complex) analysis can be carried over to the context of formal expressions and power series. Proofs for the two aforementioned theorems can be found in [FS09], as well as a little footnote which sums up the formal construction of series concisely: "for simplicity, our computation is developed using the usual language of mathematics. However, analysis is not needed in this derivation, and operations such as solving quadratic equations and expanding fractional powers can all be cast within the purely algebraic framework of formal power series" (for deeper consequences, see Part B of said book).

There are many series with well known expansions, such as the geometric or the binomial series:

$$\frac{1}{1-x} = \sum_{i\geq 0} x^i,$$
$$(1+x)^\alpha = \sum_{i\geq 0} \binom{\alpha}{i} x^i, \quad \text{for } \alpha \in \mathbb{R},$$

where the real binomial coefficient is given by $\binom{\alpha}{i} = (\alpha(\alpha-1)(\alpha-2)\dots(\alpha-i+1))/i!$. Naturally, they also hold for their combinatorial counterparts and we will use them throughout this thesis.

Now, for any sequence $(f_i)_{i\in\mathbb{N}} \in \mathrm{R}^{\mathbb{N}}$ (where R can be a ring, a field or actually any set - however, we only require the first case) we can define

$$F(x) := \sum_{i\geq 0} f_i x^i \quad \text{and} \quad \widehat{F}(x) := \sum_{i\geq 0} f_i \frac{x^i}{i!},$$

which are called the ordinary respectively the exponential generating function of the sequence. Since we will mainly work with the former ones, we will omit the term "ordinary" in this thesis. On the other hand, the expansion of a series is given by the sequence of its coefficients, which we denote by $[x^i]\, F(x)$ or $[x^i/i!]\, \widehat{F}(x)$.

To finish this section, let us recall some more, unrelated notations which we will need.
Given two complex functions $f(x), g(x)$, we say that they are asymptotically equivalent, denoted by the symbol $\sim$, if $\lim_{n\to\infty} f(n)/g(n) = 1$. We write $f(x) = O(g(x))$ if there are positive, real numbers c and x_0 such that $|f(x)| < c|g(x)|$ for all $x > x_0$.

As everywhere else in the literature, we will omit parentheses and commas when writing out permutations using the one-line notation. We call this the word representation of the permutation.

Since we will use it quite often, let us briefly and informally introduce the notion of lattice paths: given a set of allowed moves from one node of the lattice (for example $\mathbb{N}\times\mathbb{N}$, $\mathbb{Z}\times\mathbb{Z}$ or 3-dimensional lattices) to another, a lattice path is a sequence of such moves, starting with a specified starting point. A path is not allowed to visit a node twice.
A very similar concept is a lattice walk: it is a path which may revisit earlier points. Closely related are random walks, too. These need not to be restricted to a lattice and are essentially a random process which consists of discrete steps of a certain length.
These very general descriptions allow the definition of many different kinds of combinatorial objects. Their study is among the most classical subjects of combinatorics and other related fields of mathematics. Consequently, there is a vast amount of literature about this topic. Connections to the Kernel method and secondary references are provided by the papers cited in Chapters 2, 4, 5 or for example in [BM02, BG06].

2

Knuth's exercise

Following the example of [Pro04], we shall introduce the basic idea of the Kernel method by solving Knuth's quite famous exercises 2.2.1.1. - 5. from the first volume of his book "The art of computer programming" [Knu68]. It can certainly be regarded as one of the earlier appearances, if not as one of the possible origins of the technique nowadays called the Kernel method. In the book it was presented as yet another method of solving certain functional equations.

Knuth considered a data structure called a stack. It consists of a linear sequence of objects, which are added or removed at one end (the top) in a last-in, first-out manner. In his analogy, railway cars on the right hand side (the input) of a railway switching network, shown in Figure 2.1, need to be moved to the left (the output) by using an auxiliary rail (the stack).

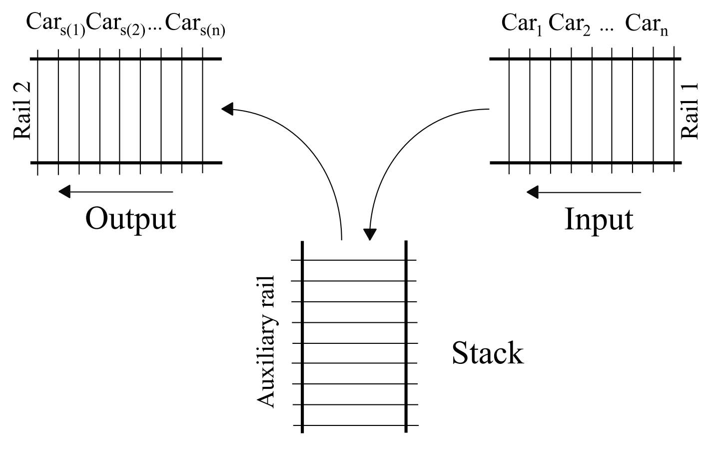

Figure 2.1: Knuth's analogy of a stack.

Only two reasonable actions are possible:

- move the leftmost car (if the input is not empty) from the input into the stack (a so-called push operation)
- move the topmost car (if the stack is not empty) from the stack into the output (a pop operation)

Let us label each car in the input end-to-end to numbers from 1 to n, starting at the leftmost position. Then, if one carries out a random sequence of these moves until all vehicles are in the output, we obtain a permutation of $\{1, 2, \ldots, n\}$ by looking at these labels, as in the following example.

Example 2.1. Starting with 1234 we carry out a sequence of random actions, which is depicted in the table below. The number moved by the current action is underlined and the active ends of input, stack and output are framed. Recall that push moves a number from the left hand end of the input to the top of the stack respectively pop from the top of the stack to the right hand end of the output.

Output	**Stack**	**Input**	**Operation**
$\emptyset$	$\emptyset$	$\boxed{1}234$	-
$\emptyset$	$\boxed{\underline{1}}$	$\boxed{2}34$	push
$\emptyset$	$\boxed{\underline{2}}1$	$\boxed{3}4$	push
$\boxed{\underline{2}}$	$\boxed{1}$	$\boxed{3}4$	pop
$\boxed{2}$	$\boxed{\underline{3}}1$	$\boxed{4}$	push
$2\boxed{\underline{3}}$	$\boxed{1}$	$\boxed{4}$	pop
$23\boxed{\underline{1}}$	$\emptyset$	$\boxed{4}$	pop
$23\boxed{1}$	$\boxed{\underline{4}}$	$\emptyset$	push
$231\underline{4}$	$\emptyset$	$\emptyset$	pop

From the output we read off the permutation 2314 as the result.

Obviously there are some permutations which will never occur on the left hand side of the switch - take for example any one starting with the pattern 312. Indeed, in exercise 5. of Knuth's book it is shown that a permutation π can be obtained using a stack if and only if there are no indices $i < j < k$ such that $\pi(j) < \pi(k) < \pi(i)$, in which case we say that π avoids the pattern 312. This also marks (part of) the beginnings of today's very popular study of pattern avoidance (we will talk a bit more about this topic in Chapter 4).

Now, the task given in Knuth's exercise is the following:

Task 2.2. Provide a simple formula for the number a_n of permutations of n elements which can be obtained using a stack as described above.

Before we proceed to solve this counting problem, let us remark that another closely related notion are one-stack-sortable permutations. They can be introduced as follows: instead of starting with the identity $12\ldots n$ on the input side, one starts with a given permutation and tries to sort it using a stack (i.e. such that the output is the identity). One can prove that this is possible if and only if the permutation does not contain the pattern 231, that is, there are no indices $i < j < k$ such that $\pi(k) < \pi(i) < \pi(j)$. By inverting (with regard to composition) such a permutation, one obtains another permutation containing 312, thus establishing a bijection (a trivial Wilf-equivalence [Wil02]) which proves that a_n counts one-stack-sortable permutations, too. See [Lim07] for an introduction and [Bón03] for further informations on this topic.

2.1 Solving the exercise with a reflection principle

In this section we will give an explicit formula for a_n by using a technique commonly attributed to Désiré André [And88] (although some [Ren08] state that the actual reflection principle is merely a variation of André's proof). It was introduced in 1887 to provide an elegant solution to the ballot problem formulated by Joseph Bertrand [Ber88] earlier that year. Interestingly, Betrand's own solution to the problem (using induction) appears only a few pages before the article by Andrè in the same journal.

Let us denote a push action by I and a pop action as O. To move all n cars from the right hand side to the left, we need exactly $2n$ operations. These can be coded as a sequence of two symbols of that length, of which n are of the type I (every car must go into the stack once) and the remaining of type O (every car is retrieved from the stack once). As stated before, not every possible sequence of length $2n$, using both symbols equally often, is reasonable - if a symbol O appears next, the auxiliary rail must not be empty, or else no car can be retrieved from the stack. Thus, assuming we are reading from the left, the number of O's never exceeds the number of I's.

Definition 2.3. In this chapter, we will call a (finite) sequence of two symbols I and O admissible iff O never outnumbers I throughout the sequence.

Examples for such sequences are $IIOIOIOO$, $IOIOIOIO$ or $IIIOOO$ (following the notation of permutations, we will omit enclosing parentheses and separating commas).
As a remark, sequences of such a type are more commonly known as Dyck words (if one replaces the symbols I and O with integers - see for example [FS09], example 1.16., or [Duc00]).
Note that different sequences give different outputs from the stack. To see this, consider two sequences of length $2n$ which agree until one of them has I and the other O as the next symbol. That means that the first one puts a number into the stack which must necessarily occur after the number which is just moved to the output by the latter one. Hence, the resulting permutations differ at this point.
The other direction is clear and thus we can establish a bijective relationship by mapping an admissible sequence of length $2n$ to the permutation of n elements given in the output after carrying out the coded actions.

Example 2.4. To give a simple example for such a correspondence, let us state it explicitly for permutations of length 3:

$$123 \leftrightarrow IOIOIO, \qquad 132 \leftrightarrow IOIIOO, \qquad 213 \leftrightarrow IIOOIO,$$
$$231 \leftrightarrow IIOIOO, \qquad 321 \leftrightarrow IIIOOO.$$

Recall that 312 can not be obtained by a stack and indeed, there is no other admissible sequence of length 6 other than those given above.

So, the task of counting permutations is translated to:

Task 2.5. Provide a simple formula for the number a_n of sequences of length $2n$, in which the symbols I and O each occur exactly n times and which are admissible.

Before attempting to solve the task, we will introduce Bertrand's ballot problem, which is closely related to it and whose proof will be applicable for our purposes.
Assume that two candidates I and O are running in an election, where i votes are cast for candidate I and o for candidate O, such that $i > o$. The question then is, what is the probability that I has strictly more votes than O throughout the counting of the ballots? Our problem is a slight variant of the above, since we additionally allow that $i = o$ and that I and O can be tied during the counting. Clearly, we can represent all such elections by sequences of two symbols I (a vote for candidate I) and O (a vote for candidate O) with length $i + o$. Using Definition 2.3 above, we are only looking for admissible sequences of a given length, in order to ensure that I never falls behind O. Hence, we can follow Pólya's suggestion [Pól04] to actually prove more than we actually need and generalize Task 2.5 to:

Task 2.6. Provide a simple formula for the number of sequences of length $i + o$, in which the symbols I and O occur exactly i and o times respectively and which are admissible.

To compute this number, we will apply an elegant reflection principle for lattice paths on the cartesian plane, using the following model:

Definition 2.7. In this section, we consider (restricted) lattice paths on $\mathbb{N} \times \mathbb{N}$ which are starting at the origin, such that the only allowed actions are: from (n, m) one can move to $(n + 1, m)$ (east) or to $(n, m + 1)$ (north).

There is a straightforward interpretation of an election or equivalently of sequences of two symbols I and O of length $i + o$ as paths as in the definition above:

- start at the origin $(0, 0)$
- whenever a vote is cast for candidate I (symbol I appears next in the sequence), move east
- whenever a vote is cast for candidate O (symbol O appears next in the sequence), move north

Every such path leads to the point with coordinates (i, o). Admissible sequences define admissible paths which never cross the main diagonal line, defined by $y(x) = x$, where the horizontal coordinate equals the vertical one. Counting them will yield our numbers a_n. Instead of doing that directly, we will determine the number of inadmissible paths and subtract them from the number of all possible ones, which gives the following theorem.

Theorem 2.8. *The number of admissible sequences of length $i + o$, as defined above, is given by* $\dfrac{i+1-o}{i+1}\dbinom{i+o}{i}$.
If furthermore $i > o$, the probability that the first candidate stays strictly ahead of the second one throughout the counting of the ballots is $\dfrac{i-o}{i+o}$*, solving Bertrand's ballot problem.*

Proof. Let $\mathbf{p} = (p_1, p_2, \ldots, p_{i+o})$ be an inadmissible sequence respectively path (we will use these terms interchangeably). Find the smallest index j such that $p_j = O$ and both symbols occur equally often to the left of p_j (i.e. j is the smallest index where O outnumbers I). Switch the roles of the symbols within the part of the sequence leading up to and including p_j by replacing every occurrence of I by O and vice versa. As an example, if $\mathbf{p} = IIOIOOOIIOIOI$, then $j = 7$ and the corresponding new sequence is $OOIOIIIIIOIOI$ (for a visualization of the corresponding paths see Figure 2.9).

Thus, we reflect the first fraction $(p_1, p_2, \ldots, p_j)$ of the path along the diagonal line given

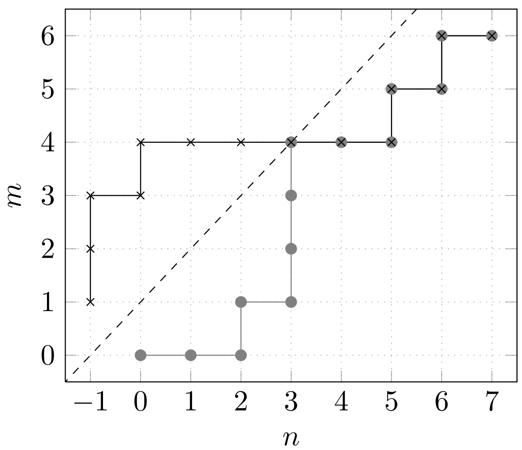

Figure 2.9: Inadmissible path (gray, dots) and path (black, crosses) partially reflected along the line $y(x) = x + 1$.

by $y(x) = x + 1$, giving rise to the name of the method. We obtain a new path $\mathbf{p}'$, which contains $i + 1$ copies of the symbol I and $o - 1$ copies of O. Note that by mirroring we do not alter the endpoint of the path, but we do change the starting point - the path now begins at $(-1, 1)$ instead of $(0, 0)$.
Conversely, given any such path, we can reconstruct the inadmissible path it must come from by reversing the aforementioned process of switching symbols.
This shows that there is a bijection between inadmissible sequences and paths leading from $(-1, 1)$ to (i, o) with the specified amount of symbols but, and this is the point of the

mirroring process, without further restrictions. It is easy to compute their number: out of $i+o$ places, exactly $i+1$ must be chosen to put I there, padding the rest with O's. There are $\binom{i+o}{i+1}$ ways to do this.
Using a similar reasoning, the number of all possible paths from $(0,0)$ to (i,o) is given by $\binom{i+o}{i}$ and we finally obtain the number of admissible paths by subtracting the inadmissible paths:

$$\binom{i+o}{i} - \binom{i+o}{i+1} = \binom{i+o}{i}\left(1 - \frac{o}{i+1}\right) = \frac{i+1-o}{i+1}\binom{i+o}{i}.$$

For completeness, we will also derive the probability from Bertrand's original problem (which requires $i > o$ and that the symbol I strictly outnumbers O at all times). The first candidate gets the initial vote with a probability of $\frac{i}{i+o}$. Using our above formula, in $\frac{i-o}{i}\binom{i-1+o}{i-1}$ cases out of $\binom{i-1+o}{i-1}$ possible ones, I will stay ahead of or be tied with O throughout the counting of the remaining $i+1-o$ ballots, giving a probability of $\frac{i-o}{i}$. Multiplying leads to the final result of $\frac{i-o}{i+o}$. □

Theorem 2.8 provides the reasonably simple formula for the numbers a_n of Knuth's exercise 2.2. By setting $i = o = n$, we obtain

$$a_n = \frac{1}{n+1}\binom{2n}{n}, \quad n \in \mathbb{N}$$

thus recovering a very well known sequence of numbers, called the Catalan numbers. They are named after the Belgian mathematician Eugène Charles Catalan, although they were already known to others before him (for example, Euler mentioned them in a letter to Goldbach [Eul]).
Apart from that, they occur in too many classic problem in combinatorics to name them all (as of December 2010, 190 applications were listed by Richard Stanley [Sta98, Sta10]), so we only mention a few examples, such as the number of full binary trees with $n+1$ leaves, the number of triangulations of a convex polygon with $n+2$ sides or the number of permutations of $\{1, 2, \ldots, n\}$ which avoid the pattern 123. The first few Catalan numbers are given by $1, 1, 2, 5, 14, 42, 132, 429, 1430, \ldots$ and the sequence is listed as entry A000108 in the on-line encyclopedia of integer sequences [OEI11], where additional references can be found.

2.2 Solving the exercise with the Kernel method

We have seen that it is not necessary to make use of the Kernel method for solving Knuth's historical exercise 2.2 or the ballot problem 2.6. Aside from some natural correspondences between sequences and paths, it involved a lot of creativity to find the reflection principle, establishing the key bijection to make counting easier. It might always be possible to employ a bijective proof, but nevertheless it can prove to be very difficult. In addition, as we have argued in the introduction to this thesis, to develop a consistent framework which can be applied to many problems of a certain kind in the same way is valuable. Therefore, in this section we will take a new, more general approach to our introductory examples and point out some concepts from the introduction. This, as well as the following chapters of this thesis, will demonstrate that the Kernel method is often a good, and sometimes the only known, way to start tackling the problem.

In order to use the Kernel method, we need to formulate a functional equation for a generating function. Again, we employ a model of lattice paths.

Definition 2.9. In this section, we consider restricted lattice paths on the grid $\mathbb{N} \times \mathbb{N}$ which are starting at the origin, such that the only allowed actions are: from (n, m) one can move to both $(n+1, m \pm 1)$ (northeast respectively southeast) if $m > 0$ or to $(n+1, 1)$ (northeast) if $m = 0$.

For any admissible sequence of two symbols I and O as in Definition 2.3 we can define such a lattice path with starting point $(0, 0)$ by:

- if a symbol I appears next, move northeast from (n, m) to $(n + 1, m + 1)$
- if a symbol O appears next, move southeast from (n, m) to $(n + 1, m - 1)$

Observe that the move for O is always well defined, as $m > 0$ holds (i.e. the stack is not empty or the symbol I outnumbers O) when this symbol occurs, given an admissible sequence.
Conversely, it is clear that a path given by Definition 2.9 ending in (n, m) can be mapped to an admissible sequence of length n in which the number of I's exceeds the number of O's by m: for every move northeast (the second coordinate may be zero), add a symbol I to the (right hand side of the) sequence and for every move down an O. Thus, another simple bijection between paths and sequences is established.
To find the formula from Task 2.2, we need to compute the number of paths with the endpoint $(2n, 0)$, for $n \in \mathbb{N}$, since they correspond to admissible sequences in which both symbols occur equally often. Note that there are no paths ending in $(2n+1, 0)$ - to reach 0 in the second coordinate, one must go down once for every time one went up earlier, thus enforcing an even number of moves. Figure 2.10 depicts the paths for the permutations from our earlier Example 2.4.

For every $n, m \in \mathbb{N}$, let $f_{n,m}$ be the number of paths as in Definition 2.9 ending in (n, m) and define a family of generating functions

$$\forall m \in \mathbb{N} : f_m(x) := \sum_{n \geq 0} f_{n,m} x^n.$$

Obtaining recursions describing the $f_{n,m}$ is straightforward. Obviously we have $f_{0,0} = 1$ (taking care of the empty path) as well as $f_{n,0} = f_{n-1,1}$ since every path from $(0, 0)$ to $(n, 0)$ corresponds to a path going to $(n - 1, 1)$, adding a step southeast at the end. Similarly, for $m \geq 1$, a path ending in (n, m) can be constructed from one ending in $(n - 1, m - 1)$ or $(n - 1, m + 1)$ by going up respectively down in the next step, leading to

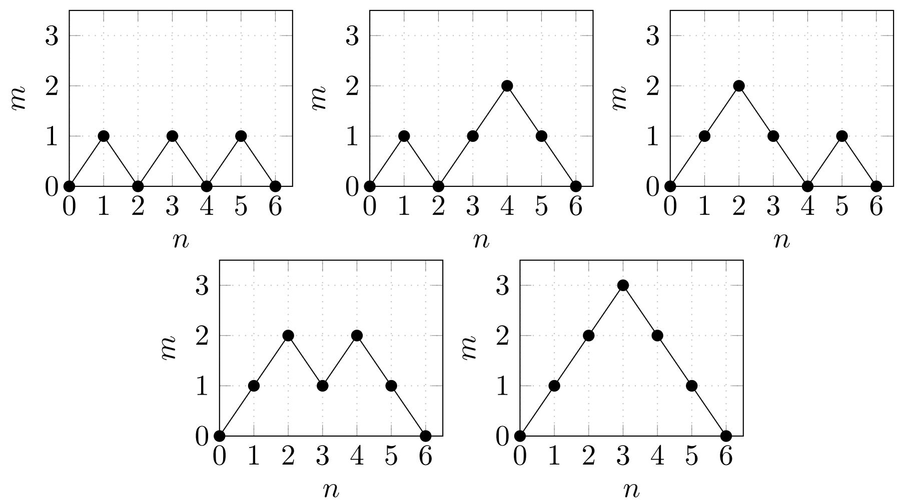

Figure 2.10: The paths corresponding to the permutations 123, 132, 213, 231 and 321 (from top left to bottom right).

$f_{n,m} = f_{n-1,m-1} + f_{n-1,m+1}$. Putting these results into the definition above yields:

$$f_0(x) = \sum_{n\geq 0} f_{n,0}x^n = 1 + \sum_{n\geq 1} f_{n-1,1}x^n = 1 + x\sum_{n\geq 0} f_{n,1}x^n = 1 + xf_1(x).$$

Using the same manipulations we obtain a recursion for $f_m(x)$ with $m \geq 1$, resulting in

Recursion 2.10.

$$f_0(x) = 1 + xf_1(x), \tag{2.10a}$$
$$f_m(x) = xf_{m-1}(x) + xf_{m+1}(x), \quad m \geq 1. \tag{2.10b}$$

Now we introduce the bivariate generating function which encodes the general solution to our problem.

Definition 2.11. Define the generating function for lattice paths as given in Definition 2.9, enumerating them by the position (n, m) of their endpoint as

$$F(x, y) := \sum_{n,m\geq 0} f_{n,m}x^n y^m.$$

In the following theorem, we will establish the desired functional equation for the application of the Kernel method:

Lemma 2.12. *The formal power series $F(x, y)$ is the unique solution of*

$$\left(xy^2 + x - y\right) F(x, y) = xF(x, 0) - y.$$

Proof. The proof is simple. Rewrite $F(x,y) = \sum_{m\geq 0} f_m(x)y^m$, multiply (2.10b) with y^m and sum for $m \geq 1$:

$$F(x,y)-f_0(x) = \sum_{m\geq 1}(xf_{m-1}(x)+xf_{m+1}(x))y^m = xyF(x,y)+\frac{x}{y}(F(x,y)-f_0(x)-f_1(x)y).$$

Adding $f_0(x)$, while using both, (2.10a) and the identity $f_0(x) = F(x,0)$, along with some further manipulations eventually yields the desired functional equation for $F(x,y)$:

$$\begin{aligned} F(x,y) &= xyF(x,y) + \frac{x}{y}(F(x,y) - F(x,0)) + 1 \\ \iff \quad \left(1 - xy - \frac{x}{y}\right) F(x,y) &= 1 - \frac{x}{y}F(x,0) \\ \iff \quad \left(xy^2 + x - y\right) F(x,y) &= xF(x,0) - y, \end{aligned}$$

which concludes the proof. This relation is equivalent to the recursion, implying uniqueness of its solution. Thus, it may also be used as an (implicit) definition of the generating function. □

The equation above is a prototypical example, suggesting the use of the Kernel method. To be more specific, Lemma 2.12 provides a linear combination involving one main formal power series and (in this case) one related series which only depends on x, i.e. not on all generating variables simultaneously. In our case, y plays the role of a catalytic variable, i.e. it vanishes from the equation by being set to zero, as described in Chapter 1.
Regardless, at first glance the equation seems to contain two unknown variables, $F(x,y)$ and its specialization $F(x,0)$, thus leading to nothing. Plugging in $y = 0$ results in an useless tautology. This is the point at which the Kernel method is applied in order to extract the necessary information (that is, additional relations) for solving the equation. As outlined in the introduction, the first step consists of setting the Kernel of the equation to zero.

The Kernel is the coefficient of the main generating function $F(x,y)$ in Lemma 2.12. Here it is a simple quadratic polynomial in y, so we can factorize it easily: $K(x,y) = xy^2 - y + x = x(y - Y_1(x))(y - Y_2(x))$ with

$$Y_{1,2}(x) = \frac{1 \mp \sqrt{1-4x^2}}{2x}.$$

For a visualization, the algebraic curve, defined by the equation $K(x,y) = 0$, is depicted in Figure 2.13 (note the different scaling for the axes). Also shown there are the roots: $Y_1(x)$ for $x \in (-0.5, 0.5)$ and the two branches of $Y_2(x)$ for $x \in (-0.5, 0.5) \setminus \{0\}$. In this domain, the discriminant $1-4x^2$ is greater than zero and hence the values are real numbers. Eventually we want to plug the roots into the generating function F. To ensure that this is a valid substitution, we need to analyze them to check if they actually define formal power series in x without a constant coefficient (otherwise the composition of power series might

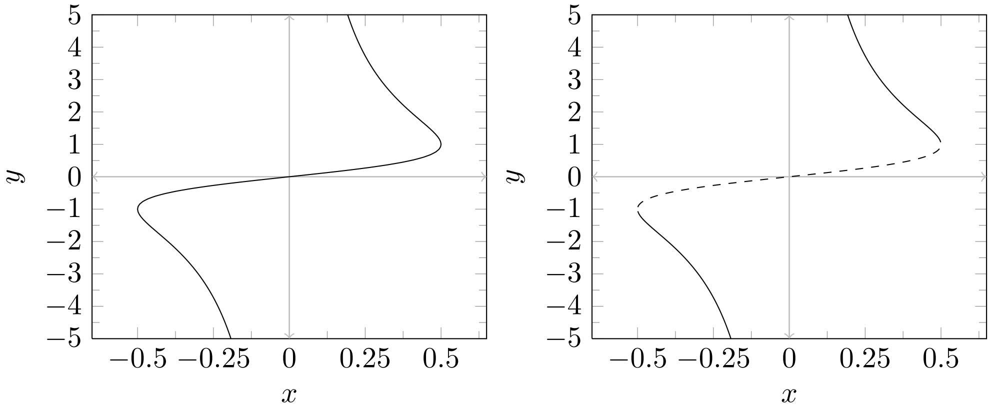

Figure 2.13: Left: The algebraic curve defined by $K(x, y) = 0$.
Right: The roots of the Kernel (Y_1: dashed line, Y_2: solid line).

not be well defined). Using the formal binomial series we can expand $Y_1(x)$:

$$Y_1(x) = \frac{1 - \sqrt{1 - 4x^2}}{2x} = \frac{1}{2x}\left(1 - \sum_{k \geq 0} \binom{1/2}{k} (-4)^k x^{2k}\right)$$
$$= -\frac{1}{2x} \sum_{k \geq 1} (-1) \cdot \binom{2(k-1)}{k-1} \frac{2x^{2k}}{k} = \sum_{k \geq 1} \binom{2(k-1)}{k-1} \frac{x^{2k-1}}{k}.$$

Hence, $\lim_{x \to 0} Y_1(x)$ exists and it is equal to zero since the series does not have a constant term. We further observe that $y - Y_1(x) \sim y - x \to 0$ if $(x, y) \to (0, 0)$.
On the other hand, by comparing with the coefficients of $K(x, y)$, we see that $Y_2(x)$ tends toward ∞ as $x \to 0$, since $Y_1(x)Y_2(x) = 1$ holds. Therefore, there is no formal power series expansion around the origin for $Y_2(x)$. Indeed, its formal Laurent series expansions involves $1/x$ as its first term, as the constant term of the square root expansion and the term one in the formula of $Y_2(x)$ do not cancel each other. This indicates a pole at the origin.
Now observe that $Y_1(x)$ and $Y_2(x)$ occur in the Kernel of 2.12, that is, the denominator of the generating function. Solving for F, we rewrite

$$F(x, y) = \frac{xF(x, 0) - y}{xy^2 + x - y},$$

which means that we have to take into account the reciprocals of the aforementioned factors. Hence, $\frac{1}{y - Y_1(x)} \to \infty$, while $\frac{1}{y - Y_2(x)} \to 0$ as $(x, y) \to (0, 0)$. Seemingly, no power series expansion exists for $F(x, y)$ around $(x, y) = (0, 0)$ given that one of its factors has a singularity at the origin.

This can not be the case, however: by definition as the generating function of the solvable Recursion 2.10, $F(x, y)$ must have a formal power series expansion with coefficients $f_{m,n} \in \mathbb{N}$. Thus, a singularity at the origin can not exist, which means that $y - Y_1(x)$ must be a factor of the numerator as well.

In particular this implies $F(x, Y_1(x)) = 0$, which holds the key information we need to solve the functional equation for F.

Consequently, it is valid to plug in $Y_1(x)$ for y. Whence we obtain a new relation $0 = F(x, Y_1(x)) = xF(x,0) - Y_1(x)$, from which the formerly unknown variable $F(x,0)$ can be computed:

$$F(x,0) = \frac{Y_1(x)}{x} = \frac{1-\sqrt{1-4x^2}}{2x^2}. \tag{2.14}$$

This is essentially the standard result after the application of the Kernel method: an additional equation for a specialization of the main generating function. In this case, the catalytic variable y has vanished as argument to F. Furthermore, comparing this to the well known generating function for the Catalan numbers (it can be obtained by using the expansion for a binomial series)

$$C(x) = \sum_{n\geq 0} \binom{2n}{n} \frac{x^n}{n+1} = \frac{1-\sqrt{1-4x}}{2x},$$

we observe that $F(x,0) = C(x^2)$. Reading off the coefficients which are the solution to our initial problem Task 2.2, recovers our result from the previous section:

$$a_n = f_{2n,0} = [x^{2n}]f_0(x) = [x^{2n}]F(x,0) = \frac{1}{n+1}\binom{2n}{n}.$$

Of course, it is also quite simple to find the expansion of $F(x,0)$ in exactly the same way as we did before for $Y_1(x)$, reducing by x^2 instead of x at the end.

Now we also have full access to the generating function $F(x,y)$ in general, so we can proceed to provide a solution to the problem of counting restricted paths. This computation involves only standard techniques for manipulating formal power series and extracting their coefficients. We start by plugging (2.14) into the equation from Task 2.12. Note again that $Y_1(x)Y_2(x) = 1$ holds.

$$\begin{aligned} F(x,y) &= \frac{Y_1(x) - y}{x(y - Y_1(x))(y - Y_2(x))} = \frac{1}{xY_2(x)(1 - \frac{y}{Y_2(x)})} = \frac{Y_1(x)}{x(1 - Y_1(x)y)} \\ &= \frac{1}{x}\sum_{m\geq 0} Y_1(x)^{m+1} y^m. \end{aligned}$$

The last equality utilizes the formal power series expansion of the geometric series $\frac{1}{1-Y_1(x)y}$. In order to read off the coefficients $[x^n y^m]$, it is necessary to know $[x^p]Y_1(x)^q$, for $p, q \in \mathbb{N}$. The substitution $x = \frac{u}{1+u^2}$ proves to be very useful here, since

$$Y_1\left(\frac{u}{1+u^2}\right) = \frac{1-\sqrt{1-4\frac{u^2}{(1+u^2)^2}}}{2\frac{u}{1+u^2}} = \frac{1+u^2-(1-u^2)}{2u} = u.$$

Using this in Cauchy's coefficient formula, Theorem 1.2, as well as $\mathrm{d}x = \frac{1-u^2}{(1+u^2)^2}\,\mathrm{d}u$, yields:

$$
\begin{aligned}
[x^p]Y_1(x)^q &= \frac{1}{2\pi\mathrm{i}}\oint \frac{Y_1(x)^q}{x^{p+1}}\,\mathrm{d}x = \frac{1}{2\pi\mathrm{i}}\oint u^q\frac{(1+u^2)^{p+1}}{u^{p+1}}\frac{1-u^2}{(1+u^2)^2}\,\mathrm{d}u \\
&= \frac{1}{2\pi\mathrm{i}}\oint \frac{(1-u^2)(1+u^2)^{p-1}}{u^{p+1-q}}\,\mathrm{d}u = [u^{p-q}](1-u^2)(1+u^2)^{p-1} \\
&= [u^{p-q}]\sum_{k=0}^{p-1}\binom{p-1}{k}u^{2k} - [u^{p-q-2}]\sum_{k=0}^{p-1}\binom{p-1}{k}u^{2k} \\
&= \begin{cases} 0 & \text{if } p-q \text{ odd,} \\ \binom{p-1}{\frac{p-q}{2}} - \binom{p-1}{\frac{p-q}{2}-1} & \text{if } p-q \text{ even.} \end{cases}
\end{aligned}
$$

It is easy to extract coefficients now, as $[x^n y^m]F(x,y) = [x^{n+1}]Y_1(x)^{m+1}$. Thus, we obtain $[x^n y^m]F(x,y) = 0$ if either n or m are odd. This obviously reflects the fact that there are no restricted paths of odd length ending in a point of even height respectively no paths of even length ending at odd height. The other, more interesting cases are

$$
\begin{aligned}
[x^{2n}y^{2m}]F(x,y) &= \binom{2n}{n-m} - \binom{2n}{n-m-1} = \frac{2m+1}{2n+1}\binom{2n+1}{n-m}, \\
[x^{2n+1}y^{2m+1}]F(x,y) &= \binom{2n+1}{n-m} - \binom{2n+1}{n-m-1} = \frac{2m+2}{2n+2}\binom{2n+2}{n-m}.
\end{aligned}
$$

Clearly, this implies our earlier result for $f_{2n,0}$, considering that $\frac{1}{2n+1}\binom{2n+1}{n} = \frac{1}{n+1}\binom{2n}{n}$. This method also provides yet another way to prove Theorem 2.8 (set $i = (n+m)/2$ and $o = (n-m)/2$).

We summarize the findings in

Theorem 2.14. *Let $f_{n,m}$ be the number of restricted paths defined in Definition 2.9 from the origin to the point $(n,m) \in \mathbb{N}\times\mathbb{N}$. Then*

$$
f_{n,m} = \begin{cases} 0 & \textit{if either } n \textit{ or } m \textit{ is odd,} \\ \dfrac{m+1}{n+1}\dbinom{n+1}{\frac{n-m}{2}} & \textit{if } n \textit{ and } m \textit{ are even,} \\ \dfrac{m+2}{n+2}\dbinom{n+2}{\frac{n-m}{2}} & \textit{if } n \textit{ and } m \textit{ are odd.} \end{cases}
$$

At first glance and in the case of an easy problem such as the one we solved in this chapter, the real usefulness and elegance of the Kernel method might not be really obvious. The author hopes that this will change in the following chapters.
Nevertheless, we have seen that after obtaining the initial recursion we only used standard techniques for manipulating generating functions and employed the Kernel method

to provide the missing information about the unknown specialization of the main generating series. The key here was finding the unknown entity $F(x, 0)$ in (2.14), an equation obtained by setting the Kernel to zero.

With some practice, this becomes a standard procedure for solving certain functional equations stemming from combinatorial problems, which is one of the reasons why the Kernel method is very attractive. While that is not a very ”combinatorial” way to deal with counting problems for some, it certainly does provide a procedure to start working towards new results.

3

Defective parking functions

After the introductory example in the preceding chapter, we will now look at a more sophisticated application of the Kernel method, as presented in [CJPS08]. To begin with, we introduce the notion of a parking function.

Consider a car park, consisting of parking spaces in line along a one-way street, labeled with numbers 1 to n from end to end. There are $m \leq n$ cars, all of their drivers having a favorite parking space, which were chosen independently from each other. Thus, as the cars arrive consecutively, it is possible that a driver's preferred place is already occupied - in this case, he continues his search and drives on in the car park towards the last lot with number n. On his way, he takes the first place which is empty and parks there. If there is none, he (frustratedly) leaves the car park and goes somewhere else.
This intuitive parking strategy (with applications in our daily life) essentially describes a greedy algorithm. It is simple, as it only takes into account the driver currently searching, but clearly it may fail to ensure that there is a parking space for every of the m arriving cars.
Either way, we can define a function by mapping each driver to his favorite place. We call this assignment a parking function if it leads to everyone parking successfully, using the search method outlined above. If exactly k drivers fail to park, we say that the parking function has a defect k (i.e. usual parking functions have defect 0 and we omit mentioning it). Or, more formally:

Definition 3.1. A function $f : \{1, 2, \ldots, m\} \to \{1, 2, \ldots, n\}$ is a parking function of defect k if for all $i \in \{1, 2, \ldots, n\}$, the cardinality of $f^{-1}[\{n+i-1, n+i, \ldots, n\}]$ is at most $k+i$. Additionally, if $k > 0$, then at least one of these sets has a size of exactly $k + i$.

Indeed, assume that $g : \{1, 2, \ldots, m\} \to \{1, 2, \ldots, n\}$ is a function which violates the first condition, such that there exists a preimage with $|g^{-1}[\{n+i-1, n+i, \ldots, n\}]| > k+i$. This would imply that more than k cars have to leave the car park, since more than $k+i$ cars have chosen one of the i places in $\{n+i-1, n+i, \ldots, n\}$ as their favorite. Furthermore, the second requirement ensures that at least $k > 0$ cars do not find a parking space. Hence, together they formalize the intuitive notion of parking functions. However, the easy to understand analogy of a car park will suffice for our purposes.

Before we proceed with a short example, let us comment on our notation first. Since there seems to be no convention in the literature, we will use use the letters m and n for the sizes of the domain (i.e. the number of cars) respectively the codomain (i.e. the number of parking spaces) of functions throughout this chapter. Both of them have an impact on whether or not a function is a parking function, but unlike the defect they are not mentioned explicitly.

Example 3.2. Let $n = 7, m = 6$ and consider the following parking function f encoded by the sequence $(f(1), f(2), \ldots, f(6)) = (1, 3, 4, 6, 3, 5)$. While the first 4 cars can be parked without problems, the fifth car tries to park in a space which is already occupied, so it has to drive ahead up to place 5. Nevertheless, everybody finds a space successfully, as seen in Figure 3.2. Observe that the above sequence would not be a parking function if n was

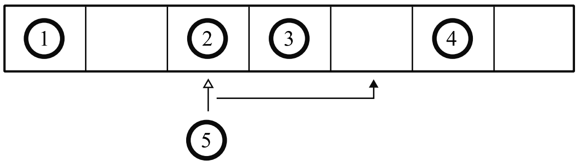

Figure 3.1: Greedy parking strategy

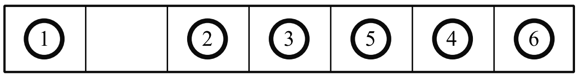

Figure 3.2: Final distribution of cars

changed. If $n = 6$, it has a defect of 1, since the last driver has to leave the car park, and similar for other values of n smaller than 7.

Note that there are many other definitions given in the literature, for example in [Sta97, Hai94, CP02]. In most cases, ours is slightly more general as usually only $m = n$ is considered or the notion of defect is omitted. Defective parking functions can also be obtained as a special case of x-parking functions introduced in [SP02], but these are not within the scope of this thesis.

Today there are many applications of these combinatorial objects. An overview of some early results was presented by Knuth in [Knu73] or more recently in the thesis [Sei09]. Also see [CJPS08] for further references. The starting point for the study of parking functions was the analysis of a hashing algorithm in [KW66]. A good hashing method aims for a low probability of data collisions, so that most of the arriving data packages can be stored immediately in a data storage device or a data structure without further adjustments. Therefore, if the greedy parking strategy is employed as part of an algorithm, it is interesting to know how many of the n^m possible functions are actually parking functions, since from this number we can easily derive the desired probability.

Task 3.3. Provide a formula for $p_{m,n,k}$, the number of defective parking functions $f : \{1, 2, \ldots, m\} \to \{1, 2, \ldots, n\}$ of defect k, where $m, n, k \in \mathbb{N}$.

In this chapter, we will establish a recursion for these numbers and obtain a functional equation for a generating function from it. The difficult part is that this equation involves two unknown variables and thus seems useless. However, remembering the success from the last chapter, we will then proceed to solve the equation using the Kernel method. Essentially, this means producing additional relations from the main equation by exploiting certain couplings of variables. Eventually this enables us to find a formula for the generating function and read off its coefficients.

3.1 Obtaining a recursion

Instead of deriving a recursion for the numbers $p_{m,n,k}$ directly, we present the approach of [CJPS08]. We will first transform the parameters to a more feasible form and extend their domain to all integers. This simply allows us to write the recursion more compactly, avoiding the need to deal with special cases.

Definition 3.4. Let $r, s, k \in \mathbb{Z}$. If one or more of r, s and k are smaller than 0, then $f_{r,s,k} = 0$. Otherwise, $f_{r,s,k}$ is the number of assignments of cars to parking spaces such that, after all cars entered the car park once, r parking spaces remain empty and s spaces are occupied, while k drivers have to search elsewhere (i.e. the defect is k).

Provided that $r, s, k \in \mathbb{N}$, these newly introduced variables have obvious connections to our original ones. There are $m = k + s$ drivers looking for a place to park and $n = r + s$ spaces available. Therefore, a solution to this problem is equivalent to a solution for Task 3.3, due to $p_{m,n,k} = f_{n+k-m,m-k,k}$. The following lemma establishes a recursive formula.

Recursion 3.5 ([CJPS08])**.** *For $r, s, k \in \mathbb{N}$ the numbers $f_{r,s,k}$ as given in Definition 3.4, can be obtained recursively by*

$$f_{r,s,k} = \begin{cases} 1 & \text{if } r = s = k = 0, \\ f_{r-1,s,0} + \sum_{i=0}^{k+1} \binom{k+s}{k+1-i} f_{r,s-1,i} & \text{if } k = 0 \text{ and either } r > 0 \text{ or } s > 0 \\ \sum_{i=0}^{k+1} \binom{k+s}{k+1-i} f_{r,s-1,i} & \text{if } k > 0. \end{cases}$$

Proof. Case $r = s = k = 0$: Obviously there exists only the empty assignment.
Case $k = 0$ and either $r > 0$ or $s > 0$: If the last parking space with number $r + s$ remains empty, the s drivers can actually be distributed among the first $r - 1 + s$ places. By definition, there are $f_{r-1,s,0}$ ways to arrange this.

If the last space is occupied in the end, then exactly one driver arrives there during the whole process - otherwise more than $k = 0$ cars had to leave or the last space would be left unoccupied again. Out of the s drivers, one (and only one) might have chosen it as his favorite parking lot, while the remaining drivers are parking successfully and independently from him within the forepart of the car park, leaving r spaces empty. Thus, there are $\binom{s}{1} f_{r,s-1,0}$ possible assignments to accomplish this. Similarly, if no one wants to park at the end of the car park, but still one car has to, then there are $\binom{s}{0} f_{r,s-1,1}$ ways to do this.
In total, $f_{r,s,0} = f_{r-1,s,0} + s f_{r,s-1,0} + f_{r,s-1,1}$. Formally, this is exactly the recursion given in the lemma above - expressing it in the same way as the last case will suit our purposes later on.
Case $k > 0$: We can generalize the idea from the former case to an arbitrary $k > 0$. Since at least one driver has to leave the car park, the last space can not remain empty and exactly $k+1$ cars must arrive at the end of the car park during the whole process, whether they wanted to park there or not.
Out of those $k + 1$ drivers, $k + 1 - i$, for an $i \in \{1, 2, \ldots, k + 1\}$, might favor parking space number $r + s$, while the remaining i do not but still reach it in their search for an unoccupied lot. Now there are $\binom{k+s}{k+1-i}$ possible ways to choose drivers who like to park at the last space and $f_{r,s-1,i}$ possibilities to distribute $s - 1 + i$ cars among the first $r + s - 1$ spaces, such that exactly i drivers are not able to park within that part of the car park. As before, these choices and assignments are independent from each other, whence we obtain $\binom{k+s}{k+1-i} f_{r,s-1,i}$ possibilities in total.
Finally, note that for $i \neq j$, all of the occurring mappings of drivers to parking spaces must differ. Hence, summing over all possible values for i yields the recursion. □

3.2 Obtaining a functional equation

From the recursive equation above we will now derive a functional equation which implicitly defines the generating function of the numbers $f_{r,s,k}$, and thus the solution to our problem. First, we will reformulate the recursion to analyze the parameters we are working with and to understand which kind of generating function captures their nature best. By multiplying with characteristic functions $\mathbb{1}_y(x)$, which evaluate to 1 if and only if $x = y$ and 0 otherwise (similar for multiple arguments), we unify the different cases of Recursion 3.5:

$$f_{r,s,k} = \mathbb{1}_{0,0,0}(r, s, k) + \mathbb{1}_0(k) f_{r-1,s,0} + \sum_{i=0}^{k+1} \binom{k+s}{k+1-i} f_{r,s-1,i}, \quad r, s, k \geq 0.$$

Note that the last sum is empty if $k = r = s = 0$ and that $f_{r,s,k}$ is zero by definition, if one of the parameters is smaller than zero, so the equation is indeed valid for all $r, s, k \geq 0$. Additionally, observe that the parameters k and s occur inside a binomial coefficient, while r does not. This indicates that the generating function which we will use should be ordinary in r and exponential in k and s.
Now, dividing the equation above by $\binom{k+s}{s}$ splits the binomial coefficient in the sum into two binomial coefficients. The advantage is that each of them depends on only one of the parameters anymore, instead of both of them. Mathematically:

$$\frac{\binom{k+s}{k+1-i}}{\binom{k+s}{s}} = \frac{(k+s)!k!s!}{(k+i-1)!(s-1+i)!(k+s)!} = \frac{s}{k+1}\frac{(k+1)!}{i!(k+1-i)!}\frac{i!(s-1)!}{(s-1+i)!} = \frac{s}{k+1}\frac{\binom{k+1}{i}}{\binom{s-1+i}{i}}.$$

This also further strengthens our observation from above and yields, keeping in mind that $\binom{0+s}{0} = 1$:

$$\frac{f_{r,s,k}}{\binom{k+s}{k}} = \mathbb{1}_{0,0,0}(r,s,k) + \mathbb{1}_0(k) f_{r-1,s,0} + \frac{s}{k+1}\sum_{i=0}^{k+1}\binom{k+1}{i}\frac{f_{r,s-1,i}}{\binom{s-1+i}{i}}, \quad r,s,k \geq 0. \tag{3.6}$$

Hence, we define our generating function accordingly.

Definition 3.6. Let $f_{r,s,k}$ be given as in Definition 3.4 and define their generating function as

$$F(x,y,z) := \sum_{r,s,k\geq 0} f_{r,s,k} x^r \frac{y^s z^k}{(s+k)!}.$$

We proceed to derive a functional equation from (3.6) in the following lemma.

Lemma 3.7. *The formal power series $F(x,y,z)$, given in Definition 3.6, is the unique solution of*

$$\left(1 - \frac{y}{z}e^z\right)F(x,y,z) = 1 + \left(x - \frac{y}{z}\right)F(x,y,0).$$

Proof. This proof, as well as some of the following, might seem technical but it is important to note that they mostly only involve standard techniques for the manipulation of formal power series. We start by multiplying (3.6) with $x^r \frac{y^s}{s!}\frac{z^k}{k!}$ and summing for $r,s,k \geq 0$.
On the left hand side of the equation we obtain $\sum_{r,s,k\geq 0} f_{r,s,k} x^r \frac{y^s z^k}{(s+k)!}$ which is exactly $F(x,y,z)$ by definition.
Now for the right hand side:

$$\begin{aligned}
&\sum_{r,s,k\geq 0}\left(\mathbb{1}_{0,0,0}(r,s,k) + \mathbb{1}_0(k) f_{r-1,s,0} + \frac{s}{k+1}\sum_{i=0}^{k+1}\binom{k+1}{i}\frac{f_{r,s-1,i}}{\binom{s-1+i}{i}}\right) x^r \frac{y^s z^k}{k!s!} \\
&= 1 + \underbrace{\sum_{r,s\geq 0} f_{r-1,s,0} x^r \frac{y^s}{s!}}_{\text{(a)}} + \underbrace{\sum_{r,s,k\geq 0}\left(\frac{s}{k+1}\sum_{i=0}^{k+1}\binom{k+1}{i}\frac{f_{r,s-1,i}}{\binom{s-1+i}{i}}\right) x^r \frac{y^s z^k}{k!s!}}_{\text{(b)}}.
\end{aligned}$$

To evaluate sum (a), we apply an index shift $r-1 \to r$ and the definition of our generating function:

$$\text{(a)} = \sum_{r,s\geq 0} f_{r,s,0} x^{r+1}\frac{y^s}{s!} = xF(x,y,0).$$

For sum (b), note that because of the term $\frac{s}{k+1}$, the sum actually starts at $s=1$. We begin by canceling the common factors of the occurring binomial coefficients and the factors $s!$, $k!$ and $\frac{s}{k+1}$.

To simplify the result, we continue by shifting the indices $k+1 \to k$ and $s-1 \to s$:

$$(\mathrm{b}) = \sum_{\substack{s\geq 1\\ r,k\geq 0}} \left(\sum_{i=0}^{k+1} \frac{f_{r,s-1,i}}{(s-1+i)!(k+1-i)!} \right) x^r y^s z^k = \sum_{\substack{k\geq 1\\ r,s\geq 0}} \left(\sum_{i=0}^{k} \frac{f_{r,s,i}}{(s+1)!(k-i)!} \right) x^r y^{s+1} z^{k-1}$$

$$= \frac{y}{z} \sum_{r,s,k\geq 0} \left(\sum_{i=0}^{k} \frac{f_{r,s,i}}{(s+1)!(k-i)!} \right) x^r y^s z^k - \frac{y}{z} \sum_{r,s\geq 0} f_{r,s,0} x^r \frac{y^s}{s!}.$$

For the last equality, we simply add the summands which occur for $k = 0$ and subtract them again, while singling out the factor $\frac{y}{z}$. The latter sum can be easily identified as $\frac{y}{z}F(x,y,0)$. The first one, arranged slightly different, is the Cauchy product of two well known formal power series in the variable z:

$$\frac{y}{z} \sum_{r,s,k\geq 0} \left(\sum_{i=0}^{k} \frac{f_{r,s,i}}{(s+1)!(k-i)!} \right) x^r y^s z^k = \frac{y}{z} \sum_{r,s,k\geq 0} \left(\sum_{i=0}^{k} f_{r,s,i} \frac{z^i}{(s+i)!} \frac{z^{k-i}}{(k-i)!} \right) x^r y^s$$

$$= \frac{y}{z} \sum_{k\geq 0} \frac{z^k}{k!} \sum_{r,s,k\geq 0} f_{r,s,k} x^r y^s \frac{z^k}{(s+k)!} = \frac{y}{z} \mathrm{e}^z F(x,y,z).$$

Altogether, we obtain for the left- and right-hand side

$$F(x,y,z) = 1 + xF(x,y,0) + \frac{y}{z}\mathrm{e}^z F(x,y,z) - \frac{y}{z}F(x,y,0),$$

which, after a slight rearrangement, yields the equation as given in the statement of the lemma. $\square$

Again, note that the functional equation for F is equivalent to the recursion for the numbers $f_{r,s,k}$, which implies the uniqueness as stated in the lemma. The same argument will hold for all similar results still to come in the following chapters.

3.3 Obtaining a closed formula

To find an explicit expression for the numbers $f_{r,s,k}$, and subsequently for $p_{m,n,k}$, we would like to use the formal power series expansion of $F(x,y,z)$ around the origin $(0,0,0)$ and read off the coefficients. Hence, we need to solve the equation

$$F(x,y,z) = \frac{1 + \left(x - \frac{y}{z}\right) F(x,y,0)}{1 - \frac{y}{z}\mathrm{e}^z}, \tag{3.8}$$

which, as we have seen in the preceding section, implicitly defines the generating function. Observe that this is usually not possible, since both, $F(x,y,z)$ as well as $F(x,y,0)$ are unknown and plugging in $z = 0$ leads to a tautology.

Overall, the situation is remarkably similar to Lemma 2.12 in Section 2.2. There, we have successfully applied the Kernel method, so we will try it once more, even if we have to deal with a third generating variable now. Recall that the denominator of $F(x,y,z)$ is called the Kernel $K(y,z) = 1 - \frac{y}{z}\mathrm{e}^z$ of the equation.

We follow the standard procedure and start by setting $K(y,z)$ to zero in order to recover $F(x,y,0)$. It is not a polynomial this time, so there is no general way to find its roots. But we may look for a formal power series in the variable y, i.e. $z = Z(y)$, such that $K(y, Z(y)) = 0$. This leads to the equation $z = y\mathrm{e}^z$. As presented in, e.g., [FS09], the solution to it is the so-called tree function (often denoted by T in the literature, for obvious reasons), the generating function of (rooted) non-plane labeled trees. In Figure 3.9 the curve defined by $K(y,z) = 0$ is shown. Note that the tree function only defines the lower part of the curve up to $y = 1/\mathrm{e}$, which is exactly its radius of convergence.

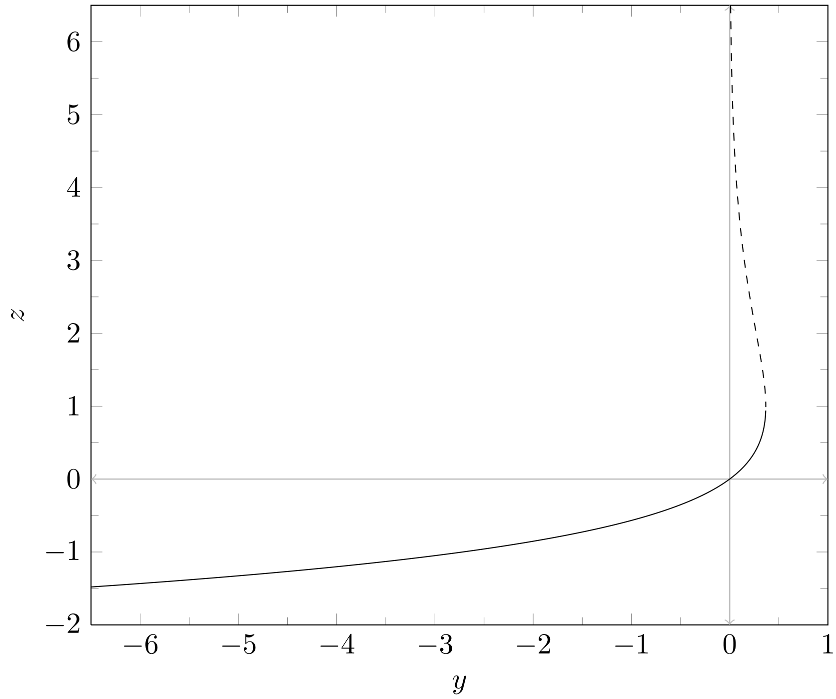

Figure 3.9: The algebraic curve defined by $K(y,z) = 0$ (the part given by the Tree function is drawn solid).

To obtain the formal power series expansion of the tree function, one might use its close relationship to the Lambert w-Function (see e.g. [CGH⁺96]), due to $Z(y) = -w(-y)$. It is named after the swiss mathematician Johann Heinrich Lambert, who proved that π is an irrational number, among other things.

Or we can use Lagrange inversion, Theorem 1.1, for the alternate form of the defining equation $y = \frac{z}{\mathrm{e}^z}$. Since we will need the result later on, we will actually extract the coefficients from $z^j = Z(y)^j$, for $j \in \mathbb{N}$.

$$
\begin{aligned}
\left[y^i\right] z^j &= \left[z^i\right] z^j = 0, \quad i < j, \\
\left[y^i\right] z^j &= \frac{1}{i}\left[z^{i-1}\right] j z^{j-1}\mathrm{e}^{iz} = \frac{j}{i}\left[z^{i-j}\right]\mathrm{e}^{iz} = \frac{j}{i}\frac{i^{i-j}}{(i-j)!}, \quad i \geq j.
\end{aligned}
\tag{3.10}
$$

Thus, if $j = 1$, the number of non-plane labeled trees with i nodes is i^{i-1}, recovering the famous enumeration result by Arthur Cayley [Cay88], frequently called Cayley's formula. Note that his result actually is i^{i-2}, which counts unrooted trees with i nodes. However, these can be converted to rooted trees by simply marking one node as the root - and for this, there are obviously i choices. Furthermore, we have

$$z = Z(y) = \sum_{i \geq 1} \frac{i^{i-1}}{i!} y^i.$$

We see that $Z(y)$ has a formal power series expansion with coefficients in $\mathbb{N}$ and without a constant term, so its substitution into the Kernel is valid. Clearly, by doing this the Kernel vanishes. However, it also seems to cause a singularity at the origin $(0,0,0)$, since $Z(y) = y + y^2 + \frac{3}{2}y^3 + \ldots \sim y$ and therefore $\frac{y}{Z(y)}\mathrm{e}^{Z(y)} \to 1$, as $x, y \to 0$. This can not be the case, though, and we can use the values at which the Kernel is zero to recover the missing information about our generating function:

By definition as the generating function of the solvable recursion given in Recursion 3.5, $F(x,y,z)$ must have a formal power series expansion around $(0,0,0)$ with coefficients $f_{r,s,k} \in \mathbb{N}$. Hence, if the Kernel equals zero, then $1 - \frac{y}{Z(y)}\mathrm{e}^{Z(y)}$ must be a factor of the numerator, too. In particular this implies $F(x, y, Z(y)) = 0$, providing the additional relation we wanted to find.

This ensures that the generating functions we are working with do not have poles in an area around the origin. We proceed with a lemma which gives the form of $F(x,y,0)$, putting the relationship of F and Z to good use:

Lemma 3.11. *The specialization $F(x,y,0)$ is given by*

$$F(x,y,0) = \frac{e^{Z(y)}}{1 - xe^{Z(y)}},$$

admitting the formal power series expansion

$$F(x,y,0) = \sum_{r,s \geq 0} (r+1)(r+s+1)^{s-1} x^r \frac{y^s}{s!}.$$

First proof. The first equation in the statement of the lemma above stems from the fact that $F(x,y,Z(y)) = 0$. This, together with the defining equation for $Z(y) = y\mathrm{e}^{Z(y)}$ yields

$$0 = 1 + \left(x - \frac{y}{Z(y)}\right) F(x,y,0) \Longleftrightarrow F(x,y,0) = \frac{1}{\frac{1}{\mathrm{e}^{Z(y)}} - x} = \frac{\mathrm{e}^{Z(y)}}{1 - x\mathrm{e}^{Z(y)}}.$$

Our main tool for the rest of the proof will be Lagrange inversion. To start with, we read off the coefficients for x and reformulate the equation as

$$x = \frac{F(x,y,0) - \mathrm{e}^{Z(y)}}{F(x,y,0)\mathrm{e}^{Z(y)}}.$$

Now define the new variable $u := F(x,y,0) - \mathrm{e}^{Z(y)}$ to obtain the form necessary for Theorem 1.1. It follows that $x = u/\left(u\mathrm{e}^{Z(y)} + \mathrm{e}^{2Z(y)}\right)$ and we can proceed to read off the coefficients from $F(x,y,0) = u + \mathrm{e}^{Z(y)}$:

$$\begin{aligned}
\left[x^0\right] u + \mathrm{e}^{Z(y)} &= \left[u^0\right] u + \mathrm{e}^{Z(y)} = \mathrm{e}^{Z(y)}, \\
[x^r]\, u + \mathrm{e}^{Z(y)} &= \frac{1}{r}\left[u^{r-1}\right]\left(u\mathrm{e}^{Z(y)} + \mathrm{e}^{2Z(y)}\right)^r = \frac{1}{r}\binom{s}{r-1}\mathrm{e}^{(r-1)Z(y)}\mathrm{e}^{2Z(y)} = \mathrm{e}^{(r+1)Z(y)},
\end{aligned}$$

where $r \geq 1$. Note that the formal power series $Z(y)$ is the solution to the equation $y = \frac{z}{\mathrm{e}^z}$, so for all $j \in \mathbb{N}$, $\mathrm{e}^{jZ(y)} = \left(\frac{Z(y)}{y}\right)^j$ holds. Therefore, we can use the result (3.10) from earlier

$$Z(y)^j = j\sum_{i\geq j}\frac{i^{i-j-1}}{(i-j)!}y^i = j\sum_{i\geq 0}\frac{(i+j)^{i-1}}{i!}y^{i+j},$$

where we applied the shift $i - j \to i$ for the second equality. Now it is easy to finish the proof:

$$\left[x^r\frac{y^s}{s!}\right]F(x,y,0) = \left[\frac{y^s}{s!}\right]\mathrm{e}^{(r+1)Z(y)} = \left[\frac{y^s}{s!}\right]\left(\frac{Z(y)}{y}\right)^{r+1} = (r+1)(r+s+1)^{s-1},$$

which yields the formal power series expansion for $F(x,y,0)$, as given in the lemma. $\square$

Second proof. There is also an alternative proof for this statement which uses a clever idea due to Pollak (see [FR74]). Since many papers related to parking functions mention it, we shall not omit it here. Furthermore it relates to our earlier observations: the Kernel method provides a standard way of doing things, but there may also be great insights which give a different perspective (likely less generatingfunctional) of the problem.
Recall that there is relationship between the number of parking functions of defect k, denoted by $p_{m,n,k}$, and the numbers $f_{r,s,k}$. If $k = 0$, then $n = r + s$ and $m = s$, so in this case it is given by $f_{r,s,0} = p_{n-m,m,0}$.
To obtain a formula for the numbers, replace the linear car park with n places by a circular one with $n + 1$ spaces, again labeled by the numbers in $\{1, 2, \ldots, n + 1\}$. We also keep the same rules for parking the $m \leq n$ cars. Obviously everyone finds a place now (they keep going around the closed circle until an empty place shows up) and no one has to drive home, thus leaving $n - m + 1$ spaces empty in the end.
A mapping of the m cars to the $n + 1$ spaces in this setting gives a parking function of the original problem if and only if the space with number $n + 1$, which has no counterpart in the linear park, is among the unoccupied ones. The probability that this happens is $(n + 1 - m)/(n + 1)$ and multiplying with $(n + 1)^m$, the number of all possible mappings, gives $(n + 1 - m)(n + 1)^{m-1}$.
Therefore we obtain the same formal power series expansion as in the first proof, since $f_{r,s,0} = p_{n-m,m,0} = (n + 1 - m)(n + 1)^{m-1} = (r + 1)(r + s + 1)^{s-1}$. $\square$

Now that we have access to the first ”unknown” in equation (3.8), we can proceed to solve it for the generating function $F(x,y,z)$ in general. By simply plugging in $F(x,y,0)$ we obtain

Lemma 3.12 ([CJPS08])**.** *The generating function for the numbers $f_{r,s,k}$ is given by*

$$F(x,y,z) = \frac{1}{1-\frac{y}{z}e^z} + \frac{x-\frac{y}{z}}{1-\frac{y}{z}e^z}\frac{e^{Z(y)}}{1-xe^{Z(y)}}.$$

Given in this form, it is not immediate that $F(x,y,z)$ is actually a formal power series. Both of its summands are not in $\mathbb{Z}[[x,y,z]]$ and thus it might seem that it is rather a formal Laurent series in the variables x,y,z. But as mentioned before, our combinatorial interpretation of $F(x,y,z)$ as a generating function ensures that occurring negative powers must disappear by canceling each other while summing. As an example, looking at critical values where $K(x,y)$ vanishes, we observe that $F(x,y,z)$ simplifies to $F(x,y,z) = 1/\left(1-x\mathrm{e}^{Z(y)}\right)$ by canceling the Kernel in denominator and numerator. This series is nothing but a geometric series with a proper formal power series expansion.

Keeping this in mind, we are now ready to extract the coefficients $f_{r,s,k}$ and subsequently give a formula for the car parking numbers $p_{m,n,k}$. To express them concisely, we will make use of so-called Abel-type partial sums. They are similar to the sums occurring in Abel's binomial theorem, which we will briefly introduce below.

Definition 3.13. Let $m,n,k \in \mathbb{N}$. Then

$$A(m,n,k) := \begin{cases} n^m & \text{if } k \le m-n, \\ \displaystyle\sum_{i=0}^{m-k} \binom{m}{i}(n-m+k)(n-m+k+i)^{i-1}(m-k-i)^{m-i} & \text{otherwise.} \end{cases}$$

Using this definition, we can formulate the final lemma for this chapter.

Lemma 3.14. *The generating function of the numbers $f_{r,s,k}$ has a formal power series expansion around the origin $(0,0,0)$ given by*

$$F(x,y,z) = \sum_{r,s,k\ge 0} \left(A(s+k,r+s,k) - A(s+k,r+s,k+1)\right) x^r \frac{y^s z^k}{(s+k)!}.$$

Proof. To find the coefficients of $F(x,y,z)$, our computations will take place within the ring of formal Laurent series $\mathbb{Z}((x,y,z))$, as negative powers of generating variables occur. But we know a-priori that these must cancel each other and disappear in the end, which we can use to our advantage.
The starting point is the equation for $F(x,y,z)$ in Lemma 3.12. Its first summand is $1/(1-\frac{y}{z}\mathrm{e}^z) \in \mathbb{Z}((x,y,z))$, which has a formal Laurent series expansion as a geometric series.

$$\frac{1}{1-\frac{y}{z}\mathrm{e}z} = \sum_{s\ge 0} y^s z^{-s}\mathrm{e}^{tz} = \sum_{s\ge 0} y^s z^{-s} \sum_{k\ge 0}\frac{(tz)^k}{k!} = \sum_{s\ge 0}\sum_{k\ge 0}\frac{s^k}{k!}y^s z^{k-s} = \sum_{s\ge 0}\sum_{k\ge -s}\frac{s^{s+k}}{(s+k)!}y^s z^k, \tag{3.15}$$

using a shift $k - s \to k$ for the last equality. Using this together with Lemma 3.11, we can expand the second summand as a Cauchy product of Laurent series in the variable y.

$$\begin{aligned}
\frac{x-\frac{y}{z}}{1-\frac{y}{z}\mathrm{e}^z}\frac{\mathrm{e}^{Z(y)}}{1-x\mathrm{e}^{Z(y)}} &= \left(x-\frac{y}{z}\right)\left(\sum_{s\geq 0}\sum_{k\geq 0}\frac{s^k}{k!}y^s z^{k-s}\right)\left(\sum_{s\geq 0}\sum_{r\geq 0}(r+1)(r+s+1)^{s-1}x^r\frac{y^s}{s!}\right)\\
&= \left(x-\frac{y}{z}\right)\sum_{s\geq 0}\left(\sum_{i=0}^{s}\left(\sum_{k\geq 0}\frac{(s-i)^k}{k!}z^{k-(s-i)}\right)\left(\sum_{r\geq 0}(r+1)(r+i+1)^{i-1}x^r\frac{1}{i!}\right)\right)y^s\\
&= \left(x-\frac{y}{z}\right)\sum_{r,s,k\geq 0}\sum_{i=0}^{s}(r+1)(r+i+1)^{i-1}\frac{(s-i)^k}{k!i!}x^r y^s z^{k-s+i}\\
&= \sum_{r,s,k\geq 0}\sum_{i=0}^{s}(r+1)(r+i+1)^{i-1}\frac{(s-i)^k}{k!i!}\left(x^{r+1}y^s z^{k-s+i} - x^r y^{s+1} z^{k-s+i-1}\right).
\end{aligned}$$

Note that because of the factor $s - i$, the inner sum for i actually stops at $i = s - 1$. We replace $1/(k!i!)$ by $\binom{k+i}{i}/(k+i)!$ and split the sum into two, shifting $k - s + i \to k$. Additionally, for the first part of the result we apply another shift $r + 1 \to r$ and for the second one $s + 1 \to s$. This yields

$$\begin{aligned}
\frac{x-\frac{y}{z}}{1-\frac{y}{z}\mathrm{e}^z}\frac{\mathrm{e}^{Z(y)}}{1-x\mathrm{e}^{Z(y)}} &= \sum_{r\geq 1}\sum_{s\geq 0}\sum_{i=0}^{s}\sum_{k\geq -s+i}\binom{k+s}{i}r(r+i)^{i-1}(s-i)^{k+s-i}x^r\frac{y^s z^k}{(s+k)!}\\
&-\sum_{r\geq 0}\sum_{s\geq 1}\sum_{i=0}^{s-1}\sum_{k\geq -s+i}\binom{k+s}{i}(r+1)(r+i+1)^{i-1}(s-1-i)^{k+s-i}x^r\frac{y^s z^k}{(s+k)!}.
\end{aligned}\tag{3.16}$$

Because of the definition as a generating function, which implies that $F(x, y, z)$ has a proper formal power series expansion around the origin, the negative powers of variables, i.e. all summands for $k < 0$, must cancel each other during the summation and we can omit them. This gives a correspondence to Abel's binomial theorem, to be discussed shortly. Hence,

$$\begin{aligned}
F(x,y,z) &= \sum_{s\geq 0}\sum_{k\geq 0}s^{s+k}\frac{y^s z^k}{(s+k)!} + \sum_{r\geq 1}\sum_{s\geq 0}\sum_{k\geq 0}\sum_{i=0}^{s}\binom{k+s}{i}r(r+i)^{i-1}(s-i)^{k+s-i}x^r\frac{y^s z^k}{(s+k)!}\\
&-\sum_{r\geq 0}\sum_{s\geq 1}\sum_{k\geq 0}\sum_{i=0}^{s-1}\binom{k+s}{i}(r+1)(r+i+1)^{i-1}(s-1-i)^{k+s-i}x^r\frac{y^s z^k}{(s+k)!}.
\end{aligned}$$

The Abel-type partial sums from Definition 3.13 turn out to be very useful for shortening the expressions of the coefficients of $F(x, y, z)$. As we always did in this chapter, we plug in $s + k$ for m and $r + s$ for n, to obtain

$$A(s+k, r+s, k) = \begin{cases} s^{s+k} & \text{if } r = 0,\\ \displaystyle\sum_{i=0}^{s}\binom{k+s}{i}r(r+i)^{i-1}(s-i)^{k+s-i} & \text{if } r > 0,\end{cases}$$

and

$$A(s+k, r+s, k+1) = \begin{cases} s^{s+k} & \text{if } r = 0, \\ \sum_{i=0}^{s-1} \binom{k+s}{i} (r+1)(r+i+1)^{i-1}(s-1-i)^{k+s-i} & \text{if } r > 0. \end{cases}$$

Note that $A(s+k, r+s, k+1) = 0$, if $s = 0$. Comparing this with the equation for $F(x, y, z)$ above yields

$$\left[x^r \frac{y^s z^k}{(s+k)!}\right] F(x, y, z) = f_{r,s,k} = A(s+k, r+s, k) - A(s+k, r+s, k+1),$$

thus finishing the proof. □

We summarize our results in the last theorem for this chapter, completing the solution to Task 3.3.

Theorem 3.17 ([CJPS08]). *Let $m, n, k \in \mathbb{N}$. The number of defective parking functions of defect k, denoted by $p_{m,n,k}$, is given by*

$$p_{m,n,k} = A(m, n, k) - A(m, n, k+1).$$

Equivalently, the sum $A(m, n, k)$ counts the number of mappings from m cars to n spaces such that at least k drivers do not find an unoccupied parking space, that means

$$A(m, n, k) = \sum_{j=k}^{m} p_{m,n,j}.$$

Proof. As a reminder, m is the number of cars entering the car park, n the number of available spaces and k drivers have to go home. On the other hand, r and s count the unoccupied respectively occupied spaces. From the relationships $m = k + s$ and $n = r + s$ we conclude that $p_{m,n,k} = f_{n+k-m,m-k,k}$. Plugging these values into the results from Lemma 3.14 yields the statement. □

To illustrate these numbers, Table 3.18 shows some values for $p_{m,n,k}$. In the on-line encyclopedia of integers [OEI11] one can find the (shifted) sequence for $k = 0$ as entry A000272 (i.e. the numbers counting normal parking functions) and $k = 1$ as A140647.

Before we proceed to give some closing remarks, we will make the connection to Abel's binomial theorem clear, which states that

$$(x+y)^q = \sum_{i=0}^{q} \binom{n}{i} x(x+iw)^{i-1}(y-iw)^{q-i} \tag{3.19}$$

holds for all $q \in \mathbb{N}$ and $w, x, y \in \mathbb{R}$. There are many other theorems of this kind, however, in this form it was studied by the Norwegian Nils Henrik Abel [Abe26].

$m \diagdown n$	1	2	3	4	5	6	7	8	9	10	
1	1	2	3	4	5	6	7	8	9	10	
2		3	8	15	24	35	48	63	80	99	
3			16	50	108	196	320	486	700	968	
4				125	432	1029	2048	3645	6000	9317	
5					1296	4802	12288	26244	50000	87846	$k=0$
6						16807	65536	177147	400000	805255	
7							262144	1062882	3000000	7086244	
8								4782969	20000000	58461513	
9									100000000	428717762	
10										2357947691	
2		1	1	1	1	1	1	1	1	1	
3			10	13	16	19	22	25	28	31	
4				107	165	235	317	411	517	635	
5					1346	2341	3716	5531	7846	10721	
6						19917	37883	65389	105255	160661	$k=1$
7							341986	697089	1286244	2206891	
8								6713975	14461513	28175767	
9									148717762	335073709	
10										3674435393	
3			1	1	1	1	1	1	1	1	
4				23	27	31	35	39	43	47	
5					436	581	746	931	1136	1361	
6						8402	12373	17394	23585	31066	$k=2$
7							173860	277397	420106	610597	
8								3924685	6685815	10773725	
9									96920092	174346021	
10										2612981360	
6						1	1	1	1	1	
7							162	169	176	183	
8								12357	13737	15173	$k=5$
9									710314	840367	
10										36046214	

Table 3.18: Values of $p_{m,n,k}$ for various m, n and k (omitted values are zero).

To this end, we collect the negative powers of generating variables from equations (3.15) and (3.16). Because of our underlying combinatorial interpretation we know that they must vanish during the summation, whence

$$\begin{aligned}0 = \sum_{s\geq 0}\sum_{k=-s}^{-1} s^{s+k}\frac{y^s z^k}{(s+k)!} + \sum_{r\geq 1}\sum_{s\geq 0}\sum_{i=0}^{s-1}\sum_{k=-s+i}^{-1}\binom{k+s}{i} r(r+i)^{i-1}(s-i)^{k+s-i}x^r\frac{y^s z^k}{(s+k)!} \\ -\sum_{r\geq 0}\sum_{s\geq 1}\sum_{i=0}^{s-1}\sum_{k=-s+i}^{-1}\binom{k+s}{i}(r+1)(r+i+1)^{i-1}(s-1-i)^{k+s-i}x^r\frac{y^s z^k}{(s+k)!}.\end{aligned}$$

Alternatively, we can use the binomial identity (3.19). By switching the sums for i and k, we now sum from $i=0$ to $i=k+s$. Using the formula yields

$$\sum_{i=0}^{k+s} \binom{k+s}{i} r(r+i)^{i-1}(s-i)^{k+s-i} = (r+s)^{k+s},$$
$$\sum_{i=0}^{k+s} \binom{k+s}{i} (r+1)(r+i+1)^{i-1}(s-1-i)^{k+s-i} = (r+s)^{k+s}.$$

Keeping in mind that the sums for s actually start at 1, we can simplify the right hand side of the equation above and obtain

$$\sum_{s\geq 1}\sum_{k=-s}^{-1} s^{s+k}\frac{y^s z^k}{(s+k)!} + \sum_{r\geq 1}\sum_{s\geq 1}\sum_{k=-s}^{-1}(r+s)^{k+s}x^r\frac{y^s z^k}{(s+k)!} - \sum_{r\geq 0}\sum_{s\geq 1}\sum_{k=-s}^{-1}(r+s)^{k+s}x^r\frac{y^s z^k}{(s+k)!}$$
$$= \sum_{s\geq 1}\sum_{k=-s}^{-1} s^{s+k}\frac{y^s z^k}{(s+k)!} - \sum_{s\geq 1}\sum_{k=-s}^{-1}(0+s)^{s+k}x^r\frac{y^s z^k}{(s+k)!} = 0,$$

verifying our argument from before.

Now, in the other direction, we take a look at the fact that $A(m, n, k)$ counts all defective parking functions with defect greater or equal to k. Clearly, if we set $k = 0$ then any function from $\{1, 2, \ldots, m\}$ to $\{1, 2, \ldots, n\}$ occurs in that enumeration. We know that the number of all functions is n^m, whence

$$n^m = A(m, n, 0) = \sum_{i=0}^{m}\binom{m}{i}(n-m)(n-m+i)^{i-1}(m-i)^{m-i}.$$

But this is a proof of a special case of Abel's identity, setting $q = m, x = n-m, y = m$ and $w = 1$. Admittedly it is also very complicated, considering the work required to obtain $A(m, n, k)$.
Besides this correspondence, Abel's theorem was also used in [CJPS08] to obtain further asymptotic results.

In this example, we have seen that the Kernel method is still applicable in a more difficult situation than in Chapter 2. Here the Kernel is not a polynomial (but the roots remain tractable enough) and there are more generating variables to consider.
It provides the necessary starting point to solve the functional equation (3.8) derived from Recursion 3.5, where it is normally not possible to solve such an equation with two unknown variables. Additionally, the underlying combinatorial interpretation ensures that the final result really is a formal power series and that negative powers of generating variables, indicating singularities at the origin, must vanish in the end. Thus, computations can be simplified.

Similar to the preceding chapter, the Kernel method is not the only way to obtain our solution. Alternatively, there are other methods (especially for asymptotic results) or the framework of x-parking functions can be applied. See for example [Sei09] for an overview. However, we have only used standard methods of manipulating formal Laurent respectively formal power series. This makes the proofs very accessible (even for computer algebra systems), albeit lengthy sometimes. No tricky bijections or concepts are involved, which might require a more in-depth explanation for a trained generatingfunctionologist.

4

Vexillary involutions

In the last two chapters we have learned how the Kernel method can be applied to solve functional equations which seem to contain too many unknowns to be solved using standard techniques. We will now look at a different flavor of the method. Until now, producing one coupling of variables which sets the Kernel to zero was enough to provide the missing information about the generating function and its specializations. However, this is not always the case, as we will see soon. Thus, one must not give up and simply keep on producing as many roots as possible, in order to obtain additional relations for the occurring entities. Indeed, this obstinate version of the Kernel method was aptly named and introduced by Bousquet-Mélou, who in turn was inspired by the book [FIM99].
As a demonstration, we will take a look at pattern-avoiding permutations, or more specifically vexillary involutions, following the corresponding chapter in the article [BM03], while filling in the omitted details.

To begin with, we need to formalize the notion of pattern-avoidance, a subject which earned a lot of popularity in the recent years due to its intriguing results and many connections to other mathematical disciplines and computer science. Indeed, we have already encountered it in Chapter 2 - Knuth [Knu68] showed that a permutation can be sorted using a stack if and only if the permutation avoids the pattern 231. For a thorough introduction see for example [Bón04] or for some questions and problems which are studied within this field of research, see [Wil02]. Now for the definition, which can be grasped very quickly.

Definition 4.1. Denote $\mathrm{S}_n := \{\pi : \{1,2,\dots,n\} \to \{1,2,\dots,n\} \;:\; \pi \text{ bijective}\}$. Let $m \leq n$, $\sigma = \sigma_1\sigma_2\dots\sigma_m \in \mathrm{S}_m$ and $\pi = \pi_1\pi_2\pi_n \in \mathrm{S}_n$. The permutation π is said to contain the pattern σ of length m, if there are $i_1 < i_2 < \dots < i_m \in \mathbb{N}$ such that $\pi_{i_j} < \pi_{ik}$ if and only if $\sigma_j < \sigma_k$. If π does not contain σ, then it is said that it avoids this pattern.

Thus, the elements of the extracted subpermutation satisfy the same ordering relations as the numbers in the given pattern. Note that this definition generalizes some very familiar concepts such as descents and ascents. They can be described as special patterns of type 21 and 12, with the additional requirement that this pattern is made out of consecutive letters within the permutation.

Example 4.2. As an example, take the permutation $\pi = 751938624$. Clearly, it contains descents and ascents (and thus patterns 21 and 12) and all 6 patterns of length 3, e.g. the pattern 231 might correspond to the subpermutations $\pi_2\pi_4\pi_5 = 593$ or $\pi_5\pi_6\pi_8 = 382$. However, as there is no increasing subsequence of length 4, it avoids 1234 or e.g. 2341 as well. It does contain 2143 though, for example given by $\pi_1\pi_2\pi_4\pi_6$, which will be the single most important pattern in this chapter.

Although the definition is very simple, there is a lot of theory behind it. In fact, there are many challenging problems regarding the study of pattern-avoidance, such as counting the number of permutations avoiding a certain pattern or finding general results for Wilf-equivalences (two patterns σ and τ are said to be Wilf-equivalent if they are both equally hard to avoid, i.e. the number of permutations avoiding σ is equal to the number of permutations avoiding τ). For more information about these topics, [Man04, Sta96, Wes96] will provide some starting points. The latter article additionally introduces generating trees for the study of pattern-avoiding permutations, a technique also used by Bousquet-Mélou in the article on which this chapter is based on.
However, the simple notion in Definition 4.1 will suffice for our purposes and leads to another definition.

Definition 4.3. Let $\pi \in \mathrm{S}_n$ be an involution, i.e. $\pi = \pi^{-1}$ holds. We call π vexillary if it avoids the pattern 2143 and we denote by V_n the set of all vexillary involutions of length n.

The name vexillary (meaning "flag-like" and having its roots in the latin word vexillum) stems from the appearance of these permutations in [LS85]. In this paper the authors studied Schubert polynomials, as well as sequences which occur in geometry and correspond to so-called flags of modules. Without going into the details, in linear algebra a flag is a sequence of subspaces of a finite-dimensional vector space, where each member of the sequence is a proper subspace of the next one. Naturally, one can also study them for modules, which are basically a generalization of vector space.
Many further references about these permutations can be found in [GPP01], where the authors present a bijective proof for the rather surprising fact that vexillary involutions are counted by the well known Motzkin numbers. One of them already conjectured that this would be the case in his PhD thesis in 1995 [Gui95], about 6 years earlier. But as Bousquet-Mélou states, it was very "vexing" that despite vexillary involutions admit this simple solution, no proof could be found for a few years time. However, she continues that a straightforward description (i.e. a method for the enumeration of vexillary involutions) given by Guibert in terms of generating trees was known. That did not help very much though, as it leads to a functional equation for a generating function which involves too many unknowns to be solved by conventional means.

In this chapter we will rederive this equation and solve it using the obstinate Kernel method as presented by Bousquet-Mélou. This is in accordance with the earlier chapters - again,

it is not the only method available to solve the counting problem. But unlike the bijective proof it does not require a very deep understanding of the underlying combinatorial objects or their relationships to each other. Instead, all we need to do is to derive a recursion and obtain a functional equation. After that only algebraic manipulations of generating functions occur, even if they are much more delicate than in the preceding chapters. There will be essentially two steps involved to solve the functional equation. Both aim to make finding the encoded solution easier and more accessible.
The first step will be to apply the Kernel method multiple times, which means finding several different couplings of variables to set the Kernel to zero. The initial functional equation is thus transformed into a system of equations, which only involve the generating function at special values and describe their relations. This system still contains too many variables to be solved directly, hence the second step is to extract the positive part of the occurring functions in the easiest way possible. This eventually provides the necessary informations by obtaining even more equations.

Indeed, this procedure provides a more general result than the bijective proof. Let us state our tasks precisely. First off,

Task 4.4. Show that the number of vexillary involutions of length n is given by the n-th Motzkin number.

The resulting numbers are named after Theodore Motzkin, who introduced them in his article [Mot48]. They occur frequently, with many applications in various branches of mathematics, and enumerate several combinatorial objects, 14 of which are given in [DS77]. An overview of their connections to e.g. the Catalan numbers can be found in [Ber99].
Additionally, Bousquet-Mélou's method gives full access to the solution of said functional equation, so we will also do

Task 4.5. Provide an expression for the generating function of vexillary involutions.

This function will count our combinatorial objects not only by their length, but also by two other, secondary statistics. This approach is even applicable to other very similar situations concerning pattern-avoiding permutations in connection with generating trees, all of them demonstrated in the article [BM03]. Examples for this are 1234-avoiding permutations and vexillary permutations (note: not involutions). A reason for this might be that bijections can be found between these objects and vexillary involutions [GPP01, Wes90]. Furthermore, it was used in the study of lattice paths [BM05] and osculating walks [BM06, BMM08].

4.1 Obtaining a recursive description

As in the chapters before, we will start by finding a recursive description for vexillary involutions. Recall the cycle notation for permutations, which enables us to write a permutation as the product of cycles. A k-cycle, or cycle of length k, $(i_1, i_2, \ldots, i_k)$ is nothing but a permutation of length greater or equal to k that maps i_1 to i_2, i_2 to i_3 and so forth.

Finally, i_k is mapped to i_1 (closing the circle) and the other numbers remain fixed (i.e. they form a 1-cycle).

Now, let $\pi \in \mathrm{V}_n$. To obtain new vexillary involutions of greater length from π, we can add a new fixed point $(n+1)$. Whence we get $\pi' \in \mathrm{V}_{n+1}$, as this insertion does not introduce a 2143-pattern within the new involution.
We may also add a new cycle, of the type $(i, n+2)$ with $1 \leq i \leq n+1$. This is clearly sufficient as involutions only consist of cycles of length at most two, but the result is not necessarily vexillary.

One way to properly define this process is the following: in every cycle of π, regardless of its length (it may be one or two), replace j by $j+1$ if $j \geq i$ and add the new 2-cycle $(i, n+2)$ to obtain the cycle representation of π'. Note that this obviously implies that π' is an involution, too.
Alternatively, one might look at the word representation of π. First, add one to all $j \geq i$. Then shift all the letters to the right by one, starting at the i-th place, and put $n+2$ at position i. Lastly, put i at the end.
For the graphically inclined, in the geometric variant one is required to move all the points on or above the horizontal line $y = i$ up by one unit. Analogously, increase the x-coordinate of the points on or to the right to the vertical line $x = i$ by one (of course, some points satisfy both properties). Lastly, add the points $(i, n+2)$ and $(n+2, i)$.
However, we can not add arbitrary cycles to π and expect to obtain another vexillary involution, as the example below demonstrates. This leads to the following definition, introducing two parameters which are very helpful for the proper construction of new involutions.

Definition 4.6. Let $\pi \in \mathrm{V}_n$. For $1 \leq i \leq n+1$ we say that the site i is active, if the insertion of the cycle $(i, n+2)$ according to the rules given above leads to another vexillary involution of length $n+2$.
Additionally, we denote by q the number of active sites of π and by p the position of the first descent, or more precisely

$$p = \begin{cases} \min\{k \geq 2 : \pi_{k-1} > \pi_k\} & \text{if } \pi \neq 12\ldots n, \\ n+1 & \text{if } \pi = 12\ldots n, \text{ i.e. it does not contain a descent.} \end{cases}$$

Before we move on to state some facts about vexillary involutions and explain why the statistic p is interesting, we will give a short example to demonstrate the construction principles.

Example 4.7. Let $\pi = (15)(46) = 523614 \in \mathrm{V}_6$ and let us insert the cycle (58). Thus, the new involution has the cycle representation $\pi^5 = (1\underline{6})(4\underline{7})\underline{(58)}$ (changes to π are underlined) and our second method gives the equivalent word representation:
$\pi \rightarrow 623714 \rightarrow 6237\ 8\ 14 \Rightarrow \pi^5 = 62378145$.
For the sake of completeness, see the figure below for a demonstration of the graphical method to add a cycle.

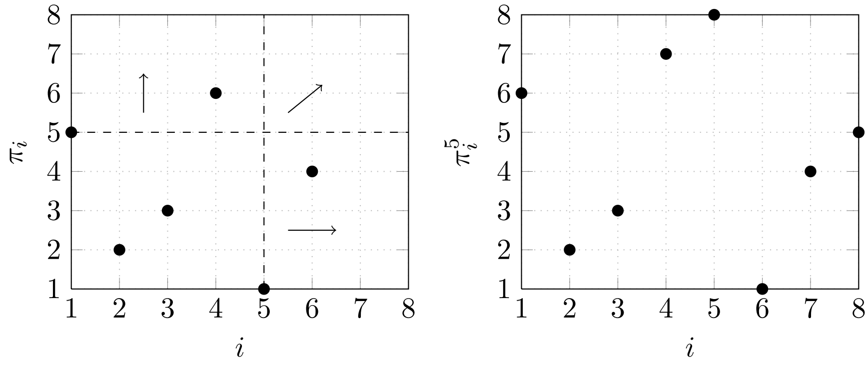

Figure 4.8: Graphical insertion of (58) into π.

Similarily, we can insert the 2-cycles from (18) up to (78) and get the 6 other involutions π^1 up to π^7: $\pi^1 = (18)(26)(57) = 86347251, \pi^2 = (16)(28)(57) = 68347152, \pi^3 = (16)(38)(57) = 62847153, \pi^4 = (16)(48)(57) = 62387154, \pi^6 = (15)(47)(68) = 52371846$, $\pi^7 = (15)(46)(78) = 52361487$. Lastly, we might also add the fixed point at the end, giving $\pi^8 = (15)(46) = 5236147$.
But only π^1, π^2, π^5 (and π^8) are vexillary again, as all the others contain one of the patterns $6287, 5276$ or 5287 which, after proper relabeling, give the inadmissible sequence 2143. Hence, π has the parameters $p = 2$ and $q = 3$.

Observe that the example also shows that active sites are not necessarily consecutive. The next lemma (also see Remark 3.3 in [GPP01]) analyzes the distribution of active sites within a vexillary involution and summarizes some useful statements that we need to know about vexillary involutions for our purposes.

Lemma 4.9. *Let $\pi \in V_n$ with $\pi \neq 12\ldots n$ and parameters p and q. Then the following properties hold:*

(a) All sites i, for $1 \leq i \leq p$, which are to the left of the first descent, are active. This implies $p \leq q$.

(b) The last site $n+1$ is inactive.

(c) Let π' be obtained by adding the fixed point $(n+1)$ to π. Then π' is a vexillary involution of length $n+1$ and all of its sites i, where $i > p$, are inactive.

(d) Let π' be the vexillary involution obtained by inserting the cycle $(i, n+2)$ into an active site i of π. Then the activity of sites j located to the right of $n+2$ in the word representation of π' remains unchanged. That is, the state of site $i < j \leq n+2$ in π' equals the state of $j-1$ in π. Furthermore, if $i > p$, then all sites for $p < j \leq i$ are inactive.

Finally, all sites of the vexillary involution $12\ldots n$ are active, thus it has parameters $p = q = n+1$.

Proof. For (a), let us insert a cycle $(i, n+2)$ into a site i with $1 \le i \le p$ and look at the word representation of the obtained involution. To the left of the newly inserted largest element, $n+2$, the letters are strictly increasing (as they were located to the left of the first descent) and thus $n+2$ can not correspond to letter 4 in the pattern 2143. Now recall that the inverse of a permutation maps each letter to its position within the word representation. In our case it is especially easy since π is an involution. As p indicates the first descent, we have $\pi_1 < \pi_2 < \ldots < \pi_{p-1}$, hence, the positions of the elements up to $p-1$ are increasing, which is to say that these elements form an increasing subsequence of π. Thus, there is no 21-pattern made of elements strictly smaller than i, which implies that it can not correspond to 3 in the pattern 2143.
Statement (b) is trivial, as subsequence $\pi_{p-1}\pi_p(n+2)(n+1)$ is inadmissible.
Statement (c) is clear, too. As we mentioned before, adding the new fixed point does not change the rest of the permutation π. Hence, the new involution is vexillary, as $(n+1)$ can not play the role of the letter 3 in 2143 either. Nevertheless, we can find a subsequence of π' of the type 213, made by the elements $\pi_{p-1}\pi_p(n+1)$. Inserting a cycle $(i, n+3)$, for $p < i < n+2$ thus creates the forbidden pattern 2143 in the form of $\pi_{p-1}\pi_p(n+3)(n+2)$. Additionally, site $n+2$ is inactive because of (b).
Now for (d). Inserting a new cycle according to the rules of this chapter retains the order of the letters - some might be shifted to the right, but small elements stay small and big ones get bigger by the same amount. If we write blocks of corresponding letters on top of each other, the general transformation looks like

$$\begin{array}{llllllll} \pi = \pi_1 & \pi_2 & \ldots & \pi_{i-1} & & \pi_i \; \pi_{i+1} & \ldots \; \pi_n & \\ \Downarrow & & & & & & & \\ \pi' = \pi_1^+ & \pi_2^+ & \ldots & \pi_{i-1}^+ & (n+2) & \pi_i^+ \; \pi_{i+1}^+ & \ldots \; \pi_n^+ & i, \end{array}$$

where $\pi_j^+ = \pi_j$ if $\pi_j < i$, or else $\pi_j^+ = \pi_j + 1$. So, if the 2143 pattern emerges after the insertion of a new cycle $(i, n+2)$, then i must play the role of the 3 or $n+2$ the role of 4, or both. Therefore, let $j > i$ be an inactive site of π' and insert $(j, n+4)$ into it. By definition, we find a 2143 pattern in the new involution π''. If $n+4$ corresponds to 4, then the subsequence looks like $\pi''_{i_1}\pi''_{i_2}(n+4)\pi''_{i_3}$ with $i_1 < i_2 < j < i_3$. After replacing $n+4$ by $n+2$ and subtracting ones from the remaining letters if necessary (depending on whether they were larger than or equal to j), this gives a 2143 pattern within the involution obtained by adding the cycle $(j-1, n+2)$ to π, thus rendering site $j-1$ inactive. The other case follows similarly.
If $i > p$, then we can use the reasoning from (c) again: the insertion of the 2-cycle does not change the order of the letters of the permutation up to and including site p, so we can find a subsequence of type 213 in π' in the form of $\pi'_{p-1}\pi'_p(n+2)$. All the sites $p < j \le i$ must be inactive then, or else we would create a 2143 pattern given by $\pi'_{p-1}\pi'_p(n+4)(n+3)$.
As for the last remark, by inserting a new cycle $(i, n+2)$, for $1 \le i \le n+1$, into the identity, we clearly obtain an involution in which neither $n+2$ can play the role of 4, nor i the role of 3 in 2143. □

With the help of this lemma, it is pretty clear how to adjust the parameters after the insertion of new cycles into a given vexillary involution. This is essential for the inductive description, which is established in the next lemma. It also shows that our method is sufficient to really generate all vexillary involutions. Essentially the same description lead in [GPP01] to a rewriting rule for generating trees of vexillary involutions.

Lemma 4.10 (Inductive description of vexillary involutions, [BM03])**.** *Let π be a vexillary involution of length n. By (p, q) we denote the corresponding pair of parameters.*

- *If $\pi = 12\dots n$, then the insertion of a new fixed point leads to one vexillary involution of length $n+1$ with parameters $(n+2, n+2)$.*
  The insertion of a cycle $(i, n{+}2)$ into an active site $1 \le i \le n{+}1$ leads to $n{+}1$ vexillary involutions of length $n+2$ with parameters $(2, n+2), (3, n+2), \dots, (n+2, n+2)$.

- *If $\pi \neq 12\dots n$, then the insertion of a new fixed point leads to one vexillary involution of length $n+1$ with parameters (p, p).*
  Furthermore, the insertion of a cycle $(i, n+2)$ into an active site of π leads to q vexillary involutions of length $n+2$ with parameters

$$(2, q+1), (3, q+1), \dots, (p+1, q+1), \underbrace{(p, q), (p, q-1), \dots (p, p+1)}_{\text{if } p<q}.$$

Conversely, removing the cycle which contains n (i.e. (n) or (i, n), where $i = \pi_n$) and replacing each remaining letter $j > i$ by $j-1$ gives a vexillary involution of length $n-1$ respectively $n-2$.

Proof. Most of the work for this proof was already done in Lemma 4.9.
Adding a new fixed point to $\pi = 12\dots n$ simply leads to the identity permutation of length $n+1$ with known parameters. All sites of π are active, thus giving $n+1$ new vexillary involutions. So, let us insert a cycle $(i, n+2)$. Clearly, the first descent will be at position $i+1$ (right after the letter $n+2$). By the aforementioned lemma, the $i+1$ sites to the left of it (including i sites of π plus the site of $n+2$) are all active and activity of the remaining $n+1-i$ sites of π does not change to the right of the inserted letter $n+2$. Summing, we obtain $n+2$ active sites. This holds for all values $i \in \{1, 2, \dots, 1, 2, \dots, n\}$ and gives the statement in the formulation of this lemma.
Now let $\pi \neq 12\dots n$. The first property follows directly from (c) in Lemma 4.9. For the second one, we insert the cycle $(i, n+2)$ and look at the two possible cases:
If $i \le p$, we get a new first descent at position $i+1$. As above, to the right of $n+2$ are $q-i$ sites whose activity does not change, so we get $q+1$ active sites in total.
In the other case, $i > p$ (note that this is equivalent to $p < q$), the first descent remains at position p. By (d) of Lemma 4.9, we may lose some active sites. To be more exact, if we insert the cycle into the j-th active site after the position of the first descent in π, we lose $j-1$ active sites to the left of it. Thus, depending on the value i, zero up to $q-p-1$ of the q active sites in π become inactive.
Of course, the method described in this chapter also works in the opposite direction. If π does not contain 2143, then removing the cycle which contains n can not add this pattern.

Indeed, all the remaining elements (after subtracting one if necessary) retain their order with respect to each other. □

As a remark, no vexillary involution is constructed twice with our method, as the starting permutations differ (an insertion of a fixed point or a cycle does not change that).

4.2 Obtaining a functional equation

After finding an inductive description in the last section, we can now basically stop thinking about vexillary involutions and start working with generating functions. As usual, the first step will be to get a functional equation which seems to be impossible to solve. The very first step, however, will be to define our generating function.

Definition 4.11. Let $f_{n,p,q}$ be the number of vexillary involutions of length n and the secondary statistics p and q as given in Definition 4.6 and let

$$F(t,x,y) := \sum_{\substack{n\geq 0\\ p,q\geq 1}} f_{n,p,q} t^n x^p y^q$$

be the corresponding generating function.

Now we make use of our construction from Lemma 4.10. For (almost) all of the $f_{n,p,q}$ involutions of the length n and parameters p and q, we obtain new permutations with an increased length and changed parameters, which were explicitly given there. We can express that directly in the language of generating functions by multiplying with our generating variables:

$$f_{n,p,q}\left(\underbrace{t^{n+2}(x^2+x^3+\ldots+x^{p+1})y^{q+1}}_{\text{insertion of } (i,n+2),\ i\leq p}+\underbrace{t^{n+2}x^p(y^{p+1}+y^{p+2}+\ldots+y^q)}_{\text{insertion of } (i,n+2),\ i>p}+\underbrace{t^{n+1}x^py^p}_{\text{insertion of } (n+1)}\right).$$

The only exception is $12\ldots n$, for which the term to multiply with is given by

$$\underbrace{t^{n+2}(x^2+x^3+\ldots+x^{n+2})y^{n+2}}_{\text{insertion of } (i,n+2)}+\underbrace{t^{n+1}x^{n+2}y^{n+2}}_{\text{insertion of } (n+1)}.$$

We will compensate the slight difference to the usual scheme (which actually only occurs when adding a new fixed point) later on. Finally, we must not forget the empty involution. It is obviously vexillary, and has parameters $p=1$, $q=1$, giving the term xy.
To carry out the inductive construction, we sum over all possible values for $n\geq 0$ and $p,q\geq 1$. Thus, we recover all vexillary involutions, or, in other words, our generating function $F(t,x,y)$, leading to the equation

$$F(t,x,y) = xy + \sum_{\substack{n\geq 0\\ p,q\geq 1}}\left(f_{n,p,q}\left(t^{n+2}x^2\frac{1-x^p}{1-x}y^{q+1}+t^{n+2}x^py^{p+1}\frac{1-y^{q-p}}{1-y}+t^{n+1}x^py^p\right)\right.$$
$$\left.-t^{n+1}x^{n+1}y^{n+1}(1-xy)\right), \tag{4.12}$$

where we applied the formula for a finite geometric series. The last term $t^{n+1}x^{n+1}y^{n+1}(1-xy) = -t^{n+1}x^{n+1}y^{n+1} + t^{n+1}x^{n+2}y^{n+2}$ handles the special case $12\dots n$ where $p = q = n+1$ (note that $f_{n,n+1,n+1} = 1$ holds) by subtracting the incorrect and adding the correct terms.

Of course, this is not really a nice functional equation to work with. The following lemma will transform it into a shape which is very similar to the other ones we have already encountered so far.

Lemma 4.13 ([BM03])**.** *The formal power series $F(t,x,y)$, given in Definition 4.11, is the unique solution of*

$$\left(1 + \frac{t^2x^2y}{1-x} + \frac{t^2y}{1-y}\right)F(t,x,y) = \frac{xy(1-t)}{1-txy} + t\left(1 + \frac{ty}{1-y}\right)F(t,xy,1) + \frac{t^2x^2y}{1-x}F(t,1,y).$$

Proof. The proof is merely a matter of rewriting (4.12) in a more fashionable way. We reformulate the right hand side by plugging in the definition of $F(t,x,y)$:

$$\begin{aligned} F(t,x,y) =& xy + \frac{t^2x^2y}{1-x}\sum_{\substack{n\geq 0\\ p,q\geq 1}} f_{n,p,q}t^n(1-x^p)y^q + \frac{t^2y}{1-y}\sum_{\substack{n\geq 0\\ p,q\geq 1}} f_{n,p,q}t^nx^py^p(1-y^{q-p}) \\ &+ t\sum_{\substack{n\geq 0\\ p,q\geq 1}} t^nx^py^p - txy\sum_{n\geq 0}(txy)^n + \sum_{n\geq 1} t^n(xy)^{n+1} \\ \iff F(t,x,y) =& \frac{t^2x^2y}{1-x}F(t,1,y) - \frac{t^2x^2y}{1-x}F(t,x,y) + \frac{t^2y}{1-y}F(t,xy,1) - \frac{t^2y}{1-y}F(t,x,y) \\ &+ tF(t,xy,1) - \frac{txy}{1-txy} + \frac{xy}{1-txy}. \end{aligned}$$

Hence, bringing all the $F(t,x,y)$ terms to the left hand side gives the equation as in the statement of the lemma. ☐

As before, this is just another (implicit) definition of the function and it is equivalent to the recursion. Although there is no immediate way to solve the equation and obtain one of its variables, it looks like the usual Kernel form. That is, it is actually a linear combination of the main formal power series and some of its specializations, which do not depend on all the catalytic variables at once. The Kernel is given as the coefficient (or denominator) of the general generating series $F(t,x,y)$.
Indeed, it is another prototype for certain classes of equations, with more examples given in [BM03]. Some of these are astonishingly similar to this one, especially for vexillary permutations (not involutions) or of permutations avoiding 1234 - essentially the same Kernel occurs in the equations for their generating functions (the only adjustment necessary is to replace t^2 by t). The applications mentioned at the beginning of this chapter, which lie outside the study of pattern permutations (for example counting lattice paths), are of a nearly identical type, too.

These are good news, obviously, as we may try our earlier method of setting the Kernel to zero again, and hope to recover the missing information we need. On the other hand, it is clear that it will be substantially more difficult in this case. There are now three unknowns, the main series and two of its offsprings, as well as two catalytic variables involved, unlike in the earlier chapters where we only had to consider one derivation of the generating function and one variable fixed to a special value.

This is where a new flavor of the Kernel method comes into play to provide more relations between the occurring unknowns, some of which might help to obtain explicit clues about our generating function. This will not be enough, however, and we need to extract even more connections (i.e. equations) by looking at the positive parts of the involved series. This second part will be easier if we substitute the variables x and y. As the term xy needs to be plugged into F in the equation above, it is very natural to define a new variable $z := xy$. This will still not suffice, however, as the goal is to apply the following observation.

Lemma 4.14 ([BM05])**.** *Let $G_1(t,\bar{x}), G_2(t,\bar{x})$ and $F(t,u,v)$ be Laurent series in t, with the following properties:*
F has coefficients in $\mathbb{C}[u,v]$ and is symmetric in u,v, i.e., $F(t,u,v) = F(t,v,u)$. The coefficients of $G_1(t,\bar{x})$ and $G_2(t,\bar{x})$ are in $\mathbb{C}[x,\bar{x}]$. Additionally, it holds that the elementary symmetric functions $G_1 + G_2$ and G_1G_2 are polynomials in $\mathbb{C}[\bar{x}]$ without a constant term (that is, only negative powers of x occur).
Then the series $F(t, G_1(t,\bar{x}), G_2(t,\bar{x}))$, if well defined, is a Laurent series in t with polynomial coefficients in $\bar{x}$. Furthermore, if viewed as a power series in $\bar{x}$, the constant term is given by $F(t,0,0)$.

Proof. As F is symmetric in u,v, its coefficients must be symmetric polynomials (in u,v). These can be written as polynomials in the elementary symmetric functions $u+v$ and uv with coefficients in $\mathbb{C}$ (this is, of course, true for any number of variables, with an appropriately defined notion of "elementary" - see e.g. [Sta99b] for more details).
So, if we plug G_1 and G_2 into F, then the coefficients are indeed polynomials in $\bar{x}$, given that this is true for $G_1 + G_2$ and G_1G_2. Clearly, the constant term in $\bar{x}$ can be obtained by setting $u = v = 0$ as $G_1 + G_2$ and G_1G_2 only involve positive powers of $\bar{x}$ and do not contribute. □

This lemma, albeit simple, is very important in a number of Bousquet-Mélou's papers (besides the paper on which this chapter is based on, it occurs in, e.g., [BM05, BM02]). It provides a method to quickly extract the constant term and subsequently the positive part of certain series, giving more information to work with. We will explain later how the change of variables helps exactly to make use of this lemma, but basically at some point of our computations it would become natural to make a substitution. Hence, let us introduce two new variables and apply the transformation to the functional equation in Lemma 4.13 below.

Lemma 4.15. *Let u, v be two new variables such that $x = (1+\bar{u})/(1+v)$ and $y = 1+v$. Then the generating function F satisfies the equation*

$$\begin{aligned} &K(t,u,v)F\left(t, \frac{1+\bar{u}}{1+v}, 1+v\right) \\ &= \frac{uv(uv-1)(1+u)(1-t)}{u(1-t)-t} + t(uv-1)(v(1-t)-t)G(u) + t^2(1+u)^2H(v), \end{aligned}$$

where the Kernel is given by $K(t,u,v) = uv(uv-1) + t^2(u+v+3uv-u^2v^2)$ and the specializations of F are $G(u) = uF(t, 1+\bar{u}, 1)$, as well as $H(v) = vF(t,1,1+v)$.

Proof. We start by dividing the functional equation we obtained earlier by t^2y and plugging in the newly defined variables. This gives

$$\begin{aligned} &\left(\frac{1}{t^2(v+1)} + \frac{(1+u)^2}{u(uv-1)(1+v)} - \frac{1}{v}\right) F\left(t, \frac{1+\bar{u}}{1+v}, 1+v\right) \\ &= \frac{(1-t)(1+u)}{t^2(1+v)(u(1-t)-t)} + \left(\frac{1}{t(1+v)} - \frac{1}{v}\right) F(t, 1+\bar{u}, 1) + \frac{(1+u)^2}{u(1+v)(uv-1)} F(t,1,1+v). \end{aligned}$$

Now multiply by the common denominator of the left hand side, $t^2uv(1+v)(uv-1)$, whence we obtain the Kernel as the coefficient of F:

$$\begin{aligned} &\left(uv(uv-1) + t^2v(1+u)^2 - t^2u(1+v)(uv-1)\right) F\left(t, \frac{1+\bar{u}}{1+v}, 1+v\right) \\ &= \left(uv(uv-1) + t^2(u+v+3uv-u^2v^2)\right) F\left(t, \frac{1+\bar{u}}{1+v}, 1+v\right). \end{aligned}$$

On the right hand side we obtain

$$\frac{uv(uv-1)(1+u)(1-t)}{u(1-t)-t} + tu(uv-1)(v-t(1+v))F(t, 1+\bar{u}, 1) + t^2v(1+u)^2F(t,1,1+v).$$

Putting both sides together and introducing $G(u)$ and $H(v)$ yields the functional equation as presented above. □

Note that the Kernel is symmetric after the substitution of x and y (whereas it would not be if we continued without the change of variables - see the remark at the end of this chapter). This is a nice coincidence and will make things easier during the coming computations (because the roots of the Kernel for u are essentially the same ones as for v). In Figure 4.16 the algebraic curve defined by the equation $K(t,u,v) = 0$ is shown for some specific values of t. Note how the symmetry of the Kernel is translated in the picture into a symmetry with the main diagonal line as axis.

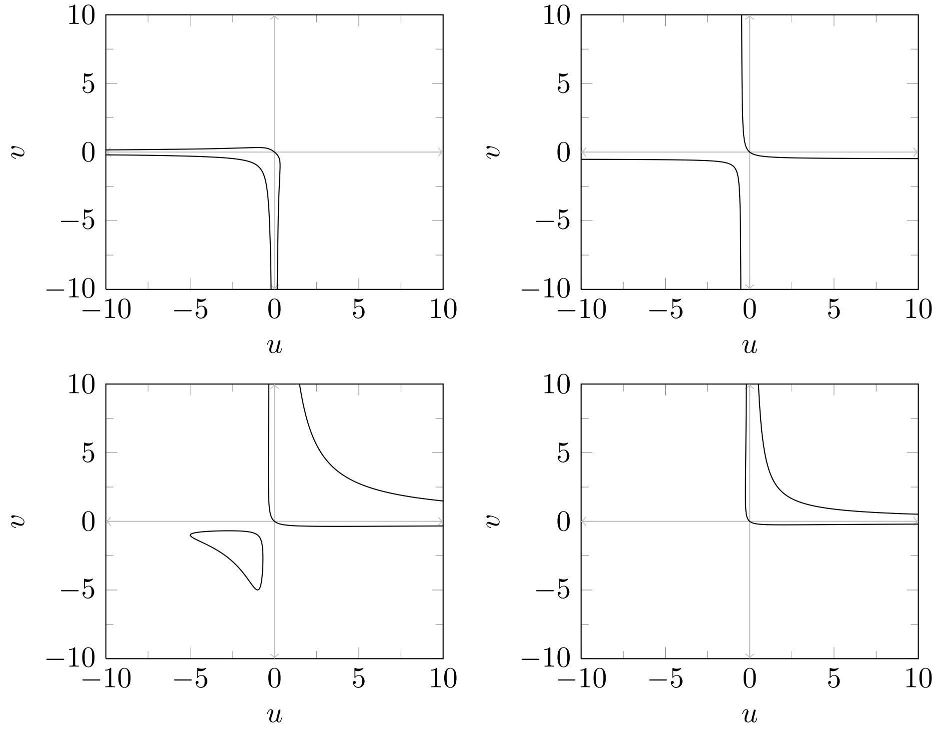

Figure 4.16: Algebraic curve defined by the Kernel $K(t, u, v)$, for various values of t. (Figures in top row: $t = 0.5$ and $t = 1$, bottom row: $t = \sqrt{1.25}$ and $t = 5$)

4.3 The obstinate Kernel method

Now that we have found a functional equation for our generating function F, we can proceed by applying the standard Kernel method. The Kernel $K(v) = v^2u^2(1-t^2)+v(t^2(1+3u)-u)+t^2u$ is a quadratic polynomial in v, so, for fixed u and t we can easily find its roots using the standard formula. After applying some minor algebraic transformations, such as factorizing and reducing the fraction, we obtain

$$V_{1,2}(u) = \frac{1 - t^2\bar{u} - 3t^2 \mp \sqrt{(1 - t^2(1 + \bar{u}))(1 - 5t^2 - 4t^2u - t^2\bar{u})}}{2u(1 - t^2)}.$$

Since we want to plug them into the Kernel to set it to zero, we need to check if they are proper formal power series in t and if $F\left(t, \frac{1+\bar{u}}{1+V_i}, 1 + V_i\right)$, $i \in \{1, 2\}$, is well defined, too. A quick analysis is enough to ensure the first point:

Both roots can be written as the product of the geometric series $1/(1 - t^2)$ and a power series in t, whose expansion is essentially given by the binomial series of the square root (with some additional terms). This latter series has polynomial coefficients in $\mathbb{Z}[\bar{u}, u]$. Additionally, by setting $t = 0$ we observe that V_2 (having a positive sign before the square root) has a constant term, given by $\bar{u}$, while V_1 does not. This is clear, since the constant term of the aforementioned binomial series vanishes after subtracting it from one in the numerator. Thus, the first root starts at t^2.

Now for the second point, which calls for a closer look. The composition of (multivariate) formal power series is (in general) not defined, if at least one of the substituted series has a constant term not equal to zero (as it is clearly the case for $1 + V_{1,2}$). However, recall our Definition 4.11 of the main generating function and that $1 \leq p \leq q \leq n+1$ holds according to Lemma 4.9. Therefore, after replacing x and y, F can actually be viewed as a power series in t with polynomial coefficients in $\mathbb{Z}[\bar{u}, v]$ and rewritten as

$$F\left(t, \frac{1+\bar{u}}{1+v}, 1+v\right) = \sum_{n\geq 0}\left(\sum_{q=1}^{n+1}\sum_{p=1}^{q} f_{n,p,q}(1+\bar{u})^p(1+v)^{q-p}\right)t^n.$$

This enables us to read off coefficients for all $n \in \mathbb{N}$ after we carry out the substitution:

$$[t^n]\, F\left(t, \frac{1+\bar{u}}{1+V_i(t)}, 1+V_i(t)\right) = \sum_{i=0}^{n}\sum_{q=1}^{i+1}\sum_{p=1}^{q} f_{n,p,q}(1+\bar{u})^p\left[t^i\right](1+V_j(t))^{q-p},$$

where $j \in \{1, 2\}$. All of the occurring sums are finite and determining $\left[t^i\right]$ is possible, since the term $(1 + V_j(t))^{q-p}$ is a finite power of a formal power series and thus a formal power series itself. It also has polynomial coefficients in u and $\bar{u}$, so we can proceed to read off coefficients for fixed powers of $u, \bar{u}$ and v. Hence, $[t^n\bar{u}^p v^q]\, F\left(t, (1+\bar{u})/(1+V_j(t)), 1+V_j(t)\right)$, for $n, p, q \in \mathbb{N}$, only depends on a finite number of coefficients of F and V_j.
The same argument may be applied if u is replaced by some formal power series with polynomial coefficients (or both, u and v simultaneously).

Also, it is not obvious that $(1 + \bar{u})/(1 + V_{1,2})$ actually has a power series expansion in t. Now, if R is a ring, then a formal power series $Z \in \mathrm{R}[[t]]$ is invertible, that is $1/Z \in \mathrm{R}[[t]]$ holds, if and only if the constant term $[t^0]Z$ is invertible in R (also see the introductory Section 1.3).
In our case, we may choose $\mathrm{R} = \mathbb{Z}[\bar{u}, u]$. For example, $1/V_1$ does not exist as the constant term is zero, while $1/V_2$ has a formal power series expansion (this will become important later on). Likewise, $1/(1 + V_1)$ is a formal power series in t with a constant term one. Hence, the expression $(1 + \bar{u})/(1 + V_1)$ admits a power series expansion with coefficients in the aforementioned ring.
It is a bit more subtle that the same holds if we use V_2 instead. The series $1/(1 + V_2)$ is not well defined, at least for our choice of R (it only has a power series expansion in $\mathbb{Z}((u))[t]$). Its constant term is $1 + \bar{u}$, which is not invertible in $\mathbb{Z}[\bar{u}, u]$. Still, the following computations suggest that this term can be singled out when doing the full substitution:

$$\begin{aligned} V_2 - \bar{u} &= \frac{1 - t^2\bar{u} - 3t^2 + \sqrt{(1-t^2(1+\bar{u}))(1-5t^2-4t^2u-t^2\bar{u})} - 2(1-t^2)}{2u(1-t^2)} \\ &= \frac{-t^2(1+\bar{u}) - 1 + \sum_{i\geq 0}\binom{1/2}{i}(-t)^i(1+\bar{u})^i \cdot \sum_{i\geq 0}\binom{1/2}{i}(-t)^i(5+4u+\bar{u})^i}{2u(1-t^2)}. \end{aligned}$$

Here we simply used the binomial expansion for the square root. The Cauchy product of the two sums has a constant term of one, which is canceled by the one in front of it. If we draw the factor $\bar{u}$ from the denominator into the second sum, we can rewrite

$\bar{u}(5+4u+\bar{u}) = (1+\bar{u})(4+\bar{u})$. This means that the factor $1+\bar{u}$ occurs in both parts of the product. Thus, it can be singled out. In total we have

$$\frac{1+\bar{u}}{1+V_2} = \frac{1+\bar{u}}{(1+\bar{u})V_2'} = \frac{1}{V_2'},$$

where V_2' is the series such that $(1+\bar{u})V_2' = 1+V_2$. It follows that $[t^0]V_2' = 1$.
Together with our result for F above, this ensures that the substitutions for x and y in the main functional equation are valid.

Furthermore, let us take a look at the elementary symmetric functions of the roots. By summing, the square roots cancel each other because of their different signs and we get

$$V_1 + V_2 = \frac{\bar{u}(1-t^2\bar{u}-3t^2)}{1-t^2}. \tag{4.17}$$

On the other hand, since $K(t,u,v) = (v-V_1(t,u))(v-V_2(t,u))/(u^2(1-t^2))$, the product of the roots is given by the constant term of the Kernel (divided by the coefficient of v^2):

$$V_1V_2 = \frac{\bar{u}t^2}{1-t^2}. \tag{4.18}$$

Note that both only involve negative powers of u, which is to say that they are polynomials in $\bar{u}$ with coefficients in $\mathbb{Q}[[t]]$, and that they do not have constant terms. This is one of the main goals we wanted to achieve by transforming our initial variables x, y to u, v. Clearly, this is essential for the application of Lemma 4.14, which will be very helpful below.

We have seen that the pairs $(u, V_1(u))$ and $(u, V_2(u))$ both set the Kernel to zero. Plugging them into the functional equation from Lemma 4.15 is valid and gives us access to two equations involving $G(u)$ and two new, unknown series $H(V_1), H(V_2)$. This does not really solve the situation, as it usually did in the earlier chapters. On the contrary, we still have too many variables and not enough relations to extract any explicit information about them. The standard Kernel method is not sufficient in this case and we need to keep on pushing for more equations, we need to be obstinate.
Bousquet-Mélou states in [BM05] that this next step is inspired by Section 2.4 of the book [FIM99], albeit the context and method is different. We will proceed as follows:

Recall that the Kernel is quadratic in both u and v. Thus, if we have two Laurent series in t, say $(U(t), V(t)) \neq (0,0)$, such that $K(t, U(t), V(t)) = 0$, then we can always produce other pairs which set the Kernel to zero, too. The coefficients of these series lie in an appropriate field, such as $\mathbb{Q}((u, \bar{u}, v, \bar{v}))$.
The (straightforward) key idea is that there are two possible solutions for u respectively v to choose from. To be more specific, define a transformation $\varphi(U,V) := (U', V)$ such that U' is the other root of the Kernel, if viewed as a quadratic polynomial in u. The same applies for v of course: $\psi(U,V) := (U,V')$ where V' is the second root if K is viewed as a polynomial in v.

These actions are particularly easy in our situation, since the Kernel is symmetric in u and v. Hence, if we solve it as a quadratic polynomial in u and for fixed v, we obtain two

roots $U_1(v)$ and $U_2(v)$. Again, let us denote the solution with the negative sign before the square root by U_1. Then the symmetry simply means that $U_1(v,t) = V_1(v,t)$, as well as $U_2(v,t) = V_2(v,t)$, where V_1 and V_2 are given above. In other words, the solutions are equal if we view them as formal series in t.
We also know how to relate the two solutions of $K(t,U,V) = 0$ to each other by looking at their product (4.18). Thanks to the form of the Kernel, both kinds of roots satisfy the same elementary symmetric formulas (one only needs to replace every occurrence of U by V and vice-versa):

$$U_i = \frac{\overline{U_j v} t^2}{1-t^2}, \quad V_i = \frac{\overline{V_j u} t^2}{1-t^2},$$

where $i,j \in \{1,2\}$ such that $i \neq j$. An alternative way to define the new pairs of Laurent series is thus given by:

$$\varphi(U,V) = \left(\frac{\overline{UV}t^2}{1-t^2}, V\right), \quad \psi(U,V) = \left(U, \frac{\overline{UV}t^2}{1-t^2}\right).$$

Indeed, one can easily verify that this procedure gives new pairs which cancel the Kernel:

$$\begin{aligned}
&K\left(t, \frac{\overline{UV}t^2}{1-t^2}, V\right)\\
=&\frac{t^2}{U(1-t^2)}\left(\frac{t^2}{U(1-t^2)} - 1\right) + t^2\left(\frac{t^2}{UV(1-t^2)} + V + \frac{3t^2}{U(1-t^2)} - \frac{t^4}{U^2(1-t^2)^2}\right)\\
=&\frac{t^2}{U^2V(1-t^2)^2}\left(t^2V - UV(1-t^2) + t^2U(1-t^2) + U^2V^2(1-t^2)^2 + 3t^2UV(1-t^2) - t^4V\right)\\
=&\frac{t^2}{U^2V(1-t^2)}(UV(UV-1) + t^2(U+V+3UV-U^2V^2)) = \frac{t^2}{U^2V(1-t^2)}K(t,U,V).
\end{aligned}$$

Therefore, under our assumption that the series U, V are not equal to 0 and that $K(t,U,V) = 0$, the Kernel also vanishes when we plug in the new pair we obtain by applying φ. Clearly, the same computations work for ψ as well (after switching the roles of U and V).
Note that these transformations actually depend on the Kernel only and not on the explicit knowledge of its roots. The reason is that the elementary symmetric functions of the roots can be expressed in terms of the coefficients of the Kernel.

Now, we already know two pairs which satisfy the properties we are looking for. Let us start with the pair (u, V_1) and see which pairs we can produce by applying the two previously defined transformations. Obviously they are involutions, so we shall not apply the same action twice in a row. Diagram 4.19 displays the orbits of both actions, similar to Figure 6 in [BM03].

The rather abstract description above has a very intuitive geometric interpretation. Recall that the equation $K(t,u,v) = 0$ describes a geometric curve, which consists of multiple branches. Let us fix t and choose a starting point on the curve, say (u_0, v_0) (or, choose u_0 only and then obtain the second coordinate by plugging it into one of the roots $V_1(u)$ or $V_2(u)$). By applying our transformations, we simply travel parallel to the axes to find

$$
\begin{tikzcd}
 & & (u,V_1) \arrow[dl, <->, "\varphi"'] \arrow[dr, <->, "\psi"] & & \\
\left(\frac{\overline{uV_1}t^2}{1-t^2}, V_1\right) = & (V_2,V_1) \arrow[d, <->, "\psi"'] & & (u,V_2) \arrow[d, <->, "\varphi"] & = \left(u, \frac{\overline{uV_1}t^2}{1-t^2}\right) \\
\left(V_2, \frac{\overline{V_2V_1}t^2}{1-t^2}\right) = & (V_2,u) \arrow[dr, <->, "\varphi"'] & & (V_1,V_2) \arrow[dl, <->, "\psi"] & = \left(\frac{\overline{uV_2}t^2}{1-t^2}, V_2\right) \\
\left(\frac{\overline{V_2u}t^2}{1-t^2}, u\right) = & & (V_1,u) & & = \left(V_1, \frac{\overline{V_1V_2}t^2}{1-t^2}\right)
\end{tikzcd}
$$

Figure 4.19: Pairs produced by applying φ and ψ.

new points on the curve. To be more precise, φ changes the u-coordinate of the point while v remains unchanged, and the other way around for ψ. Figure 4.20 (corresponding to Figure 6 in [BM03]) shows a (closed) path described by tracing these transformations, switching from one branch of the curve to another. It corresponds to the (rounded) values $(u_0, v_0) = (-3, 0.675) \overset{\psi}{\to} (-3, -0.475) \overset{\varphi}{\to} (0.675, -0.475) \overset{\psi}{\to} (0.675, -3) \overset{\varphi}{\to} (-0.475, -3) \overset{\psi}{\to} (-0.475, 0.675) \overset{\varphi}{\to} (u_0, v_0)$. While all of the 6 pairs within the hexagon above set $K(t, U, V)$

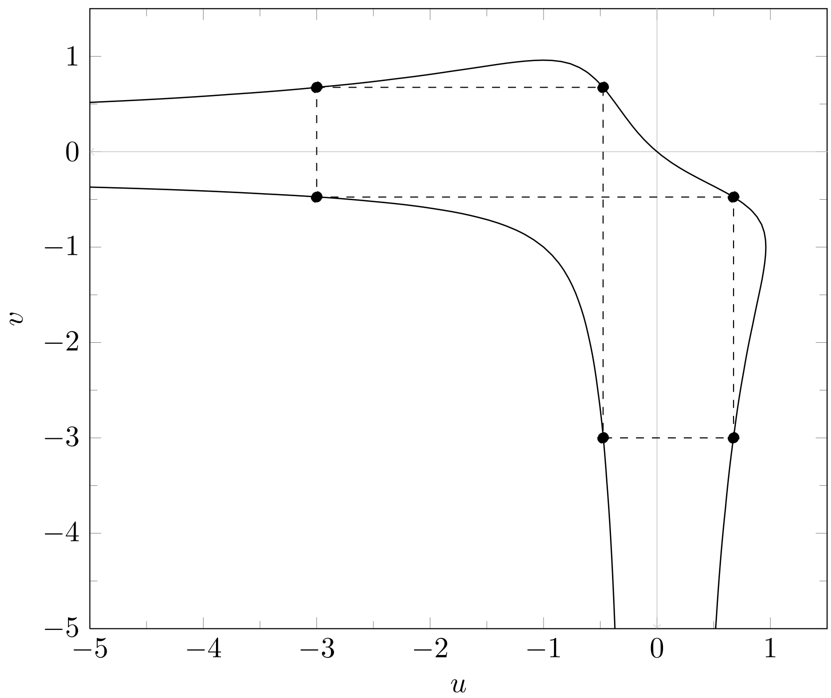

Figure 4.20: Tracing the transformations φ and ψ for $t = 0.7$ and a starting value $u_0 = -3$.

to zero, not all of them can be used in the equation from Lemma 4.15. It is not ensured that all of the involved series are still well defined as formal power series in t after applying the substitutions. Thus, as we did before for (u, V_1) and (u, V_2), we have to check this again.
Keep in mind that $1/V_2, 1/(1+V_1), (1+\bar{u})/(1+V_2) \in \mathbb{Q}[u,\bar{u},v,\bar{v}][[t]]$, as we also showed there. Furthermore, we also know already that for all the following pairs, the replacements for y admit power series expansions.

(V_2, V_1): The substitutions looks like $x = (1+1/V_2)/(1+V_1)$. This case is simple, as all of the involved reciprocals exist as formal power series in t.

(V_2, u): Or $x = (1+1/V_2)/(1+u)$. Here $1/(1+u)$ is not an element of $\mathbb{Q}[u,\bar{u}]$. But it holds that

$$\frac{1+\frac{1}{V_2}}{1+u} = \frac{1+V_2}{(1+u)V_2} = \frac{(1+\bar{u})V_2'}{(1+u)V_2} = \frac{1}{V_2}\bar{u}V_2',$$

where V_2' is again defined such that $(1+\bar{u})V_2' = 1+V_2$. In this form it is immediate that the substitution is valid.

(V_1, u): Or $x = (1+1/V_1)/(1+u)$. But the series $V_1 \cdot (1+u)$ does not have a constant term (as V_1 starts at t^2) and so is not invertible. Therefore $(V_1+1)/(V_1 \cdot (1+u)) = (1+1/V_1)/(1+u)$ is not a proper formal power series in t. We must not replace x by this expression.

(V_1, V_2): Or $x = (1+1/V_1)/(1+V_2)$. Similarly, this substitution involves the series $V_1 \cdot (1+V_2)$ which is not invertible due to the same reasons as in the point above. The exchange of x and $(1+V_1)/(V_1 \cdot (1+V_2)) = (1+1/V_1)/(1+V_2)$ is not possible.

So, by being obstinate we found two more pairs such that the Kernel vanishes. We proceed as in the chapters before by plugging the 4 admissible solutions $(u, V_1), (u, V_2), (V_2, V_1), (V_2, u)$ into the functional equation for vexillary involutions in Lemma 4.15. As it was our goal, this gives us the following system of equations (4.21) in which only the specializations of our main generating function, the series G and H, occur (at special values). If we had used the standard Kernel method, we would merely have produced I or II, yielding little helpful information.

$$\begin{aligned}
\text{I:}\quad & \frac{uV_1 \cdot (uV_1-1)(1+u)(t-1)}{u(1-t)-t} && = t(uV_1-1)(V_1 \cdot (1-t)-t)G(u) + t^2(1+u)^2H(V_1) \\
\text{II:}\quad & \frac{uV_2 \cdot (uV_2-1)(1+u)(t-1)}{u(1-t)-t} && = t(uV_2-1)(V_2 \cdot (1-t)-t)G(u) + t^2(1+u)^2H(V_2) \\
\text{III:}\quad & \frac{V_2V_1 \cdot (V_2V_1-1)(1+V_2)(t-1)}{V_2 \cdot (1-t)-t} && = t(V_2V_1-1)(V_1 \cdot (1-t)-t)G(V_2) + t^2(1+V_2)^2H(V_1) \\
\text{IV:}\quad & \frac{V_2u(V_2u-1)(1+V_2)(t-1)}{V_2 \cdot (1-t)-t} && = t(V_2u-1)(u(1-t)-t)G(V_2) + t^2(1+V_2)^2H(u)
\end{aligned} \tag{4.21}$$

Even though this procedure provides more relations between our generating series, it is still not enough. There are now 5 unknowns in these 4 equations and thus, it is still not possible to solve the system with the usual algebraic methods. It seems that the problem was only delayed, but not solved. However, as mentioned before, there is a second, rather creative step introduced by Bousquet-Mélou.

4.4 Towards a formula for the generating function

In this section we will obtain even more information about the generating function of vexillary involutions. We will do this by looking at the positive parts of the involved series, as defined in the introduction. To do this, our goal is to form nice relations from system (4.21) so that this can be done easily. This is where Lemma 4.14 finally comes into play. We will build symmetric functions in V_1 and V_2 and apply the aforementioned lemma.

For the first relation we eliminate $G(u)$ from equations I and II of (4.21). This can be done in the following way:

$$\begin{aligned}
&\mathrm{I}\cdot(uV_2-1)(V_2\cdot(1-t)-t)-\mathrm{II}\cdot(uV_1-1)(V_1\cdot(1-t)-t)\\
\iff\quad &\frac{u(1+u)(t-1)}{u(1-t)-t}(uV_1-1)(uV_2-1)(V_1\cdot(V_2\cdot(1-t)-t)-V_2\cdot(V_1\cdot(1-t)-t))\\
=\quad &t^2(1+u)^2((uV_2-1)(V_2\cdot(1-t)-t)H(V_1)-(uV_1-1)(V_1\cdot(1-t)-t)H(V_2))
\end{aligned} \tag{4.22}$$

Of course, this expression can be simplified a lot further. The expression $(uV_1-1)(uV_2-1)$ will be an important one, so let's start here. Recall equations (4.17) and (4.18) as the elementary symmetric functions of the roots of the Kernel will be useful here.

$$\begin{aligned}
(uV_1-1)(uV_2-1)=u^2V_1V_2-u(V_1+V_2)+1&=\frac{t^2u}{1-t^2}-\frac{1-t^2\bar{u}-3t^2}{1-t^2}+1\\
&=\frac{t^2(u+\bar{u}+2)}{1-t^2}=\frac{t^2\bar{u}(1+u)^2}{1-t^2}.
\end{aligned} \tag{4.23}$$

Additionally, we have $(V_1\cdot(V_2\cdot(1-t)-t)-V_2\cdot(V_1\cdot(1-t)-t))=t(V_2-V_1)$. Thus, after dividing by $t^2(1+u)^2$, we obtain the left hand side

$$\frac{u(1+u)(t-1)}{u(1-t)-t}\cdot\frac{t^2\bar{u}(1+u)^2}{1-t^2}\cdot\frac{t}{t^2(1+u)^2}(V_2-V_1)=\frac{-t(1+u)}{(1+t)(u(1-t)-t)}(V_2-V_1).$$

Lastly, we put both sides together and bring $V_1-V_2=-(V_2-V_1)$ to the right:

$$\frac{t(1+u)}{(1+t)(u(1-t)-t)}=\frac{(uV_2-1)(V_2\cdot(1-t)-t)H(V_1)-(uV_1-1)(V_1\cdot(1-t)-t)H(V_2)}{V_1-V_2} \tag{4.24}$$

The second symmetric expression will be a little more complicated. We start by repeating exactly the same computations as for the first two equations in order to get rid of $G(V_2)$ in III and IV:

$$\mathrm{III}\cdot(uV_2-1)(u(1-t)-t)-\mathrm{IV}\cdot(V_1V_2-1)(V_1\cdot(1-t)-t).$$

The equation we obtain is virtually the same as (4.22) and leads to a new version of (4.24), only with switched roles of u and V_2.

$$\frac{t(1+V_2)}{(1+t)(V_2\cdot(1-t)-t)} = \frac{(uV_2-1)(u(1-t)-t)H(V_1)-(V_2V_1-1)(V_1\cdot(1-t)-t)H(u)}{V_1-u} \tag{4.25}$$

As a remark, the involved equations stem from the pairs (V_2, u) and (V_2, V_1) which set the Kernel to zero. Thus, for the fixed value V_2 for u, the two roots for v are V_1 and u, which must satisfy the same equations as in (4.17) and (4.18) (again, after the replacement of u with V_2 and vice versa). Therefore the calculations can be performed as before and the relation above holds.

We combine these last two equation now, such that V_1 and V_2 play symmetric roles. To this end, we compute

$$\begin{gathered}(4.24)\cdot(1+t)(u(1-t)-t)(V_1-V_2)-2\cdot(4.25)\cdot(1+t)(V_2\cdot(1-t)-t)(V_1-u)\\ \iff \qquad t(1+u)(V_1-V_2)-2t(1+V_2)(V_1-u)\\ =-(1+t)(u(1-t)-t)\big((uV_2-1)(V_2\cdot(1-t)-t)H(V_1)-(uV_1-1)(V_1\cdot(1-t)-t)H(V_2)\big)\\ +2(1+t)(V_2V_1-1)(V_1\cdot(1-t)-t)(V_2\cdot(1-t)-t)H(u).\end{gathered}$$

This pretty long expression is subject to various simplifications, thanks to the known relations of the roots. It is also not yet immediate that it is actually symmetric. We begin by taking a look at the coefficients of $H(u)$ and start by simply plugging in the product into

$$V_1V_2-1=\frac{\bar{u}t^2}{1-t^2}-1=\frac{t^2(1+\bar{u})-1}{1-t^2}. \tag{4.26}$$

For the rest, we have

$$\begin{aligned}(1+t)(V_1\cdot(1-t)-t)(V_2\cdot(1-t)-t)&=(1+t)(V_1V_2\cdot(1-t)^2-t(1-t)(V_1+V_2)+t^2)\\ =(1+t)\left(\frac{t^2\bar{u}(1-t)}{1+t}-\frac{t\bar{u}(1-t^2\bar{u}-3t^2)}{1+t}+t^2\right)&=t^2\bar{u}(1-t)+t^2(1+t)-t\bar{u}(1-t^2\bar{u}-3t^2)\\ &=t\bar{u}(t+2t^2+tu+t^2u+t^2\bar{u}-1).\end{aligned} \tag{4.27}$$

Now we divide the whole equation by V_1V_2-1 in the form we have just derived. While not obvious, this will remove the occurrences of the roots on the left hand side:

$$\begin{aligned}&\frac{t(1+u)(V_1-V_2)-2t(1+V_2)(V_1-u)}{V_1V_2-1}\\ &\qquad=\frac{t(1-t^2)}{t^2(1+\bar{u})-1}(u(V_1+V_2)-(V_1+V_2)-2V_1V_2+2u)\\ &\qquad=\frac{t(1-t^2)}{t^2(1+\bar{u})-1}\cdot\frac{1-t^2\bar{u}-3t^2-\bar{u}+t^2\bar{u}^2+3t^2\bar{u}-2t^2\bar{u}+2u(1-t^2)}{1-t^2}\\ &\qquad=t\cdot\frac{t^2(\bar{u}^2-3-2u)-\bar{u}+1+2u}{t^2(1+\bar{u})-1}\end{aligned}$$

Using the factorization $\bar{u}^2 - 3 - 2u = (1+\bar{u})(\bar{u} - 1 - 2u)$ yields

$$t \cdot \frac{t^2(\bar{u}^2 - 3 - 2u) - \bar{u} + 1 + 2u}{t^2(1+\bar{u}) - 1} = t(\bar{u} - 1 - 2u) = t(1+\bar{u})(1-2u).$$

As a last step, we bring $H(u)$ to the left hand side and put all things together to finally obtain the following equation:

$$\begin{aligned} 2t\bar{u}(1 - t - 2t^2 - tu - t^2u - t^2\bar{u})H(u) + t(1+\bar{u})(1-2u) \\ = \frac{(1+t)(u(1-t)-t)(1-t^2)}{1-t^2(1+\bar{u})}((uV_2 - 1)(V_2 \cdot (1-t) - t)H(V_1) \\ + (uV_1 - 1)(V_1 \cdot (1-t) - t)H(V_2)). \quad (4.28) \end{aligned}$$

Indeed, the relation we have obtained is fully symmetric in V_1 and V_2. This is a very nice property but by no means mandatory for the success of the method. In the paper [BM03] this chapter is based on, there are other examples, which demonstrate how to proceed if this symmetry does not hold. One of those are the 1234-avoiding permutations, which share a lot of similarities with the vexillary involutions (as mentioned before, their functional equation has essentially the same Kernel). The difference between these two cases is that in the analog of (4.28), the asymmetric occurrences of the roots on the left hand side can not be removed.
In short, this makes it necessary to analyze this side of the equation in a special way (separating the symmetric and non-symmetric parts). Regardless, the next major steps of the approach presented here still apply (i.e. the extraction of the positive part). As another consequence, though, the generating function of 1234-avoiding permutations is not algebraic but D-finite.

Back to our computations: while the equation is symmetric, it involves no less than three unknown series. So, instead of combining it with other relations to eliminate some of them, we will gather more information in a different way. Namely by comparing the positive parts of both sides, if viewed as Laurent series in u. The other equation (4.24) we formed earlier will then be used to connect the last loose ends and eventually obtain some meaningful relations for H. To this end, we denote

$$H(t,v) = vF(t,1,1+v) = \sum_{i\geq 1} H_i(t)v^i,$$

where the H_i are power series in t with coefficients in $\mathbb{N}$ (these series must be well defined as they are coming from a specialization of the generating function F, which has a combinatorial interpretation).

Let us begin with the left hand side of (4.28). By multiplying with a power of $\bar{u}$, the positive part of H (denoted by $H^{\geq}$) is shifted. To be more specific, for the occurring terms of $\bar{u}$, we have

$$(\bar{u}H)^{\geq}(u) = \sum_{i\geq 0} H_{i+1}u^i = \bar{u}H(u) - H_1,$$

and

$$(\bar{u}^2H)^{\geq}(u) = \sum_{i\geq -1} H_{i+2}u^i = \bar{u}^2H(u) - H_2 - \bar{u}H_1.$$

So, we simply subtract the unnecessary terms and do not forget to add in the contribution from $t(\bar{u} - 1 - 2u)$. This gives the result

$$2t\bar{u}(1 - t - 2t^2 - tu - t^2u - t^2\bar{u})H(u) - 2t(1 - t - 2t^2 - t^2\bar{u})H_1 + 2t^3H_2 - 2tu.$$

Now for the right hand side. Let us restate it in the form

$$\underbrace{(1+t)(u(1-t)-t)(1-t^2)}_{\text{(a)}} \cdot \underbrace{\frac{1}{1-t^2(1+\bar{u})}}_{\text{(b)}} \cdot \widehat{H}(t, V_1, V_2),$$

where $\widehat{H}(t, V_1, V_2) = (uV_2 - 1)(V_2 \cdot (1 - t) - t)H(V_1) + (uV_1 - 1)(V_1 \cdot (1 - t) - t)H(V_2)$. Clearly, $\widehat{H}$ is symmetric in V_1 and V_2. We have seen earlier that the elementary symmetric functions of the roots of the Kernel are polynomials in $\bar{u}$ without a constant term. Thus, the preconditions for Lemma 4.14 are satisfied and eventually it plays its important role. By applying this result, we know that the coefficients of $\widehat{H}$ are in $\mathbb{Q}[\bar{u}]$, thus involving only non-negative powers of $\bar{u}$ (or non-positive of u).
The same goes for the geometric series (b) in the above equation, as well.
So, the only possible way to obtain a positive power of u on the right hand side of equation (4.28) is to multiply the factor $u(1 - t)$ from (a) with the constant terms from the series (b) and $\widehat{H}$ (this product is exactly the constant term of their Cauchy product, too). For the first series it is easy to obtain this term using the geometric series expansion and the binomial theorem:

$$\frac{1}{1-t^2(1+\bar{u})} = \sum_{i\geq 0} t^{2i}(1+\bar{u})^i = \sum_{i\geq 0} t^{2i} \sum_{j=0}^{i} \binom{i}{j} \bar{u}^j = \sum_{j\geq 0} \left(\sum_{i\geq j} \binom{i}{j} t^{2i} \right) \bar{u}^j,$$

after switching the order of summation. Thus, extracting the constant term gives

$$\left[\bar{u}^0\right] \frac{1}{1-t^2(1+\bar{u})} = \sum_{i\geq 0} t^{2i} = \frac{1}{1-t^2}.$$

Lemma 4.14 tells us how to extract the constant term from $\widehat{H}$, too. But again, we need to take a closer look before we simply plug in $V_1 = V_2 = 0$, especially where powers of u or $\bar{u}$ are involved. Hence, we use the definition of H and the usual relations between the roots to reformulate the first of the two symmetric parts:

$$\begin{aligned}
&(uV_2-1)(V_2\cdot(1-t)-t)H(V_1)\\
&\qquad= uV_2^2(1-t)H(V_1)-tuV_2H(V_1)-V_2\cdot(1-t)H(V_1)+tH(V_1)\\
&\qquad= uV_1V_2^2(1-t)H_1+\frac{t^4\bar{u}(1-t)}{(1-t^2)^2}\sum_{i\geq 2}H_iV_1^{i-2}-\frac{t^3}{1-t^2}\sum_{i\geq 1}H_iV_1^{i-1}\\
&\qquad\qquad -\frac{t^2\bar{u}}{1+t}\sum_{i\geq 1}H_iV_1^{i-1}+t\sum_{i\geq 1}H_iV_1^i.
\end{aligned}$$

In the second part $(uV_1-1)(V_1\cdot(1-t)-t)H(V_2)$ the same computations are valid, only the roles of V_1 and V_2 are exchanged. Together they yield $\widehat{H}$, so to obtain the constant term in $\bar{u}$ we can sum all the constant terms of the series involved. Of course we can omit those for which it is immediate that they only feature positive powers of $\bar{u}$, for example those which are multiplied with $\bar{u}$ to begin with. We continue with

$$\begin{aligned}
&\left[\bar{u}^0\right]\widehat{H}(t,V_1,V_2)\\
&=\left[\bar{u}^0\right]uV_1V_2\cdot(V_1+V_2)(1-t)H_1-\left[\bar{u}^0\right]\frac{t^3}{1-t^2}\sum_{i\geq 1}H_i(V_1^{i-1}+V_2^{i-1})+\left[\bar{u}^0\right]t\sum_{i\geq 1}H_i(V_1^i+V_2^i).
\end{aligned}$$

The first part does not contribute, as after plugging in both elementary symmetric functions, the whole term is multiplied by $\bar{u}^2$ (recall the form of the product V_1V_2) and thus (after reducing by u) starts at $\bar{u}$. For the other two terms, we finally set $V_1=V_2=0$ in the equation above. Only the middle one is not zero and gives $\left[\bar{u}^0\right]\widehat{H}=-(2t^3H_1)/(1-t^2)$.

Putting both sides together (remembering to multiply the constant factors on the right hand side), we obtain the new relation

$$\begin{aligned}
&2t\bar{u}(1-t-2t^2-tu-t^2u-t^2\bar{u})H(u)-2t(1-t-2t^2-t^2\bar{u})H_1+2t^3H_2-2tu\\
&\qquad\qquad= u(1+t)(1-t)(1-t^2)\cdot\frac{1}{1-t^2}\cdot\frac{-2t^3}{1-t^2}H_1,
\end{aligned}$$

which, after dividing by $2t$ and bringing everything to one side, can be simplified to

$$\bar{u}(1-t-2t^2-tu-t^2u-t^2\bar{u})H(u)-(1-t-2t^2-t^2\bar{u}-t^2u)H_1+t^2H_2-u=0. \tag{4.29}$$

Again, in this last step two new entities, H_1 and H_2, are introduced. Both are power series in t with coefficients in $\mathbb{N}$. So, we still have to keep on producing more interesting relations, especially concerning these two unknown series. A good starting point for this is equation (4.24). It involves the series H in a very similar manner to equation (4.28), from which we extracted the positive part and ended up with the relation above. In the computations we just did, H_1 and H_2 occurred as constant terms of certain series in $\bar{u}$. This suggests to apply Lemma 4.14 again.

Therefore, with regard to our next steps, we are actually interested to restate (4.24) in terms of $\bar{u}$ instead of u. This can be done by simply dividing both the denominator and numerator by u:

$$\frac{t(1+\bar{u})}{(1+t)(1-t-t\bar{u})}=\frac{(uV_2-1)(V_2\cdot(1-t)-t)H(V_1)-(uV_1-1)(V_1\cdot(1-t)-t)H(V_2)}{V_1-V_2}.$$

We are going to find the constant terms in $\bar{u}$ on both sides and compare them, much like we just did above. First off, it is clear that both sides are formal power series in t with polynomial coefficients in $\bar{u}$. For the right hand side, this follows from our lemma about power series which are symmetric in the roots of the Kernel. For the left hand side, we simply find its expansion as a geometric series:

$$\begin{aligned}\frac{t(1+\bar{u})}{(1+t)(1-t-t\bar{u})} &= \frac{t(1+\bar{u})}{1+t}\cdot\frac{1}{1-t(1+\bar{u})} = \frac{1}{1+t}\sum_{i\geq 0} t^{i+1}(1+\bar{u})^{i+1} \\ &= \frac{1}{1+t}\sum_{i\geq 1} t^i \sum_{j=0}^{i}\binom{i}{j}\bar{u}^j = \frac{1}{1+t}\sum_{j\geq 0}\sum_{i\geq \max(1,j)}\binom{i}{j} t^i\bar{u}^j.\end{aligned}$$

Hence, the constant term can be extracted easily:

$$\left[\bar{u}^0\right]\frac{t(1+\bar{u})}{(1+t)(1-t-t\bar{u})} = \frac{1}{1+t}\sum_{i\geq 1} t^i = \frac{t}{1-t^2}.$$

Now we do basically the same steps as when we extracted $\left[\bar{u}^0\right]\widehat{H}$. Only this time we have to connect the two symmetric parts by a minus and divide by $V_1 - V_2$. This leads to

$$\begin{aligned}&\frac{(uV_2-1)(V_2\cdot(1-t)-t)H(V_1)-(uV_1-1)(V_1\cdot(1-t)-t)H(V_2)}{V_1-V_2} \\ &= \frac{1}{V_1-V_2}\left(uV_1V_2\cdot(V_2-V_1)(1-t)H_1 + \frac{t^4\bar{u}(1-t)}{(1-t^2)^2}\sum_{i\geq 2} H_i\left(V_1^{i-2}-V_2^{i-2}\right)\right. \\ &\left. -\frac{t^3}{1-t^2}\sum_{i\geq 1} H_i\left(V_1^{i-1}-V_2^{i-1}\right) - \frac{t^2\bar{u}}{1+t}\sum_{i\geq 1} H_i\left(V_1^{i-1}-V_2^{i-1}\right) + t\sum_{i\geq 1} H_i\left(V_1^{i}-V_2^{i}\right)\right).\end{aligned}$$

As before, we can omit those expressions which are multiplied by $\bar{u}$ as they will not contribute to $\left[\bar{u}^0\right]$. For the rest, we carry out the division (using the factorization $V_1^k - V_2^k = (V_1-V_2)\sum_{i\geq 0}^{k-1} V_1^i V_2^{k-1-i}$) and plug in the well known relations of the roots. We shift some sums and then the constant term is given by

$$\begin{aligned}\left[\bar{u}^0\right]\frac{-t^2}{1+t}H_1 - \left[\bar{u}^0\right]\frac{t^3}{1-t^2}\sum_{i\geq 0} H_{i+2}\sum_{j=0}^{i} V_1^j V_2^{i-j} + \left[\bar{u}^0\right] t\sum_{i\geq 0} H_{i+1}\sum_{j=0}^{i} V_1^j V_2^{i-j} \\ = \frac{-t^2}{1+t}H_1 - \frac{t^3}{1-t^2}H_2 + tH_1,\end{aligned}$$

after finally setting $V_1 = V_2 = 0$. Lastly, we bring the two sides together:

$$\begin{aligned}\frac{t}{1-t^2} = \frac{-t^2}{1+t}H_1 - \frac{t^3}{1-t^2}H_2 + tH_1 \quad &\Longleftrightarrow \quad \frac{1}{1-t^2} - \left(1-\frac{t}{1+t}\right)H_1 = -\frac{t^2}{1-t^2}H_2 \\ &\Longleftrightarrow \quad \frac{H_1\cdot(1-t)-1}{t^2} = H_2. \qquad (4.30)\end{aligned}$$

As we hoped, this finally provides the connection between the two series we need to obtain some explicit information about H and subsequently the generating function for vexillary involutions.

4.5 The Kernel method again and again. A first result

Now basically everything is laid out to finish our proof, and obtain some explicit expressions for our generating functions H, G and finally F. We will begin to collect the results by using relation (4.30) in equation (4.29). To turn the coefficient of $H(u)$ into a quadratic polynomial in u, we also multiply by u^2. This yields

$$(u - tu - 2t^2u - tu^2 - t^2u^2 - t^2)H(u) + t^2u(2u + 1 + u^2)H_1 - u^2(1 + u) = 0. \tag{4.31}$$

Not surprisingly, the standard flavor of the Kernel method proves to be very useful to tackle this situation. It is the usual setting of a functional equation with a main generating function $H(t, u)$ and only one other unknown series $H_1(t)$. So, starting from the relation in Lemma 4.15, where we first established an equation defining the generating function for vexillary involutions, we have reduced the difficulty of our task significantly. In fact, by so much that we are now in the position to find some formulas for the unknown series involved and unravel the connections we have found in our preceding efforts.

Let us start by finding the roots in u of the coefficient of H, the new Kernel $K_1(u) = u^2t(-1 - t) + u(1 - t - 2t^2) - t^2$:

$$U_{1,2} = \frac{1 - t - 2t^2 \mp \sqrt{(1 - t - 2t^2)^2 - 4t^3(1 + t)}}{2t(1 + t)} = \frac{1 - t - 2t^2 \mp \sqrt{1 - 2t - 3t^2}}{2t(1 + t)}.$$

This time only the first solution U_1 (with the negative sign) is a proper formal power series in t. By computing the expansion of the square root, we observe that it starts with $\sqrt{1 - 2t - 3t^2} = 1 - t - 2t^2 + O(t^3)$. More precisely, we can use the binomial series expansion for $\sqrt{1 - 2t - 3t^2} = \sum_{i\geq 0} \binom{1/2}{i}(-1)^i(2 + 3t)^it^i$ and compute its first three coefficients as a formal power series in t. For $i = 0$, the resulting term is 1, for $i = 1$ it is $\binom{1/2}{1}(-1)(2t + 3t^2) = -t - 3/2 \cdot t^2$ and for $i = 2$ we have $\binom{1/2}{2}(2+3)^2t^2 = -1/2 \cdot t^2 + O(t^3)$. As there are no further contributions due to the multiplication with t^i, summing yields the result.
Thus, the numerator is actually a formal power series in $\mathbb{Q}[[t]]$ which starts at t^3. Multiplication with the series $1/(1 + t) = \sum_{i\geq 0}(-t)^i$ (afterwards, the Cauchy product still starts at t^3) and dividing by t (hence, the result starts at t^2) are therefore possible within the ring of formal power series in t.
On the other hand, this also shows that U_2 (having a positive sign before the square root) only has a Laurent series expansion. The Cauchy product of numerator and $1/(1 + t)$ has the constant term 1 and thus the multiplication with $1/t$ yields a pole at $t = 0$.

Plugging the admissible root U_1 into equation (4.31) sets the Kernel K_1 to zero and gives

$$\begin{aligned} &t^2U_1(1 + U_1)^2H_1 - U_1^2(1 + U_1) = 0 \\ \iff \quad &H_1 = \frac{U_1}{t^2(1 + U_1)} = \frac{1 - t - 2t^2 - \sqrt{1 - 2t - 3t^2}}{t^2(1 + t - \sqrt{1 - 2t - 3t^2})}. \end{aligned}$$

This can be further simplified by multiplying both, the numerator and denominator, by $1+t+\sqrt{1-2t-3t^2}$ and reducing the fraction. This finally provides a nice formula for H_1:

$$H_1(t) = \frac{1-t-\sqrt{1-2t-3t^2}}{2t^2}. \tag{4.32}$$

This result is actually more interesting than it might seem at first. Recall the definition of $H_1(t)$ as the coefficient of v in $H(t,v) = vF(t,1,1+v)$. In other words,

$$F(t,1,1+v) = \frac{H(t,v)}{v} = \sum_{i\geq 0} H_{i+1}(t)v^i \quad \Rightarrow \quad F(t,1,1) = H_1(t).$$

Obviously, $F(t,1,1)$ is nothing but the generating function counting vexillary involutions by their length (by setting the other two arguments to one, the secondary statistics do not matter). Indeed, we have just derived one of the main results we were aiming for, namely that the Motzkin numbers enumerate vexillary involutions, as H_1 is their generating function. We can quickly rederive this result here, applying the procedures we are accustomed to by now.
Note that there are various (more or less equivalent) definitions for Motzkin numbers (many of which can be found in [DS77]). A classical one is the following:

Definition 4.33. Consider the lattice $\mathbb{N}\times\mathbb{N}$. A Motzkin path of length n is defined as a lattice path from the origin $(0,0)$ to $(n,0)$, where one is allowed to move from (n,m) to $(n+1,m+1)$ (north), $(n+1,m-1)$ (south) or $(n+1,m)$ (east), while never crossing the horizontal axis (i.e. if $m=0$ in (n,m), then one can not do a step to the south).
Furthermore, the n-th Motzkin number M_n is the number of Motzkin paths of length n.

This problem is very similar to the one we solved in Section 2.2 of Chapter 2, only the kinds of steps we are allowed to take differ. Since our approach there worked so well, we will try to apply it again as an exercise.

Lemma 4.34. *Let $M(t)$ be the generating function of the Motzkin numbers M_n, that is $M(t) = \sum_{i\geq 0} M_i t^i$. Then*

$$M(t) = H_1(t) = \frac{1-t-\sqrt{1-2t-3t^2}}{2t^2}.$$

Proof. We have already seen the same method more in-depth, so we will be rather quick about our proof this time. Let $a_{n,m}$ be the number of restricted paths from the origin to the point (n,m), where the paths follow the same rules for taking steps as Motzkin paths as in the definition above (only the endpoint does not have to be $(n,0)$).
Additionally, define $a_m(t) := \sum_{n\geq 0} a_{n,m}t^n$. From the description of allowed steps we can derive a recursion for the numbers $a_{n,m}$, which after summing over n implies a recursion for the generating functions $a_m(t)$:

$$\begin{aligned} & a_{n,0} = a_{n-1,0} + a_{n-1,1} \quad \text{and} \quad a_{n,m} = a_{n-1,m-1} + a_{n-1,m} + a_{n-1,m+1}, \quad m \geq 1 \\ \Rightarrow \quad & a_0(t) = 1 + ta_0(t) + ta_1(t) \quad \text{and} \quad a_m(t) = t(a_{m-1}(t) + a_m(t) + a_{m+1}(t)), \quad m \geq 1. \end{aligned}$$

Now introduce the bivariate generating function $A(t,s) := \sum_{m\geq 0} a_m(t)s^m$. This means that we are interested in $M(t) = A(t,0)$. Let us proceed by multiplying the recursion above with s^m and summing for $m \geq 1$, which leads to a functional equation for A.

$$A(t,s) - a_0(t) = \sum_{m\geq 1} \frac{t}{1-t}(a_{m-1}(t) + a_{m+1}(t))s^m$$
$$= \frac{ts}{1-t}A(t,s) + \frac{t}{s(1-t)}(A(t,s) - a_0(t) - sa_1(t)).$$

Now, we plug in $a_0(t) = (1 + ta_1(t))/(1-t)$ on the left hand side (which cancels the term with $a_1(t)$ on the right) and note that we can write $A(t,0) = a_0(t)$. Bringing all the terms with $A(t,s)$ together yields

$$A(t,s)\left(1 - \frac{ts}{1-t} - \frac{t}{s(1-t)}\right) = \frac{1}{1-t} - \frac{t}{s(1-t)}A(t,0)$$
$$\iff \quad A(t,s)(ts^2 - s(1-t) + t) = tA(t,0) - s.$$

Of course, now it is time to apply the Kernel method. The roots of $K(s) = ts^2 - s(1-t) + t$, if viewed as a quadratic polynomial in s, are given by

$$S_{1,2} = \frac{1 - t \mp \sqrt{1-2t-3t^2}}{2t}.$$

We have already established that $\sqrt{1-2t-3t^2} = 1 - t - 2t^2 + O(t^3)$ holds, so it is clear that only the first solution S_1 with the negative sign is a proper formal power series in t (without a constant term), while S_2 is not (having a pole at $t = 0$). Hence, setting $s = S_1$ in the equation above makes the Kernel vanish and gives

$$A(t,0) = \frac{S_1}{t} \quad \Rightarrow \quad M(t) = \frac{1 - t - \sqrt{1-2t-3t^2}}{2t^2} = H_1(t),$$

which finishes the proof. □

Before we continue by extracting the exact formula for the Motzkin numbers M_n from this generating function, we remark that there is a slightly different definition for them, for example found in [FS09]. It stems from the notion of Motzkin trees, which is closely related to the paths of the same name. These trees, also called unary-binary trees, are defined recursively: a Motzkin tree is either a root node only or consists of a root with one or two ordered subtrees attached, both of which are Motzkin trees themselves. Using the symbolic method of combinatorics, one can immediately translate this into a functional equation for the generating function of Motzkin trees. We state it here, as it will prove to be very useful for our own task below.

Definition 4.35. Let $W(t)$ be the unique formal power series in t defined by the relation

$$W = t(1 + W + W^2).$$

Note that W has coefficients in $\mathbb{N}$, which is immediate as it has a combinatorial interpretation. Now we state our first main result as a theorem.

Theorem 4.36 ([BM03]). *The number of vexillary involutions of length n is given by the n-th Motzkin number M_n, which may be written as*

$$M_n = \sum_{i=0}^{\lfloor n/2 \rfloor} \frac{1}{i+1}\binom{n}{2i}\binom{2i}{i} = -\frac{1}{2}\sum_{i=0}^{n+2}\binom{\frac{1}{2}}{i}\binom{\frac{1}{2}}{n+2-i}(-3)^i.$$

Proof. We have already stated that $H_1(t) = F(t,1,1)$ is nothing but the length generating function of vexillary involutions. Reading off its coefficients leads to the second expression. To this end, we remark that $1-2t-3t^2 = (1+t)(1-3t)$ and use this form alongside the binomial series expansion for the square root to obtain

$$\sqrt{(1+t)(1-3t)} = \sum_{n\geq 0}\binom{\frac{1}{2}}{n}t^n \cdot \sum_{n\geq 0}\binom{\frac{1}{2}}{n}(-3)^n t^n = \sum_{n\geq 0}\left(\sum_{i=0}^{n}\binom{\frac{1}{2}}{i}\binom{\frac{1}{2}}{n-i}(-3)^i\right)t^n,$$

by the formula for the cauchy product. The coefficients $[t^0]$ and $[t^1]$ are thus given by 1 respectively -1. Therefore, after subtracting from $1-t$ the resulting series actually starts at t^2. In total, this means that

$$\begin{aligned} H_1(t) &= \frac{1}{2t^2}\left(-t^2\sum_{n\geq 2}\left(\sum_{i=0}^{n}\binom{\frac{1}{2}}{i}\binom{\frac{1}{2}}{n-i}(-3)^i\right)t^{n-2}\right) \\ &= \sum_{n\geq 0}\left(-\frac{1}{2}\sum_{i=0}^{n+2}\binom{\frac{1}{2}}{i}\binom{\frac{1}{2}}{n+2-i}(-3)^i\right)t^n, \end{aligned}$$

and as H_1 is their generating function, the Motzkin numbers are given as the coefficients of t^n.

Now we also want to derive the first, seemingly neater expression. For this, we can use the formal power series $W(t)$, which we defined above by the equation $W = t(1+W+W^2)$. As the next step, we rewrite the relation as $0 = tW^2 + W(t-1) + t$ and compute the roots of the quadratic polynomial in W. We have encountered this polynomial already in Lemma 4.34, where it occurred as a Kernel of a functional equation. However, one should not confuse this step with an application of the Kernel method, as this easy equation, involving only one unknown, can be solved directly by the means of standard algebra. In the previous lemma we found that one of the roots is a formal power series in t and is given by

$$W(t) = \frac{1-t-\sqrt{1-2t-3t^2}}{2t}.$$

Hence, it holds that $tH_1(t) = W(t)$ and we see that W also encodes the Motzkin numbers, only shifted by one (that is, $M_n = [t^{n+1}]\,W$).
Another way to see this is by substituting $t = W/(1+W+W^2)$ into H_1. Note that the formal power series $1+W+W^2$ has a constant term and is thus invertible and additionally, that W starts at t - hence, their product starts at t as well. Therefore, it is a valid exchange of variables and simplifies the square root to $(1-W^2)/(1+W+W^2)$. Which, after reducing, yields $H_1 = W/t$, as expected. Care needs to be taken at this step, though - the other

square root (given by $(W^2-1)/(1+W+W^2)$) must not be used as it leads to the expression $1/(tW)$, which is not a well defined power series in t.
Instead of extracting its coefficients directly, we want to apply the Lagrange inversion formula. In contrast to H_1, this is much easier in this case, due to the form of the functional equation satisfied by W. While we find, by simple computation, that $H_1 = 1+tH_1+t^2H_1$, we can immediately express t in terms of W by $t = W/(1+W+W^2)$. Using Theorem 1.1, this leads to

$$\begin{aligned}
\left[t^0\right] W &= \left[W^0\right] W = 0\\
\left[t^n\right] W &= \frac{1}{n}\left[W^{n-1}\right](1+W+W^2)^n = \frac{1}{n}\left[W^{n-1}\right]\sum_{j=0}^{n}\binom{n}{j}W^j(1+W)^j\\
&= \frac{1}{n}\left[W^{n-1}\right]\sum_{j=0}^{n}\sum_{i=0}^{j}\binom{n}{j}\binom{j}{i}W^{i+j}, \quad n \geq 1.
\end{aligned}$$

Let us introduce a new variable by defining $k := i+j$. Hence, the outer summation, which will be over k, starts at 0 and stops at $2n$. The bounds of the inner sum are given by the constraints of the occurring binomial coefficients:

$$\begin{aligned}
\binom{n}{j} > 0 \quad &\Rightarrow \quad n \geq j = k-i \quad \Rightarrow \quad i \geq \max(k-n,0) \quad \text{and}\\
\binom{j}{i} > 0 \quad &\Rightarrow \quad j = k-i \geq i \quad \Rightarrow \quad \frac{k}{2} \geq i.
\end{aligned}$$

Carrying out this transformation of the variables yields (for $n \geq 1$)

$$\begin{aligned}
\left[t^n\right] W &= \frac{1}{n}\left[W^{n-1}\right]\sum_{k=0}^{2n}\left(\sum_{i\geq\max(k-n,0)}^{\lfloor k/2\rfloor}\binom{n}{k-i}\binom{k-i}{i}\right)W^k\\
&= \frac{1}{n}\sum_{i=0}^{\lfloor (n-1)/2\rfloor}\binom{n}{n-1-i}\binom{n-1-i}{i}.
\end{aligned}$$

To finish the proof, we divide the first binomial coefficient by n and subsequently reduce the factorial $(n-1-i)!$ from both binomial coefficients. Then multiply the denominator and numerator by $(2i)!$ and rearrange the factors:

$$\left[t^n\right] W = \sum_{i=0}^{\lfloor (n-1)/2\rfloor}\frac{(n-1)!}{(i+1)!}\cdot\frac{1}{i!(n-1-2i)!}\cdot\frac{(2i)!}{(2i)!} = \sum_{i=0}^{\lfloor (n-1)/2\rfloor}\frac{1}{i+1}\binom{n-1}{2i}\binom{2i}{i}.$$

Considering that $M_n = \left[t^{n+1}\right] W$, we have thus found the first expression from the statement of our theorem. □

So, we have recovered the result obtained by giving a bijective proof in [GPP01], thus completing Task 4.4. The well known Motzkin numbers are listed as entry A001006 in the online encyclopedia of integer sequences [OEI11], starting with $1, 1, 2, 4, 9, 21, 51, 127, 323, \ldots$

To finish this section, we want to remark two more consequences of the last theorem, besides solving the problem of counting vexillary involutions by their length.
First, it also provides an identity of Motzkin numbers. We obtained this without much extra effort by looking at the same thing (the generating function of these numbers) from two slightly different perspectives. This is, of course, a typical example for a proof of combinatorial identities.
Furthermore, the first expression above yields a connection to the Catalan numbers C_n, which we introduced in Chapter 2 by basically the same means. This result can be reformulated as $M_n = \sum_{i=0}^{\lfloor n/2 \rfloor} 1/(i+1) \cdot \binom{n}{2i} C_i$, a well known relation between these two series of numbers [Ber99].
Thus, the Kernel method proves to be a very nice tool for recovering some interesting results "on the fly", which were usually achieved in a different way.

4.6 A formula for the generating function

Finally, in this section we reach the end of our task to find an expression for the generating function F of vexillary involutions. From now on, it will often be beneficial to remember the relation $t = W/(1 + W + W^2)$ in Definition 4.35. This makes many of the resulting formulas shorter and is one of the reasons we have introduced W above. We start to unravel the connections from the previous sections with the following lemma.

Lemma 4.37. *The formal power series $H(u) = uF(t, 1, 1 + u)$ is given by*

$$H(u) = \frac{uW \cdot (1+u)}{t(1 - uW \cdot (1+W))}.$$

Proof. Now that we know H_1, we can use this information in equation (4.31). Solving for H yields

$$H(u) = \frac{u^2(1+u) - t^2 u(1+u)^2 H_1(u)}{u - tu(1+u) - t^2(2u + u^2 + 1)}.$$

Recall that $H_1 = W/t = 1 + W + W^2$ holds. We proceed by expressing t in terms of W, giving

$$\begin{aligned} H(u) &= \frac{u^2(1+u) - \frac{W^2}{(1+W+W^2)^2} u(1+u)^2(1+W+W^2)}{u - \frac{W}{1+W+W^2} u(1+u) - \frac{W^2}{(1+W+W^2)^2}(1+u)^2} \\ &= \frac{1+u)(u^2(1+W) - uW^2)(1+W+W^2)}{(uW^2 + uW - 1)(W^2 - uW - u)} = \frac{u(1+u)(1+W+W^2)}{(1 - uW \cdot (1+W))}. \end{aligned}$$

Given the relationship of t and W, this is equivalent to the expression in the statement of the lemma. ☐

The other important series involved in the equation from Lemma 4.15 is $F(t, 1 + u, 1)$.

Lemma 4.38. *The formal power series $G(u) = uF(t, 1 + \bar{u}, 1)$ is given by*

$$G(u) = \frac{u(1+u)(uW^2 + t(u + W^3))}{t(u(1-t)-t)(u(1+W)-W^2)}.$$

Proof. We continue to go up our chain of equations. To obtain G from system (4.21), one possibility is to find $H(V_1)$ first. To this end, one could use the third and fourth equation in this system or, more quickly, relation (4.25). The latter one provides an expression for $H(V_1)$, which only involves the known formal power series $H(u)$. We will leave it as it is for now.

$$H(V_1) = \frac{t(1+V_2)(V_1-u) + (V_1V_2-1)(V_1\cdot(1-t)-t)(V_2\cdot(1-t)-t)(1+t)H(u)}{(1+t)(V_2\cdot(1-t)-t)(uV_2-1)(u(1-t)-t)}.$$

Hence, in principle we could compute $H(V_1)$. So, we can use equation I from the system (4.21), yielding

$$G(u) = \frac{-t^2(1+u)^2(u(1-t)-t)H(V_1) - uV_1\cdot(uV_1-1)(1+u)(1-t)}{t(u(1-t)-t)(uV_1-1)(V_1\cdot(1-t)-t)}.$$

Plugging in our lengthy formula $H(V_1)$ (immediately reducing by $(u(1-t)-t)$), gives an even longer expression for $G(u)$. But it is easy to split it up into smaller parts which can be simplified significantly, eventually giving rise to a decent form:

$$\begin{aligned} G(u) = \frac{1}{D}\Big(&-t^2(1+u)^2\Big(\underbrace{t(1+V_2)(V_1-u)}_{\text{(a)}} \\ &+ \underbrace{(V_1V_2-1)(V_1\cdot(1-t)-t)(V_2\cdot(1-t)-t)(1+t)H(u)}_{\text{(b)}}\Big) \\ &- \underbrace{uV_1\cdot(uV_1-1)(1+u)(1-t)(1+t)(V_2\cdot(1-t)-t)(uV_2-1)}_{\text{(c)}}\Big), \end{aligned}$$

where $D = t(1+t)(uV_1-1)(uV_2-1)(u(1-t)-t)(V_1\cdot(1-t)-t)(V_2\cdot(1-t)-t)$ is the common denominator. Recall some equations concerning the roots V_1, V_2 we have encountered earlier, namely (4.23), (4.26) and (4.27). The latter one, similar to the previous lemma, can be restated in terms of W as

$$\begin{aligned}(V_1\cdot(1-t)-t)(V_2\cdot(1-t)-t) &= \frac{t\bar{u}(t^2(2+u+\bar{u}) + t(1+u) - 1)}{1+t} \\ &= \frac{t^3(1-uW\cdot(1+W))(W^2-u(1+W))}{u^2W^2(1+t)}.\end{aligned}$$

This, alongside the first relation for $V_1V_2 - 1$ and the formula for $H(u)$ from Lemma 4.37, can be used to obtain

$$\text{(b)} = \frac{t^2(1+u)(t^2(1+\bar{u})-1)(W^2-u(1+W))}{uW\cdot(1-t^2)}.$$

For part (c), we use (4.23) again: (c) $= t^2V_1 \cdot (1+u)^3(V_2 \cdot (1-t) - t)$. Summing with (a) yields $t^2(1+u)^2$(a) + (c) $= t^2(1+u)^2(tu + tu(V_1+V_2) + V_1V_2 \cdot (1+u(t-1)))$. Here, the well known elementary symmetric functions (4.18) and (4.17) of V_1, V_2 can be applied. Now we bring the whole numerator together, single out $1/(uW \cdot (1-t^2)$ and factorize the remaining terms. All this gives

$$-t^2(1+u)^2((\mathrm{a}) + (\mathrm{b})) - (\mathrm{c}) = -\frac{t^6(1+u)^3(1-uW\cdot(1+W))(uW\cdot(W^2+W+1)+u+W^3)}{u^2W^2(1-t^2)}.$$

The denominator can be reformulated, by simply plugging in the appropriate relations and reducing, as

$$\frac{1}{D} = \frac{u^3W^2(1-t^2)}{t^6(u(1-t)-t)(1+u)^2(1-uW\cdot(1+W))(W^2-u(1+W))}.$$

Hence, the only terms that remain after the multiplication for G are given by

$$G(u) = -\frac{u(1+u)(uW\cdot(W^2+W+1)+u+W^3)}{(u(1-t)-t)(W^2-u(1+W))}.$$

Lastly, we restate $uW\cdot(W^2+W+1)+W^3+u = (uW^2+t(u+W^3))/t$, whence we obtain the expression of $G(u)$ to finish the proof. □

This leads to the final theorem of this chapter, which brings us back to the beginning and the solution for the functional equation we have derived from the inductive description of vexillary involutions. One last time, implications of the Kernel method will help us to provide a neat expression for the resulting generating function.

Theorem 4.39 ([BM03])**.** *The generating function $F(t,x,y)$ of vexillary involutions, counting them by their length, the position of the first descent and the number of active sites is given by*

$$F(t,x,y) = \frac{xy(1-ty(1+W)+t^2xy^2W)}{(1-txy)(1-txyW)(1-ty(1+W))}.$$

Proof. In the last two lemmata we have collected all the necessary informations about the specializations of F, which are involved in the Kernel equation from Lemma 4.15. All that remains is to plug them into this relation and try to simplify the result as much as possible. The starting point for this is

$$\begin{aligned}F\left(t,\frac{1+\bar{u}}{1+v},1+v\right) = \frac{1}{D}\Big(&tuv(1+u)(1-t)(uv-1)(W^2-u(1+W))(1-vW\cdot(1+W))\\ &-tu(1+u)(uv-1)(v(1-t)-t)(uW^2+t(u+W^3))(1-vW\cdot(1+W))\\ &+t^2vW\cdot(1+u)^2(1+v)(u(1-t)-t)(W^2-u(1+W))\Big),\end{aligned}$$

where $D = t(1-vW\cdot(1+W))(u(1-t)-t)(W^2-u(1+W))K(t,u,v)$ is the common denominator this time. Recall that the Kernel is further given by

$K(t,u,v) = uv(uv-1) + t^2(u+v+3uv-u^2v^2)$. As the first small steps we reduce the fraction by t and single out $(1+u)$. Then we substitute $t = W/(1+W+W^2)$ in the numerator and the Kernel to express all occurrences of t in terms of W. This makes it easier to factor the numerator (which has mixed terms in W and t). Indeed, it is not too hard (albeit lengthy) to find this factorization, as we already know one of its components - namely the Kernel.
During our computations, we have taken advantage of the fact that the Kernel vanishes for certain couplings of u and v. Now, as in the preceding chapters, this seems to imply that F can not have a formal power series expansion in t, given the form of the functional equation it has to satisfy. Said couplings might lead to a singularity at the origin $(0,0)$, making a Laurent series expansion necessary. However, as F stems from a combinatorial counting problem, it must be well defined as a power series. Therefore, the Kernel must be one of the factors in the aforementioned decomposition of the numerator. Thus, canceling it from the fraction leads to

$$\begin{aligned} &F\left(t, \frac{1+\bar{u}}{1+v}, 1+v\right) \\ &\quad = \frac{(1+u)\Big(uvW\cdot(W^3+W^2+2W+1) - u(W^3+W^2+W+1) - W^3(1+v)\Big)}{(1-vW\cdot(1+W))(u(1-t)-t)(W^2-u(1+W))}. \end{aligned}$$

Now it is only a matter of revoking the substitution we did in the lemma establishing the functional equation for F. There we defined two new variables u, v such that $x = (1+\bar{u})/(1+v)$ and $y = 1+v$. W can undo this by setting $v = y-1$ and $u = 1/(xy-1)$. This quickly leads to nice expressions for the terms in the denominator:

$$\begin{aligned} 1 - vW\cdot(1+W) &= 1+W+W^2 - yW\cdot(1+W) = \frac{W}{t}(1-ty(1+W)), \\ W^2 - u(1+W) &= \frac{1}{xy-1}(xyW^2 - W^2 - W - 1) = \frac{-W}{t(xy-1)}(1-txyW), \end{aligned}$$

as well as

$$u(1-t) - t = \frac{1}{xy-1}(1-t-t(xy-1)) = \frac{1}{xy-1}(1-txy).$$

In the numerator we get, keeping in mind the relation of t and W:

$$\begin{aligned} &\frac{xy}{xy-1}\left(\frac{y-1}{xy-1}W\cdot(W\cdot(W^2+W+1)+1+W) - \frac{1}{xy-1}(W^3+\frac{W}{t}) - yW^3\right) \\ &\quad = \frac{xyW}{t(xy-1)^2}((y-1)(W^2+W-tW) - tW^2 - 1 - tyW^2(xy-1)) \\ &\qquad = \frac{xyW}{t(xy-1)^2}(W\cdot(1+W)(y-1) - 1 - txy^2W^2). \end{aligned}$$

The fraction can therefore be reduced by $-W/(t(xy-1)^2)$. In the numerator, proceed by writing $W\cdot(1+W)(y-1) = (W/t-1)(y-1)$ and dividing by W/t to obtain its final form:

$$\frac{txy}{W}\left(1+txy^2W^2-\left(\frac{W}{t}-1\right)(y-1)\right)=xy\left(1+t^2xy^2W-v\left(1-\frac{t}{W}\right)\right)$$
$$=xy\left(1+t^2xy^2W-v\left(\frac{t(1+W+W^2)-t}{W}\right)\right)=xy(1+t^2xy^2W-ty(1+W)).$$

Putting everything together yields the desired expression for $F(t,x,y)$. □

As stated in the paper [BM03], this generating function is algebraic of degree two.

With this theorem we conclude our solution of the second Task 4.5 for this chapter and the study of vexillary involutions. Throughout our computations we have applied the Kernel method several times, in two different ways. Many of the calculations can be followed rather quickly by using a computer algebra system (of course, this is true for the earlier chapters as well - but there the computations were not as lengthy), even if it is often necessary to make various substitutions of variables manually (or choosing the right square root to continue with).
Again, this shows that the Kernel method provides basic procedures which are very helpful to solve certain functional equations derived from enumeration problems with a recursive description. It acts as a good starting point, especially in the obstinate version, and can be applied later on, too, to produce more and more interesting relations to extract explicit information from.
Still, it also showed some limits of the method: while useful, it certainly is not powerful enough to solve any problem at hand (on its own). Here Bousquet-Mélou found a way to continue (by extracting positive parts of power series) but this might not be possible for some problems. We will see other limitations in the following chapter. We close this chapter with a few remarks.

The method described here can be used in a very similar manner for other problems, as stated at the beginning of this chapter. Especially interesting is the connection to general vexillary permutations. In [GPP01, Gui95] it is established that there is a bijective relation between vexillary permutations of length n and vexillary involutions of length $2n$ without a fixed point. Hence, it would be nice to add this component - the number of fixed points - to the construction we presented in Section 4.1 of this chapter. This is possible: the only way to introduce a new fixed point is indeed to add it by inserting the cycle $(n+1)$ of length one. Otherwise the number of fixed points stays the same. Translated into the language of generating functions, this means that one defines a new variable z to encode the number of fixed points, restates Lemma 4.10 taking into account the new parameter and derives a functional equation again.
Its form is very similar to the one we derived and can be tackled by the same means we have presented here. Additional steps need to be taken though. A more precise description and examples of these steps are shown in [BM03].

Lastly, we need to comment on the substitution of variables we did for Lemma 4.15 where we established the Kernel equation for the generating function of vexillary involutions.

This step is not obvious beforehand - it aims to make computations more accessible. Nevertheless, it does become natural at a certain point. A brief explanation, as given in the paper by Bousquet-Mélou, will suffice to show that.
We go back to the functional equation for F in Lemma 4.13, before we substituted the variables x, y. After multiplying with the common denominator $(1-x)(1-y)$ of the left hand side, the Kernel of the equation, that is, the resulting coefficient of F, is given by $(1-x)(1-y) + t^2x^2y(1-y) + t^2y(1-x)$. The rest of the equation is not important for our argument, as the coming steps depend only on the form of the Kernel.
Note the term xy as an argument of F on the right hand side. This naturally suggests to introduce a new variable z such that $z = xy$. Now multiply the whole equation by y (to remove any fractions introduced by setting $x = z/y$) and obtain the final version of this Kernel:

$$\widehat{K}(t, y, z) = (y-z)(1-y) + t^2\left(z^2(1-y) + y(y-z)\right).$$

One difference to the Kernel we used throughout this chapter is immediate: this time it is not symmetric in y and z. While that does not prevent our method from succeeding, it is simply not as nice as before and leads to more computational effort as in a symmetric case. Indeed, as visualized in Figure 4.40, the curves defined by $\widehat{K}(t, y, z) = 0$ reflect this - they are not symmetric and thus more complex.

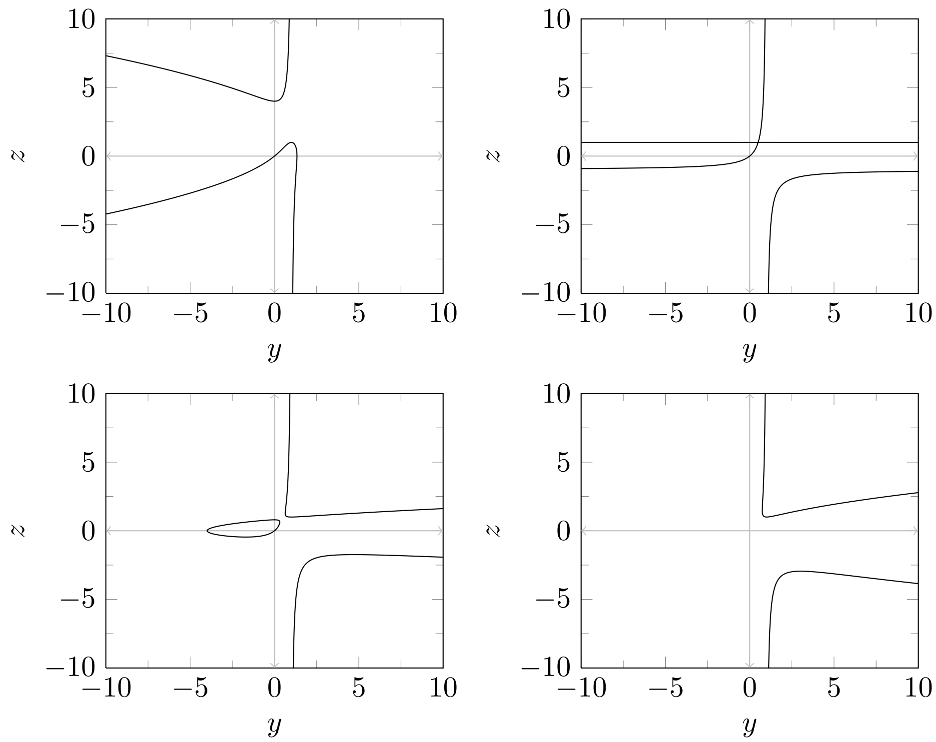

Figure 4.40: Algebraic curve defined by the Kernel $\widehat{K}(t, y, z)$, for the same values of t as in 4.16.
(Figures in top row: $t = 0.5$ and $t = 1$, bottom row: $t = \sqrt{1.25}$ and $t = 5$)

Let us proceed by computing the roots of $\widehat{K}$ if viewed as a quadratic polynomial in y:

$$Y_{1,2} = \frac{(1+z)\,(1-t^2z) \mp \sqrt{(1-z)(1-t^2z)(t^2z^2+3t^2z-z+1)}}{2(1-t^2)}.$$

Both solutions are formal power series in t with coefficients in $\mathbb{Q}[[z]]$, by the same reasons we used for V_1 and V_2 above: the square root admits a binomial series expansion and $1/(1-t^2)$ is nothing but a geometric series. Again, we can obtain their $[t^0]$ terms easily: for the solution with the negative sign before the square root, we have $Y_1 = z + O(t^2)$ and for $Y_2 = 1 + O(t^2)$. Note that this expansion requires the ring of formal power series in z (and not only polynomials).
The elementary symmetric functions of Y_1, Y_2 can be obtained from the Kernel $\widehat{K}(y) = (t^2-1)y^2 + (1+z)(1-t^2z)y - z + t^2z^2$ and are a bit more complicated this time (i.e. both contain z^2) :

$$Y_1 + Y_2 = \frac{(1+z)(1-t^2z)}{1-t^2} \quad \text{and} \quad Y_1Y_2 = \frac{z(1-t^2z)}{1-t^2}.$$

Thus, one of the crucial points of our computations in this chapter is not met: they do not admit the immediate application of Lemma 4.14 to gain further relations by extracting positive parts or constant terms from involved equations. However, this is not the only reason to make a substitution.
The next step is the obstinate use of the Kernel method. That is, we define two transformations $\varphi(Y,Z)$ and $\psi(Y,Z)$ which, starting from one pair of Laurent series that cancel the Kernel, produce another such pair. Recall that all the involved series are power series in t with coefficients in an appropriate field, such as $\mathbb{Q}((z,\bar{z},y,\bar{y}))$. The latter one was defined as $\varphi(Y,Z) := (Y',Z)$ such that Y' is the other solution for y to the quadratic equation $\widehat{K}(y) = 0$, or, more precisely, by expressing Y' in terms of Y and Z, due to the elementary symmetric functions of the roots of the Kernel.
In this particular case, let us find another relation for obtaining Y_i from Y_j, where $i \neq j$, such that only z is occurring in it. Given the form of their elementary symmetric functions, we quickly find that $(1+z)Y_1Y_2 - z(Y_1+Y_2) = 0$ (one might also apply the Euclidean algorithm to obtain this). We can solve this relation for Y_1 or Y_2, whence

$$\varphi(Y,Z) := \left(\frac{YZ}{Y-Z+YZ}, Z\right).$$

Since our current Kernel $\widehat{K}$ is not symmetric in y,z, we need to treat the case $\widehat{K}(z) = t^2(1-y)z^2 + (y(1-t^2)-1)z + y + y^2(t^2-1) = 0$ separately (if it was symmetric, we could define ψ analogously to φ, as we did above). The actual solutions Z_1, Z_2 which set the Kernel to zero are not of interest, merely their connection to the (now fixed) variable y via their symmetric functions. They depend solely on the Kernel, so we have

$$Z_1 + Z_2 = \frac{1-y(1-t^2)}{t^2(1-y)} \quad \text{and} \quad Z_1Z_2 = \frac{y+y^2(t^2-1)}{t^2(1-y)}.$$

Again, we can find a simpler relation as clearly $y(Z_1+Z_2) = Z_1Z_2$. Solving this for either of the roots leads to

$$\psi(Y,Z) := \left(Y, \frac{YZ}{Z-Y}\right).$$

$$\begin{tikzcd}
 & (Y_1, z) \arrow[dl, leftrightarrow, "\varphi"'] \arrow[dr, leftrightarrow, "\psi"] & \\
(Y_2, z) \arrow[d, leftrightarrow, "\psi"'] & & (Y_1, \frac{Y_1 z}{z-Y_1}) \arrow[d, leftrightarrow, "\varphi"] \\
\left(Y_2, \frac{Y_1}{Y_1-1}\right) \arrow[dr, leftrightarrow, "\varphi"'] & & \left(\frac{z}{z-1}, \frac{Y_1 z}{z-Y_1}\right) \arrow[dl, leftrightarrow, "\psi"] \\
 & \left(\frac{z}{z-1}, \frac{Y_1}{Y_1-1}\right) &
\end{tikzcd}$$

Figure 4.41: Pairs produced by applying φ and ψ.

Starting with the pair (Y_1, z) (which is a valid substitution setting the Kernel to zero), we apply these two transformations (while not doing the same one twice in a row) and obtain a diagram 4.41 (similar to Figure 7 in [BM03]).
The equation $(Y_2 z)/(z - Y_2) = Y_1/(Y_1 - 1)$, which can be derived by plugging $Y_2 = (Y_1 z)/(Y_1 - z + Y_1 z)$ into the right hand side, was used here to make the occurring expressions shorter. Additionally, it shows that the solutions from the right path and the left path are actually equal.
Now we need to check which of the possible six pairs of solutions for $\widehat{K}(y, z) = 0$ are formal power series in t and thus can be substituted into the Kernel. The first root Y_1 has the constant term z. Therefore $z - Y_1$, having no constant term, is not invertible and further, this implies that $(Y_1 z)/(z - Y_1)$ only has a formal Laurent series expansion in t. The other four pairs not containing this product are admissible, though: $z/(z - 1) \in \mathbb{Z}[[z]]$ is in the ring of coefficients for our series and $Y_1 - 1$ has the constant term $z - 1$, which is invertible (in $\mathbb{Z}[[z]]$).
Hence, the four pairs $(Y_1, z), (Y_2, z), (Y_2, Y_1/(Y_1 - 1))$ and $(z/(z - 1), Y_1/(Y_1 - 1))$ give us again four equations with five unknown specializations of the generating function F, similar to system (4.21). This time the series $F(t, z, 1)$ and $F(t, Y_1/(Y_1 - 1), 1))$ can be eliminated from this system and the remaining series are $F(t, 1, Y_1), F(t, 1, Y_2)$, as well as $F(t, 1, z/(z - 1))$. At this point one is again lead to the exchange of variables we did in Lemma 4.13.
Setting $z = 1 + \bar{u}$ yields $z/(z - 1) = 1 + u$, so the latter specialization of the generating function only involves non-negative powers of u. This allowed us to define it as a formal power series in a variable u and extract the positive part of a certain equation (namely (4.28)). Furthermore, this transforms the elementary symmetric functions of the roots of $\widehat{K}$ into polynomials in $\bar{u}$, which makes the computations easier by applying Lemma 4.14.
Lastly, the equations also involve $F(Y_1/(Y_1 - 1), 1)$ and so it is also sensible to set $y = 1 + v$. This finally leads to the substitution as specified in Lemma 4.15. As we have seen, this exchange of variables makes the computations much quicker, especially because the Kernel becomes symmetric in u and v. Note however, that this is merely a particularly nice coincidence and the reason why this problem has such a well behaved solution.

5

Partially directed paths in a wedge

In the last chapter we added a twist to the Kernel method by applying it several times in succession. We obtained a finite sequence of formal series which set the Kernel to zero, thus giving us more equations to work with. Taking this one step further, one might also look for infinitely many such roots.

As a demonstration, we come back to lattice paths and walks again. One can imagine now that, as stated in the introduction to this thesis, they are a traditional and wide field of study within enumerative combinatorics. A classical way to tackle the counting problems for related objects is the one we have already employed ample times: starting from the definition of the combinatorial object, find a recursive description, derive a functional equation for a generating function and finally solve it. Thus, one has access to the solution in form of an explicit formal power series expansion (if available) or it is possible to determine its asymptotic behavior.
One of the difficulties in walk and path enumeration stems from the many restrictions that one can impose on them, destroying invariance properties (such as symmetries) which might make the task easier. So, even if the first step is tractable, the second one of actually solving the resulting equation might be very hard, if at all possible with the current methods, and is the subject of this thesis. We will take on the problem of counting partially directed paths in a wedge, introduced below, and of course try to apply the Kernel method to obtain a solution. This example originally appeared in [vRPR08]. It will also clearly point out some limits of the Kernel method for practical use. Let us begin by defining the model of lattice walks we will work with in this chapter.

Definition 5.1. In this chapter, a partially directed walk on the lattice $\mathbb{Z} \times \mathbb{Z}$ starts at the origin $(0, 0)$ and the allowed moves are from (n, m) to $(n + 1, m)$ (east), $(n, m + 1)$ (north) or $(n, m - 1)$ (south) with the added restriction that no point of the lattice is visited twice (hence, one is not allowed to do steps north/south in immediate succession).

The special condition turns our walks into a specific case of general self-avoiding walks, which never intersect themselves. An overview of the topic can be found, for example, in [Sla] or [MS96]. Besides being interesting on their own right, these objects occur in many natural contexts, namely they provide an elementary, yet realistic model of polymers in solution (an introduction to this topic offers, for example, the book [Ter02]). Polymers are essentially macromolecules (large molecules) consisting of long, repeated chains of smaller subunits, held together by chemical bonds. Clearly, no two subunits can occupy the same volume in space, preventing intersections and making them self-avoiding. Materials based on them are ubiquitous - among them being DNA, RNA and Proteins, the building stones of life [AJL$^+$02], and many products of today's industry (e.g. Nylon, Polyethylene, ...) [CP98].
While being so important for many applications, there is currently little to no hope of giving a (more or less) complete description of their properties with the current methods of combinatorics. There are results for various aspects of self-avoiding walks, but often one has to rely on numerical simulations or simplified models, such as the one from our definition. It stems from somewhat simpler directed paths and thus might remain tractable. Also see [vRPR07] for a similar situation in the setting of directed paths.

Indeed, there are no special techniques necessary to give a solution for the following task:

Task 5.2. Provide a formula for the number a_n of paths of length n (i.e. n steps taken), restricted by the rules given in Definition 5.1.

Let us derive the answer quickly, applying our usual approach. To this end, let r_n be the number of partially directed paths of length n, such that the last step taken was to the east (right) $(n-1, m) \to (n, m)$. Similarly u_n and d_n are defined to be paths ending with a step north (up) or south (down). These latter two numbers are obviously equal, $u_n = d_n$ (instead of taking a step down, we might take a step up at the end and the other way around). Thus, by definition, we have $a_n = r_n + 2d_n$. A recursion can be found as

$$r_{n+1} = r_n + 2d_n \quad \text{and} \quad d_{n+1} = r_n + d_n, \quad n \geq 1,$$

with $r_0 = 1$ (counting the empty path) and $d_0 = 0$. The first equation simply says that a step to the right can be added to any path of length n (yielding one of length $n+1$) while the second models the self-avoidance, i.e. the restriction that a north (south) step must not follow directly after a south (north) step. Next, define the ordinary generating functions $A(t)$, $R(t)$ and $D(t)$, which encode the numbers a_n, r_n and d_n respectively. Multiplying the recursion above by t^n and summing for $n \geq 1$ yields

$$\frac{1}{t}(R(t) - r_0) = R(t) + 2D(t) \quad \text{and} \quad \frac{1}{t}(D(t) - d_0) = R(t) + D(t).$$

Nothing fancy is necessary to solve this simple system of equations. Plugging in the values for r_0, d_0 and expressing R in terms of D leads to $R = D \cdot (1/t - 1)$. Using this in the first equation gives

$$\frac{1}{t}\left(D \cdot \left(\frac{1}{t} - 1\right) - 1\right) = D \cdot \left(\frac{1}{t} + 1\right) \quad \Longleftrightarrow \quad D \cdot \left(\frac{1-t}{t^2} - \frac{1+t}{t}\right) = \frac{1}{t}$$

$$\iff \quad D(t) = \frac{t}{1-2t-t^2}.$$

Hence, we find an expression for R and eventually the generating function for partially directed paths as

$$A(t) = R(t) + 2D(t) = \frac{1-t}{1-2t-t^2} + 2\frac{t}{1-2t-t^2} = \frac{1+t}{1-2t-t^2}.$$

Now we can read off the coefficients and thus the numbers a_n. The denominator can be factorized by finding its roots $1-2t-t^2 = -(t+1-\sqrt{2})(t+1+\sqrt{2})$. Furthermore, the partial fraction decomposition of A makes it easier to extract a_n:

$$\begin{aligned}
[t^n]\, A(t) &= [t^n] - \frac{1}{2}\left(\frac{1}{t+1-\sqrt{2}} + \frac{1}{t+1+\sqrt{2}}\right) \\
&= -\frac{1}{2}\,[t^n]\left(\frac{1}{1-\sqrt{2}} \cdot \frac{1}{1+\frac{t}{1-\sqrt{2}}} + \frac{1}{1+\sqrt{2}} \cdot \frac{1}{1+\frac{t}{1+\sqrt{2}}}\right) \\
&= -\frac{1}{2}\left(\frac{1}{1-\sqrt{2}} \cdot \frac{(-1)^n}{1-\sqrt{2}} + \frac{1}{1+\sqrt{2}} \cdot \frac{(-1)^n}{1+\sqrt{2}}\right).
\end{aligned}$$

For the last equality, we simply used the expansion for a geometric series. We can proceed by computing the common denominator which is given by $(1+\sqrt{2})^{n+1}(1-\sqrt{2})^{n+1} = (-1)^{n+1}$. Using this, we obtain

$$a_n = [t^n]\, A(t) = \frac{1}{2}\left(\left(1+\sqrt{2}\right)^{n+1} + \left(1-\sqrt{2}\right)^{n+1}\right).$$

The first few values of this sequence are given by $1, 3, 7, 17, 41, 99, 239, 577, 1393, \ldots$ and it can be found as entry A078057 in the on-line encyclopedia of integer sequences [OEI11]. From this, one can find an explicit connection to statistical mechanics via the asymptotics (see [vRPR08]). For us it suffices to see that this model is relatively easy to understand and allows us to solve the counting problem Task 5.2 completely.

However, besides directedness, one can impose other restrictions onto the paths such as limiting the area in which it may grow. This is also relevant regarding applications, modeling polymers in confined spaces. Indeed, the walls of the confinement interact with the molecules and similarly the form of the surrounding space is of importance as well.
In this chapter, we will take a look at a simplified model for self-avoiding walks taking into account these two forms of constraints. As usual, our approach will be to start with a recursive description. However, instead of formulating it explicitly, we will immediately derive a functional equation for a generating function.

5.1 Obtaining a functional equation

A brief remark to begin with: in the following sections of this thesis, unless specified otherwise, we use the terms walk and path interchangeably and refer to partially directed paths as defined in Definition 5.1.
Now let us state our task precisely. We will restrict paths not only by imposing directedness onto them (which proved to be easy to solve, so we want to increase the difficulty) but also by limiting them to a wedge:

Definition 5.3. From now on, the walks as given by Definition 5.1 are additionally confined within the (symmetric) wedge $\mathrm{W} \subset \mathbb{Z}^2$, given by

$$\mathrm{W} = \{(m, n) \in \mathbb{Z}^2 | m \geq 0 \text{ and } -m \leq n \leq m\}.$$

Thus, for all pairs (m, n) visited by the path we have $(m, n) \in \mathrm{W}$.

Examples for walks in this space are given in Figure 5.4.

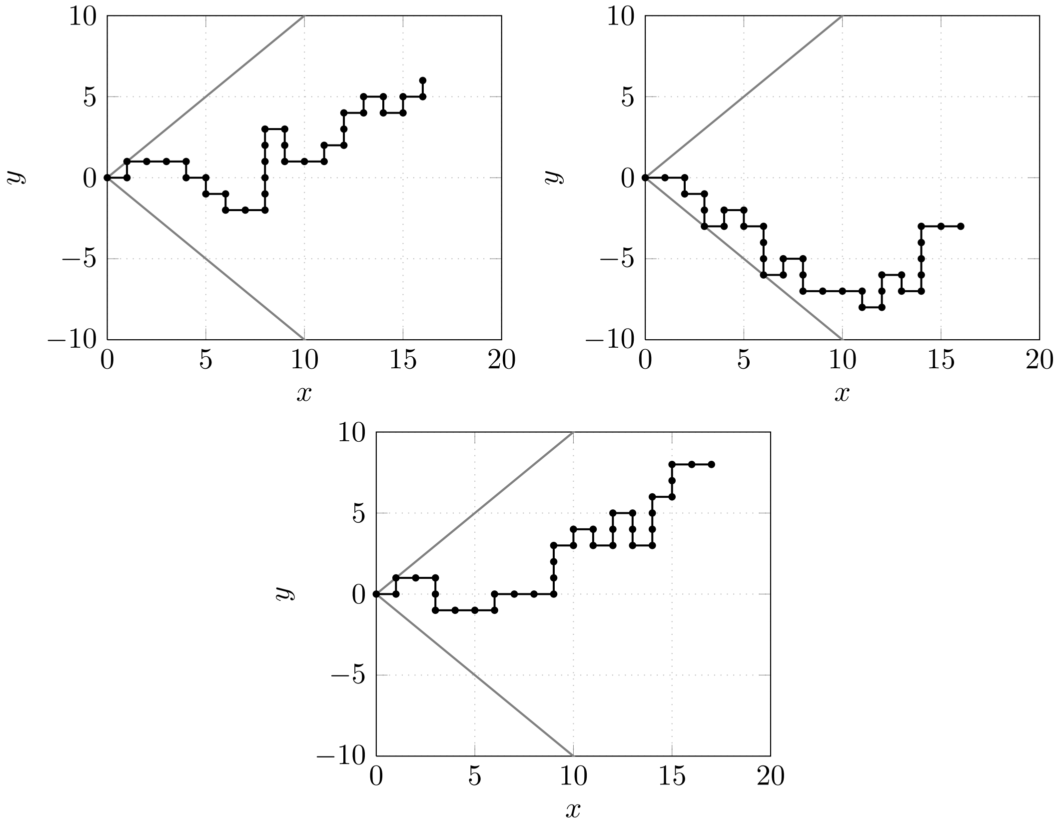

Figure 5.4: Examples for random partially directed paths of length 35 in a symmetric wedge (grey lines).

Now, as discussed in the underlying paper [vRPR08], this could be generalized in multiple ways. One is to make the wedge asymmetric and use the x-axis as the bottom line of the wedge (such that we have $0 \leq n \leq m$). While this makes the task of finding a recurrence and a functional equation not much harder, it significantly increases the difficulty of finding a solution for it. The authors show that it is possible by using the same methods we will demonstrate here. However, the computations, which mostly consist of simplifying the result from the new flavor of the Kernel method we are going to introduce, are much more lengthy. This is in accordance to the preceding chapter, where we have observed that a symmetric Kernel makes everything much easier to work with, but is not essential for the working out of the general approach.

On the other hand, one might change the angle of the boundary lines of either wedge (symmetric or asymmetric), i.e. the restrictions for the second coordinate become $-\alpha m \leq n \leq \alpha m$ respectively $0 \leq n \leq \alpha m$ for $\alpha \in \mathbb{N} \setminus \{0\}$. While possible in theory (as proposed in the paper), actually solving the enumeration problem for walks in these spaces seems to be beyond the practical limit of working with the occurring expressions. We will see that even when $\alpha = 1$, while tractable, we need to do a lot of polishing to obtain orderly results. This is especially obvious for the asymmetric model and suggests that even the most simple case of this model of self-avoiding walks poses numerous, challenging mathematical problems.

In this chapter we will therefore concentrate on the simplest setting:

Task 5.4. Find the generating function of partially directed walks within the symmetric wedge as in Definition 5.3, enumerating them by their length n, i.e. the number n of edges in total.

While we will not give an explicit number of such paths, access to the generating function admits asymptotic results and is therefore very useful (see [vRPR08] for the details). So, as usual, let us find a recursive description of our combinatorial objects.
Unlike we did before, we will not enumerate them directly by their length and the coordinates of the endpoint (which is an alternative way to obtain a functional equation). Instead, we introduce the generating function as follows.

Definition 5.5. Let $F(u, v, x, y)$ be defined as the generating function of partially directed paths constrained to the symmetric wedge W, such that it enumerates the walks by the following four statistics:

- the variables u and v correspond to the distance of the endpoint of the walk to the upper and bottom boundary line of the wedge W. More precisely, if the last point is (m, n) then the walk contributes the terms u^{m-n} respectively v^{m-n} to the generating function $F(u, v, x, y)$.
- the variables x and y encode the number of steps taken by the walk - x counts the horizontal edges and y the vertical ones. That is, if there are k horizontal edges in the path, then the contribution to $F(u, v, x, y)$ is x^k, and similar for y.

Thus, to obtain the generating function we are looking for, we will eventually set $x = y = t$ to count the number of edges, regardless of their direction, and $u = v = 1$, as the coordinates of the endpoint do not matter. To further simplify our task (which means a simpler functional equation), we will make one more restriction.

Denote by $G(u, v, x, y)$ the generating function of paths which end in a step to the east (or have no steps at all). The connection to F is obvious: we can easily turn any walk contributing to F into one ending horizontally by simply appending a step to the east. This means that the path constructed this way has one more edge parallel to the x-axis and its endpoint is one unit farther away from the boundary lines. In the language of generating functions, this is accomplished by multiplying with the term uvx. Clearly, this way we obtain all possible such walks (not forgetting about the path consisting of a single vertex at the origin only), leading to the simple relation

$$G(u, v, x, y) = 1 + uvxF(u, v, x, y). \tag{5.6}$$

So, finding an expression for G immediately gives one for F, too. Thus, we can turn to a recursive description of our walks and derive a functional equation for G in the following theorem.

Lemma 5.7 ([vRPR08]). *The generating function $G(u, v, x, y)$, enumerating partially directed walks obeying the rules of Definition 5.1, restricted to the symmetric wedge W as defined in Definition 5.3 and ending in a horizontal step, satisfies the functional equation*

$$\begin{aligned} K(u, v)G(u, v, x, y) = {} & (u - vy)(v - uy) - u^2vxy(u - vy)G(u, uy, x, y) \\ & - uv^2xy(v - uy)G(vy, v, x, y), \end{aligned}$$

where the Kernel is given by $K(u, v) = (u - vy)(v - uy)(1 - uvx) - uvxy(u^2 + v^2 - 2uvy)$.

Proof. Constructing new walks starting with a given path is done by appending a sequence of steps to the shorter one - either this sequence is a step east only or a number of steps south (or north, but recall that we are not allowed to take south/north steps in direct succession) ending with a single step east. In the latter case, care must be taken not to leave the wedge, so not all possible combinations of steps are admissible and we have to subtract them accordingly. Let us state the contributions to the generating function G of each case.

- Appending a single step to the east: to obtain the generating function of such walks, we have to multiply $G(u, v, x, y)$ by uvx, for the same reasons as above (as for the relation given in (5.6)).
- Appending south-steps followed by an east-step: note that in this case we do not care whether or not the path leaves the wedge, so any number of steps vertically is allowed for now. We will remove the wrong contributions below. So, again the horizontal step at the end gives the term uvx. Every vertical step adds one y term. Furthermore, stepping south increases the distance to the upper line, as well as "reduces" the distance to the bottom line by one, thus adding a u/v term (negative powers of v correspond to a path which leaves the wedge). Summing all contributions from taking sequences of steps of increasing length (i.e. for length $i > 0$) yields the geometric series $\frac{1}{1-yu/v} - 1$.
  Overall, the generating function for paths constructed this way is given by $uvx\frac{yu/v}{1-yu/v}G(u, v, x, y)$.
- Removing south-steps which leave the wedge: to make up for the inadmissible addition of south-steps without a restriction of length, we need to remove all contributions from walks leaving the wedge. These can be constructed in the following way: start with a path touching the bottom line (that is, the endpoint has coordinates $(m, -m)$)

and append a sequence of steps south ending with a horizontal step (modeling the part outside the wedge).
Consider a path (within the wedge) such that its endpoint has a distance of k to the bottom line. Hence, by appending k steps down, it touches the lower boundary. This corresponds to an increase of the distance to the upper line by k, hence to multiplying the main generating function G by $u^k y^k / v^k$. In other words, the variable v is replaced by uy which means that the generating function for paths ending on the bottom line is given by $G(u, uy, x, y)$.
The enumeration of the overhanging pieces is now done as in the point above, resulting in $uvx\frac{yu/v}{1-yu/v}G(u, uy, x, y)$, encoding the walks leaving the wedge.

- Appending north-steps followed by an east-step: we essentially repeat the arguments as for taking south-steps, the generating function for this case is given by $uvx\frac{yv/u}{1-yv/u}G(u, v, x, y)$.
- Removing north-steps which leave the wedge: as above, we need to subtract overhanging walks, enumerated by $uvx\frac{yv/u}{1-yv/u}G(vy, v, x, y)$ (analogously to the south-steps case).

Hence, to obtain the generating function of all partially directed paths ending in a horizontal step, we simply need to carry out the construction as described here. This means to add all the generating functions for the 5 cases, leading (after some minor algebraic transformations) to

$$\begin{aligned} G(u, v, x, y) = 1 + uvxG(u, v, x, y) &+ \frac{u^2vxy}{v - uy}(G(u, v, x, y) - G(u, uy, x, y)) \\ &+ \frac{uv^2xy}{u - vy}(G(u, v, x, y) - G(vy, v, x, y)). \end{aligned}$$

Since we want to apply the Kernel method, we will rewrite it to obtain the shape we are used to work with. That is, we bring all the $G(u, v, x, y)$ terms to the left hand side and multiply by the common denominator $(u - vy)(v - uy)$. This yields the equation as given in the statement of the lemma and concludes the proof. □

A note regarding the two ways to generalize this result, as mentioned before: first, this derivation is also true if we use a symmetric wedge between the lines $-\alpha x$ and αx - one could simply put this α into the index of the generating function and adjust the distances from newly constructed endpoints. In short, instead of multiplying the generating function with uv, we would have to multiply by $(uv)^\alpha$, taking into account the slope of the boundary lines. The subsequent steps will not work anymore, though.
Additionally, the functional equation for the asymmetric wedge is obtained by essentially the same means. In fact, one only needs to adjust the contributions to the distance from the bottom line, which does not change by taking the final horizontal step (i.e. a term v is removed). See [vRPR08] for more details.

5.2 The iterated Kernel method

We will now try to solve the equation from the lemma above. This kind of functional equation looks somehow familiar to us now - and as usual, trying to solve it by conventional means proves to be unsuccessful. It is the situation in which the Kernel method might prove to be helpful: the equation essentially consists of a linear combination of a main generating series and some of its offsprings with special arguments. However, once again it seems to be of a somewhat different type.
Instead of being set to one or zero, as most of the catalytic variables were in the preceding chapters, they are merely replaced by combinations of other arguments this time. Thus, the technique needs to be adjusted for our purposes again.
In the last chapter we demonstrated a way to start with a solution that sets the Kernel to zero and constructed new roots of the Kernel with it. We more or less applied the Kernel method multiple times, to obtain additional information through equations of the unknown generating functions, which originally appeared in the main functional equation. The strategy lead to a result, even though it required additional work in the end (extracting positive parts from certain relations).

To solve the functional equation we are dealing with now, the authors of the paper [vRPR08] proposed the so-called iterated Kernel method, which they based on works mainly by Bousquet-Mélou and Petkovsek. It appears to be very similar to an iterative scheme [BM96] as well as the approach of the obstinate Kernel method, outlined in the earlier chapter. However, the big difference is that it essentially consists of applying the Kernel method infinitely many times. So instead of only using a few (finitely many) roots of the Kernel, it requires an infinite sequence of roots. Clearly, this approach remains tractable only in very specific cases, when the roots can be expressed in a sufficiently simple manner. Otherwise, the method to construct new solutions to $K(u, v) = 0$ might produce increasingly complex formulas which, in theory, give the solution we are looking for but become useless for practical purposes at some point. We will see that a lot of work must be done, even in the simplest case we are showing here, for boundary lines of the wedge with a slope of one.

So, after worrying a lot about the upcoming difficulties, let us start with a very positive aspect of our example. The symmetric wedge leads to two nice properties: first, the generating function $F(u, v, x, y)$ and consequently $G(u, v, x, y)$, too, is symmetric in u and v. This stems from the fact that walks ending in a point (m, n) are in obvious bijective correspondence to walks ending in $(-n, -m)$ (by flipping them vertically).
Secondly, the Kernel K from the functional equation in Lemma 5.7 is symmetric in the variables u and v as well. As in the last chapter, this will make the computations easier and shorter. Obviously, this is not the case anymore for the asymmetric wedge and one can compare the increase in the amount of work necessary for a solution in [vRPR08].

The computations start out, as usual, with the Kernel - again, it is only a quadratic polynomial in u, v and thus its roots can found easily. The symmetry means that the resulting solutions to $K(u, v) = 0$ are equal as Laurent series, regardless whether we solve for u or v. Hence, let us simplify and write $K(u) = (v^2xy^2 - v^2x - y)u^2 + v(1 + y^2)u - v^2y$ and find its roots as a polynomial in u.

Graphical examples for the algebraic curves defined by the solutions to this equation are depicted in Figure 5.8.

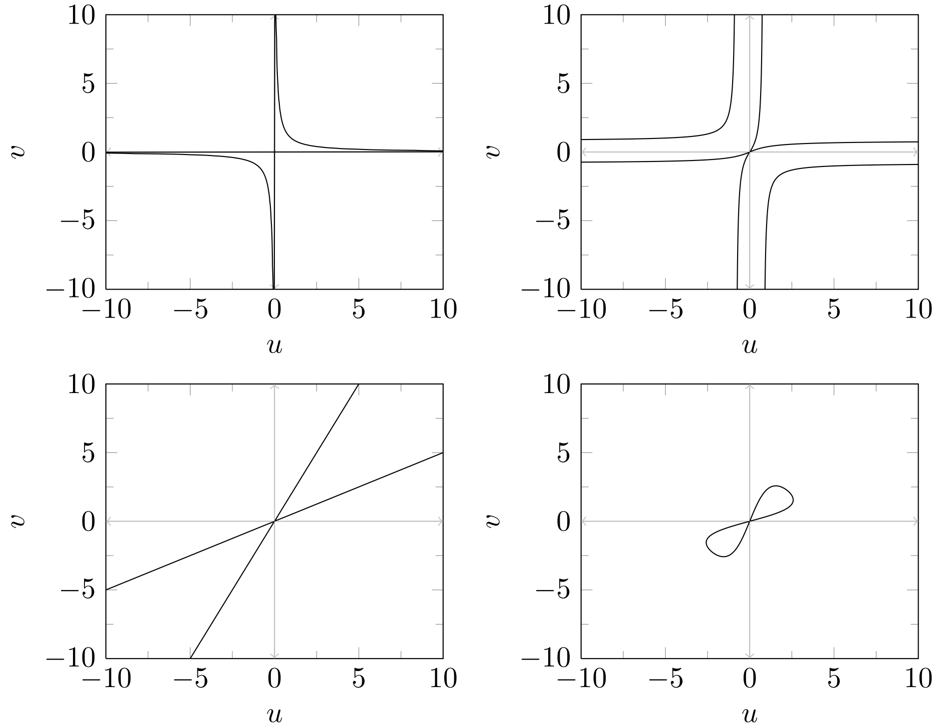

Figure 5.8: Algebraic curve defined by the Kernel $K(u, v, x, y)$, for various values of (x, y). (top row: $(x, y) = (1, 0)$ and $(x, y) = (1, 2)$, bottom row: $(x, y) = (0, 0.5)$ and $(x, y) = (-0.1, 3)$)

Arithmetically, they are given by

$$U_{1,-1}(v) = \frac{v}{2} \cdot \frac{1 + y^2 \mp \sqrt{(1 - y^2)(1 - 4v^2xy - y^2)}}{y + v^2x - v^2xy^2}. \tag{5.9}$$

Let us check which of these solutions are appropriate for our purposes and define formal power series. First off, it is easy to see that both solutions are well defined as power series in v, with coefficients in $\mathbb{Q}[x, y, \overline{y}]$. The denominator is a geometric series if written as $y + v^2x - v^2xy^2 = y(1 - v^2(xy - x/y))$. The expansion of the square root is given by the general binomial series and thus, the roots can be expressed as the product of two formal power series. Both U_1 and U_{-1} do not have a constant term, because of the multiplication with $v/2$. Furthermore, we have $[v^1]\, U_1 = y$ (also, U_1 has an expansion in $\mathbb{Q}[x, y]$) and $[v^1]\, U_{-1} = 1/y$ - this can be obtained by looking at the constant term of the roots before the multiplication of the additional $v/2$ term (when using a computer algebra system to rederive this result, one has to exercise caution and choose the "right" square root of $(1 - y^2)^2$, otherwise the roots are switched).

Furthermore, recall that we will set $x = y = t$ in the end, to count walks only by their length (the total number of steps taken). In this case, we have

$$U_1(t) = \frac{1 + t^2 - \sqrt{(1-t^2)(1-4v^2t^2-t^2)}}{t + v^2t - v^2t^3}.$$

The power series expansion of the square root has the constant term 1, which is canceled by subtraction in the numerator. Thus, the fraction can be reduced by t. That means that the expression in the denominator now has a constant term of 1 and is thus invertible in the ring of formal power series in t with coefficients in $\mathbb{Z}[v]$. Therefore, the first root with the negative sign is indeed a power series in t.
On the other hand, the constant terms in the numerator of U_{-1} do not cancel each other, so it is not well defined in t and this series must not be used in the substitutions.

The elementary symmetric functions for the roots U_1 and U_{-1} will prove to be useful again below, so let us state them now as well. They are given by

$$U_{-1} + U_1 = \frac{v(1+y^2)}{y + v^2x - v^2xy^2} \quad \text{and} \quad U_{-1}U_1 = \frac{v^2y}{y + v^2x - v^2xy^2}, \tag{5.10}$$

where the latter equation can be obtained by looking at the constant coefficient in u of the Kernel.

Now comes the crucial step in the working out of (any flavor of) the Kernel method. We have produced one solution for $K(u) = 0$ which is a formal power series without a constant term, and hence admissible for substitution into the functional relation in Lemma 5.7. This gives us one more equation to work with, in which the main generating function vanishes (because the Kernel is set to zero). However, on the right hand side we still have two specializations of it and these are still unknown, since the resulting equation can not be solved directly. So, we have to create more roots of the Kernel and try to obtain more information about them. Instead of applying the approach from the last chapter, which involved the elementary symmetric functions of the roots to produce new ones (and another step of extracting positive parts of equations afterwards), we will now try to substitute U_1 for v repeatedly. Therefore, this flavor of the Kernel method has been named the iterative Kernel method.

To be more precise, we have considered $K(u, v)$ as a quadratic polynomial in the variable u. Thus, we can also substitute U_1 (a valid formal power series with no constant term) for the other variable v and obtain $K(U_1(U_1(v)), U_1(v)) = 0$. Clearly, we can repeat that process and produce a (possibly infinite) sequence of roots of the Kernel. To this end, let us define, for all $i \in \mathbb{N}$:

$$U_i(v) := (\underbrace{U_1 \circ U_1 \circ \ldots \circ U_1}_{i \text{ times}})(v),$$

where $U_0(v) = v$.
Indeed, all of the series U_i, for $i \in \mathbb{N}$ are unique. This can be verified by looking at the first coefficient $[v^1]\, U_i = y^i$. To be more formal, an inductive argument can be used: assume that the property holds for $i > 0$ (for 0 we have stated it explicitly above) and we carry out

the substitution $U_i(U_1)$. To obtain the first term of the resulting series (we checked above that the substitution is valid), we look at the first term of U_i, which is vy^i and replace v by vy (the first term of U_1). There are no further contributions, since all the other terms involve higher powers of v, and so $[v^1]\, U_{i+1} = y^{i+1}$ holds.

We have found a countable sequence of well defined formal power series, such that two consecutive elements set the Kernel $K(u, v)$ to zero. Moreover, since it defines a formal power series in v without a constant term, too, we can similarly define U_{-i} as the composition of the other root U_{-1}. The same argument as above, starting with U_0 and carrying out an inductive step $U_{-i} \to U_{-i-1}$ shows that the series are unique for all $i \in \mathbb{Z}$.
By simply plugging in and computing the result, we observe that $U_1 \circ U_{-1} = U_{-1} \circ U_1 = v$, which means that the composition of U_i and U_{-i} also yields v. So in fact this sequence together with the composition and the identity U_0 forms a group structure. This nice property will become important later on, when we try to simplify the rather messy result of the following iterations of the Kernel method. It might also be a reason why these complicated expression can be made much easier.

Before we proceed, let us consider the geometric viewpoint and see how we move along the algebraic curve defined by the roots of the Kernel while carrying out these substitutions. In the preceding chapter, the transformations for the obstinate Kernel method consisted of switching from one branch of the algebraic curve to the other, moving parallel to the horizontal and vertical axes.
This time, we simply stay on one branch (given by $v = U_1(u)$). From the starting point $(u_0, U_1(u_0))$ (where $u_0 \neq 0$), we move along the curve towards the origin $(0, 0)$. In this iterative process, the u-coordinate of a point is given by the v-coordinate of the previous one. This can be seen exemplary in Figure 5.11, which shows a detail view of the drawing in the upper right corner in Figure 5.8. The (rounded) coordinates of the first few iterations (drawn as points in the plot) are $(u_0, U_1(u_0)) = (1, 0.372) \to (0.372, 0.175) \to (0.175, 0.086) \to (0.086, 0.0429) \to (0.0429, 0.0215) \to (0.0215, 0.011)\ldots$

Since all of the elements in the sequence of iterated roots are well defined, we can substitute U_i, for all $i \in \mathbb{N}$, into the functional equation. This gives a sequence of equations in which the Kernel is always set to zero and hence the main generating function $G(u, v, x, y)$ does not occur:

$$\begin{aligned} 0 = {} & (U_i - U_{i+1}y)(U_{i+1} - U_i y) - U_i^2 U_{i+1} xy(U_i - U_{i+1}y) G(U_i, U_i y, x, y) \\ & - U_i U_{i+1}^2 xy(U_{i+1} - U_i y) G(U_{i+1}y, U_{i+1}, x, y), \end{aligned}$$

where $i \geq 0$. We can easily express $G(U_i, U_i y)$ in terms of $G(U_{i+1}y, U_{i+1})$ by bringing it to the left hand side and dividing by the factor $U_i^2 U_{i+1} xy(U_i - U_{i+1}y)$. This gives

$$\begin{aligned} G(U_i, U_i y) &= \frac{(U_i - U_{i+1}y)(U_{i+1} - U_i y)}{U_i^2 U_{i+1} xy(U_i - U_{i+1}y)} - \frac{U_i U_{i+1}^2 xy(U_{i+1} - U_i y)}{U_i^2 U_{i+1} xy(U_i - U_{i+1}y)} G(U_{i+1}y, U_{i+1}) \\ &= \frac{U_{i+1} - U_i y}{U_i^2 U_{i+1} xy} - \frac{U_{i+1}(U_{i+1} - U_i y)}{U_i(U_i - U_{i+1}y)} G(U_{i+1}y, U_{i+1}). \end{aligned} \tag{5.12}$$

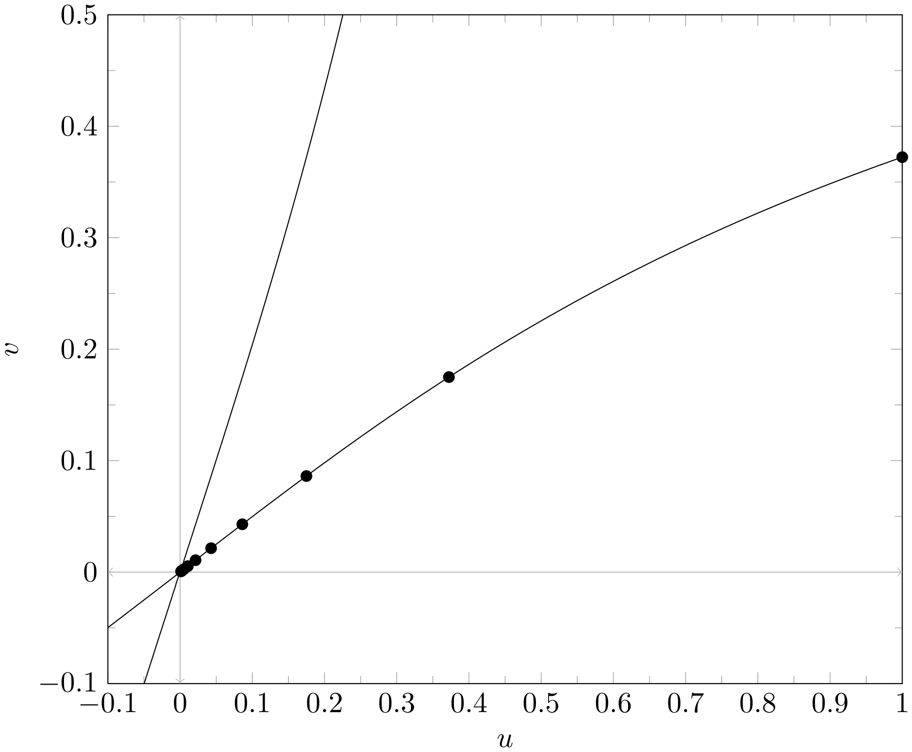

Figure 5.11: Tracing the iteration of the root, with starting point $u_0 = 1$ and $(x, y) = (1, 2)$.

Written compactly (for appropriately defined auxiliary terms), this seems to be a simple relation of the form $G_i = a_i + b_i G_{i+1}$ for $i \geq 0$.
Note that we make use of the symmetry of the generating function G here, by switching the arguments $U_{i+1}y$ and U_{i+1}. It also allows us to formulate the next equation for both unknown specializations of G without extra effort (we can simply replace u by v and switch the order of the arguments). As in the chapter before, this symmetry is not vital for the success of the method. However, we have demonstrated earlier that it does decrease subsequent difficulties and helps to make results much less complex. This is the case here, too. In [vRPR08], the authors also show the working out of this method for the asymmetric wedge. There it is required to iterate again to find G_i in terms of G_{i+2}, and even though that is possible, it proves to be significantly harder to obtain a legible result.

From (5.12) we can find $G(vy, v) = G(v, vy) = G(U_0(v), U_0(v)y)$ by applying the equation iteratively:

$$G(v, vy) = \sum_{i \geq 0} \frac{U_{i+1} - U_i y}{U_i^2 U_{i+1} xy} \prod_{j=0}^{i-1} -\frac{U_{j+1}}{U_j} \cdot \frac{U_{j+1} - U_j y}{U_j - U_{j+1} y} = \sum_{i \geq 0} \frac{U_{i+1} - U_i y}{U_i U_{i+1} vxy} (-1)^i \prod_{j=0}^{i-1} \frac{U_{j+1} - U_j y}{U_j - U_{j+1} y}. \tag{5.13}$$

The latter equality is obtained by reducing the telescope product of the terms U_{j+1}/U_j. This relation shows that the expression on the right hand side is well defined as a for-

mal power series in the variables v, x, y, since G does have a combinatorial interpretation. Otherwise, this is not immediate and we need to make substantial simplifications for verification. Along the way, it will become clear that this is indeed the case.
Moreover, we can replace v by u in the above equation. Hence, thanks to the symmetry of the generating function, this relation also gives us the second unknown series, $G(u, uy)$, which occurs in Lemma 5.7. So, once we have found a tractable expression for these specializations of the main generating function, we can solve the functional equation.

5.3 Obtaining an explicit expression

To begin with, let us state the result we have just obtained by applying the iterated Kernel method. We plug the expressions for $G(u, uy, x, y)$ and $G(vy, v, x, y)$ into the equation from Lemma 5.7:

$$\begin{aligned} G(u,v,x,y) = {} & \frac{(u-vy)(v-uy)}{K(u,v)} \\ & - \frac{u^2vxy(u-vy)}{K(u,v)} \sum_{i\geq 0} \frac{U_{i+1}(u)-U_i(u)y}{U_i(u)U_{i+1}(u)uxy}(-1)^i \prod_{j=0}^{i-1} \frac{U_{j+1}(u)-U_j(u)y}{U_j(u)-U_{j+1}(u)y} \\ & - \frac{uv^2xy(v-uy)}{K(u,v)} \sum_{i\geq 0} \frac{U_{i+1}(v)-U_i(v)y}{U_i(v)U_{i+1}(v)vxy}(-1)^i \prod_{j=0}^{i-1} \frac{U_{j+1}(v)-U_j(v)y}{U_j(v)-U_{j+1}(v)y}. \end{aligned}$$

There are a few things to do before we can call this a solution to our problem. We want to introduce various simplifications, in order to bring this expression into a form closer to a power series expansion. Secondly, recall that we are not interested in the general generating function: our goal is to enumerate partially directed paths by their length, making no distinction between horizontal and vertical steps. Furthermore, the endpoint is of no importance. Therefore, we are actually interested in a nice expression for $G(1, 1, t, t)$.

Not surprisingly, the starting point for this is the sequence of roots of the Kernel. In the chapters before, we exploited their relations to make results easier, mostly using expressions built up by their elementary symmetric functions. We will try to use these to our advantage again, even though we are now working with compositions of the solutions to $K(u, v) = 0$ and not only with pairs of corresponding roots. These seem to be rather complicated, but one can find a useful recursive description for them. To get rid of the quadratic term in the denominator of the elementary symmetric functions in (5.10), we combine them and thus obtain a simple relation for the reciprocals of the (first) roots (considered as Laurent series):

$$\frac{1}{U_1(v)} + \frac{1}{U_{-1}(v)} = \frac{U_1(v)+U_{-1}(v)}{U_1(v)U_{-1}(v)} = \frac{1+y^2}{vy}.$$

The variable v occurs only once, which makes it easy to substitute $v = U_{i-1}(v)$. By definition of U_i as the composition of U_1 respectively U_{-1}, as well as the fact that $U_{-1}(U_1(v)) = v$, we have $U_1(U_{i-1}(v)) = U_i(v)$ and $U_{-1}(U_{i-1}(v)) = U_{i-2}(v)$. Therefore, the equation yields a recursion for the iterated roots of the Kernel:

$$\frac{1}{U_i(v)} = \frac{1+y^2}{y} \cdot \frac{1}{U_{i-1}(v)} - \frac{1}{U_{i-2}(v)}, \quad i \geq 2,$$

where $U_0(v) = v$ and $U_1(v)$ given by (5.9) are available to us, providing the starting values. This recursion is not hard to solve, so we might as well employ the tools we are so used to by now.
Define a generating function for the reciprocals of the roots of the Kernel $U(z) := \sum_{i\geq 0} z^i/U_i$. Summing the recursion for $i \geq 2$ and plugging in this definition, leads, after filling in the missing first coefficients and some minor shifting operations, to

$$\begin{aligned} & U(z) - z\frac{1}{U_1} - \frac{1}{v} = \frac{1+y^2}{y} z(U(z) - \frac{1}{v}) - z^2 U(z) \\ \iff \quad & U(z)\left(1 - \frac{1+y^2}{y} z + z^2\right) = z\frac{1}{U_1} + \left(1 - \frac{1+y^2}{y} z\right)\frac{1}{v}. \end{aligned}$$

In the following we divide by the coefficient of $U(z)$ in the equation above, so first we will find a formal power series expansion for its reciprocal. To this end, we rewrite it as

$$\frac{1}{1 - \frac{1+y^2}{y} z + z^2} = \frac{y}{y - (1+y^2)z + yz^2} = \frac{y}{(1-yz)(y-z)}.$$

By doing a partial fraction decomposition and using the well known geometric series, we can easily extract the coefficients in z. So, let $i \in \mathbb{N}$, then

$$\begin{aligned} \left[z^i\right] \frac{y}{(1-yz)(y-z)} &= y\left[z^i\right]\left(\frac{1}{y(1-y^2)} \cdot \frac{1}{1-\frac{z}{y}} - \frac{y}{1-y^2} \cdot \frac{1}{1-yz}\right) \\ &= \frac{1}{1-y^2} \cdot \frac{1}{y^i} - \frac{y^2}{1-y^2} \cdot y^i = \frac{1-y^{2(i+1)}}{y^i(1-y^2)}. \end{aligned}$$

Now reading off the solution for the roots of the Kernel from $U(z)$ yields, for $i \geq 2$:

$$\begin{aligned} \frac{1}{U_i} &= \left[z^i\right] U(z) = \left[z^i\right] \frac{y}{(1-yz)(y-z)} \left(z\frac{1}{U_1} + \left(1 - \frac{1+y^2}{y} z\right)\frac{1}{v}\right) \\ &= \frac{1-y^{2i}}{y^{i-1}(1-y^2)} \cdot \frac{1}{U_1} + \left(\frac{1-y^{2(i+1)}}{y^i(1-y^2)} - \frac{1+y^2}{y} \cdot \frac{1-y^{2i}}{y^{i-1}(1-y^2)}\right)\frac{1}{v} \\ &= \frac{1-y^{2i}}{y^{i-1}(1-y^2)} \cdot \frac{1}{U_1} - \frac{y^2(1-y^{2(i-1)})}{y^i(1-y^2)} \cdot \frac{1}{v}. \end{aligned}$$

This reasonably simple formula enables us to find an expression for $G(v, vy)$, given in (5.13). We apply it immediately to compute and simplify the following two terms, for $j \in \mathbb{N}$. First,

$$\begin{aligned} \frac{U_{j+1} - U_j y}{U_j U_{j+1}} &= \frac{1}{U_j} - \frac{y}{U_{j+1}} \\ &= \frac{1-y^{2j}}{y^{j-1}(1-y^2)} \cdot \frac{1}{U_1} - \frac{y^2(1-y^{2(j-1)})}{y^j(1-y^2)} \cdot \frac{1}{v} - \left(\frac{1-y^{2(j+1)}}{y^{j-1}(1-y^2)} \cdot \frac{1}{U_1} - \frac{y^2(1-y^{2j})}{y^j(1-y^2)} \cdot \frac{1}{v}\right) \\ &= \frac{y^{2j}(y^2-1)}{y^{j-1}(1-y^2)} \cdot \frac{1}{U_1} + \frac{y^{2j}(1-y^2)}{y^j(1-y^2)} \cdot \frac{1}{v} = y^j\left(\frac{1}{v} - \frac{y}{U_1}\right). \end{aligned}$$

In the other term, only the denominator changes slightly. Clearly, the calculations remain essentially the same.

$$\frac{U_j - U_{j+1}y}{U_jU_{j+1}} = \frac{1}{U_{j+1}} - \frac{y}{U_j} = \frac{1}{y^j}\left(\frac{1}{U_1} - \frac{y}{v}\right).$$

Together, they yield new expressions for the terms occurring in the product in (5.13):

$$\frac{U_{j+1} - U_jy}{U_j - U_{j+1}y} = \frac{U_{j+1} - yU_j}{U_jU_{j+1}} \cdot \frac{U_jU_{j+1}}{U_j - U_{j+1}y} = \frac{y^j(U_1 - vy)}{U_1v} \cdot \frac{y^jU_1v}{v - U_1y} = y^{2j}\frac{U_1 - vy}{v - U_1y}.$$

This leads to a lemma, which gives a formula for the specialization of the main generating function and shows that it is indeed a formal power series.

Lemma 5.14. *The generating function for partially directed paths within the symmetric wedge, ending in a horizontal step satisfies*

$$G(v, vy, x, y) = \left(1 + \frac{H(v, x, y)}{y}\right)\sum_{i\geq 0}(-1)^i y^{i^2} H(v, x, y)^i,$$

where the formal power series H is given by

$$H(v, x, y) = \frac{(1 - y^2)(1 - 2v^2xy) - \sqrt{(1 - y^2)(1 - 4v^2xy - y^2)}}{(1 - y^2)(y + 2v^2x) + y\sqrt{(1 - y^2)(1 - 4v^2xy - y^2)}}.$$

Proof. As a proof for the statement, we simply substitute the relations we have just obtained into (5.13). Hence, we have

$$\begin{aligned} G(v, vy) &= \sum_{i\geq 0}(-1)^i \frac{y^i}{vxy}\left(\frac{1}{v} - \frac{y}{U_1}\right)\prod_{j=0}^{i-1} y^{2j}\frac{U_1 - vy}{v - U_1y} \\ &= \left(\frac{1}{v^2xy} - \frac{1}{U_1vx}\right)\sum_{i\geq 0}(-1)^i y^{i^2}\left(\frac{U_1 - vy}{v - U_1y}\right)^i. \end{aligned}$$

Let us introduce the notation $H(v, x, y) := (U_1 - vy)/(v - U_1y)$. First off, it is possible to reduce the whole fraction by v (because U_1 starts with vy - which is subtracted in the numerator, resulting in a series which starts at v^2). Consequently, the series in the denominator $1 - U_1y/v$ does have a constant term 1 and is therefore invertible. The subsequent multiplication with the series in the numerator yields a formal power series without a constant term. Also note, as U_1 does not have a constant term as power series in y, the division of H by y is possible.
Furthermore, we can rewrite $H(v, x, y) = y(1/(v^2xy) - 1/(U_1vx) - 1)$. This equality holds by definition of U_1 as a root of the Kernel:

$$\begin{aligned} \frac{U_1 - vy}{v - U_1y} &= \frac{1}{v^2x} - \frac{y}{U_1vx} - y \\ \iff \quad U_1v^2x(U_1 - vy) - U_1(v - U_1y) &+ vy(v - U_1y) + U_1v^2xy(v - U_1y) = 0 \\ \iff \quad K(U_1(v), v) &= 0. \end{aligned}$$

Therefore, the formula for $G(v, vy, x, y)$ as given in the statement of the lemma holds. Lastly, the expression for H is obtained by plugging equation (5.9) into the original definition of H, reducing the resulting fraction and collecting terms. □

Now that we know $G(v, vy) = G(vy, v)$ in the equation from Lemma 5.7, we can use the symmetry of the generating function to get the other: this significantly reduces the computations. In the earlier chapter, we had two unknown specializations and even though the Kernel was symmetric (but only the Kernel and not the main generating function itself), we could not derive one immediately from the knowledge of the other.
In this case it is possible, yielding an expression for $G(u, v, x, y)$ in general by plugging into an earlier result. We state it as a theorem.

Theorem 5.15. *The generating function of partially directed walks within the symmetric wedge ending in a horizontal step is given by*

$$\begin{aligned} G(u, v, x, y) = {} & \frac{(u - vy)(v - uy)}{K(u, v)} - \frac{u^2 vxy(u - vy)}{K(u, v)} \left(1 + \frac{H(u, x, y)}{y}\right) \sum_{i \geq 0} (-1)^i y^{i^2} H(u, x, y)^i \\ & - \frac{uv^2 xy(v - uy)}{K(u, v)} \left(1 + \frac{H(v, x, y)}{y}\right) \sum_{i \geq 0} (-1)^i y^{i^2} H(v, x, y)^i, \end{aligned}$$

where the formal power series H is defined as in Lemma 5.14.

This is the final result for the general generating function and yields a rather complicated series. In contrast to all of the chapters before, where the final results were either rational or algebraic, it is a non-holonomic series, as the authors of [vRPR08] state. In our situation, though, this is of no importance.

To close this chapter, we want to give a solution to Task 5.4 which motivated the whole exercise. The following theorem summarizes the results.

Theorem 5.16 ([vRPR08])**.** *The generating function G of partially directed walks of length n, constrained to the symmetric wedge W and ending with a horizontal step is given by*

$$G(t) \equiv G(1, 1, t, t) = \frac{1 - t}{1 - 2t - t^2} - \frac{1 - t^2 - \sqrt{(1 - t^2)(1 - 5t^2)}}{1 - 2t - t^2} \sum_{n \geq 0} (-1)^n t^{n^2} H(1, t, t)^n,$$

where

$$H(1, t, t) = \frac{1 - 3t^2 - \sqrt{(1 - t^2)(1 - 5t^2)}}{2t}.$$

Furthermore, the generating function F of partially directed walks of length n constrained to the symmetric wedge W (without the restriction of ending in a horizontal step) is given by

$$F(t) \equiv F(1, 1, t, t) = \frac{1 + t}{1 - 2t - t^2} - \frac{1 - t^2 - \sqrt{(1 - t^2)(1 - 5t^2)}}{t(1 - 2t - t^2)} \sum_{n \geq 0} (-1)^n t^{n^2} H(1, t, t)^n.$$

Proof. The proof merely consists of plugging the right values into the generating function from Theorem 5.15. As we are only interested in the length of the path, and not the number of steps taken horizontally or vertically, we simply set the generating variables corresponding to the number of these steps to $x = y = t$. Hence, both contribute equally to the length of the walk.
Similarly, the location of the endpoint does not matter either. In the language of generating functions, this translates to setting the conjugated variables u and v to one, i.e. they effectively vanish from the series.
Clearly, these two modifications simplify the equation from the preceding theorem. Carrying out the transformations yields $K(1, 1, t, t) = (1 - t)(1 - t)(1 - t) - t^2(2 - 2t) = (1 - t)(1 - 2t - t^2)$ and

$$H(1, t, t) = \frac{(1 - t^2)(1 - 2t^2) - \sqrt{(1 - t^2)(1 - 5t^2)}}{(1 - t^2)3t + t\sqrt{(1 - t^2)(1 - 5t^2)}}.$$

By multiplying both, nominator and denominator, by $(1 - t^2)3t - t\sqrt{(1 - t^2)(1 - 5t^2)}$ we get rid of the square root in the denominator. Proceed by reducing the resulting fraction by $2t(t^4 - 3t^2 + 2)$ and we obtain the reasonably simple expression

$$H(1, t, t) = \frac{1 - 3t^2 - \sqrt{(1 - t^2)(1 - 5t^2)}}{2t}.$$

Combining this in the equation for G,

$$\begin{aligned}
G(t) = {} & \frac{(1 - t)^2}{(1 - t)(1 - 2t - t^2)} - \sum_{n\geq 0}(-1)^n t^{n^2} H(1, t, t)^n \\
& \cdot \left(\frac{t^2(1 - t)}{(1 - t)(1 - 2t - t^2)} \left(1 + \frac{H(1, t, t)}{t}\right) + \frac{t^2(1 - t)}{(1 - t)(1 - 2t - t^2)} \left(1 + \frac{H(1, t, t)}{t}\right)\right) \\
= {} & \frac{1 - t}{1 - 2t - t^2} - 2\frac{t^2}{1 - 2t - t^2} \left(1 + \frac{1 - 3t^2 - \sqrt{(1 - t^2)(1 - 5t^2)}}{2t^2}\right) \sum_{n\geq 0}(-1)^n t^{n^2} H(1, t, t)^n \\
= {} & \frac{1 - t}{1 - 2t - t^2} - \frac{1 - t^2 - \sqrt{(1 - t^2)(1 - 5t^2)}}{1 - 2t - t^2} \sum_{n\geq 0}(-1)^n t^{n^2} H(1, t, t)^n,
\end{aligned}$$

yields the result as presented in the statement of the theorem.
Lastly, to obtain the generating function F, we use the simple relation (5.6). That is, $F(t) = (G(t) - 1)/t$. This leads directly to the formula in the theorem. □

The last theorem finishes our solution to the task of obtaining the generating function for partially directed walks in the symmetric wedge W. Even though the final result is a bit simpler than the general form, it is still a complicated series. An explicit expression for its coefficients is therefore not what we are looking for. Instead it is now possible to obtain asymptotic results for the number of partially directed walks by the methods of singularity analysis. Indeed, this is what the authors of [vRPR08] do as the final step in their paper. They also state that the generating functions $H(v, x, y)/y$ and $G(v, vy)$ have combinatorial interpretations, counting special kinds of paths. However, they could not derive the results obtained by the Kernel method with a more combinatorial technique in the cited paper.

For our purposes, let us recall the key to solving the functional equation given in Lemma 5.7: it is a special flavor of the Kernel method, called the iterated Kernel method. It involves finding new roots of the Kernel $K(u, v)$ by following one of the branches of the algebraic curve defined by $K(u, v) = 0$. In this way, we obtain an infinite sequence of well defined solutions which set the Kernel to zero. From this an iterative scheme can be derived which eventually yields an expression for the generating function defined by the underlying functional equation.

The computations as shown here were particularly simple because of the highly symmetric problem we have studied - the symmetry of the wedge W resulted in a symmetry of the generating function of walks restricted to W. This enabled us to find the unknown specializations of the main generating function much easier. But what happens if this nice property is not applicable?

In [vRPR08], the authors proceed to study the same counting problem where walks are not confined to W, but to an asymmetric wedge, given by the horizontal axis and the main diagonal line $y(x) = x$. The approach remains unchanged and we use the same notations as in the demonstration above. A recursive description leads to a functional equation for the generating function encoding partially directed walks ending in a horizontal step. However, the essential distinction is that the generating function, as well as the Kernel of the relation, lack the symmetry in u and v we exploited earlier. Thus, one has to study the Kernel as a (quadratic) polynomial in u and additionally in v. This gives two different kinds of roots: the solutions for u, given by $U_1(v)$ (again denoting the root which has a formal power series expansion in t when setting $x = y = t$) and $U_{-1}(v)$, respectively for v, namely $V_1(u)$ and $V_{-1}(u)$. Recall that these series were equal in the example we have studied above (i.e. $U_1 = V_1$ and $U_{-1} = V_{-1}$).
Proceed by plugging the two roots which have a formal power series expansion into the functional equation, which sets the Kernel to zero and gives two new equations. Each of them is too complicated to be applied iteratively, though. But combining the equations by considering mixed compositions of the roots (i.e. substitute U_1 for u in the equation obtained by using V_1 first) does yield a relation which can be iterated. To this end, one defines $W_1(u) := U_1(V_1(u))$ and $W_n(u) := W_{n-1}(W_1(u))$ as the counterpart of the series of roots in the symmetric case. At last, this leads to a complicated expression for the generating function. The next steps are similar to the ones we have shown here: the result is a solution to the problem, but it has to be simplified significantly to be legible. The lengthy computations necessary to do this can be found in [vRPR08].

To close this chapter, we want to consider the case of slightly more general wedges we have mentioned before. That is, their boundary lines are given by $y(x) = -\alpha x$ and $y(x) = \alpha x$ in the symmetric, and the x-axis and $y(x) = \alpha x$ in the asymmetric case - such that $\alpha \in \mathbb{R} \setminus \{0, 1\}$. In theory, the problem works out just as we have demonstrated here. But that is obviously not enough to obtain results - practical reasons prevent one from actually computing a solution. Hence, it certainly needs more work to improve the working out

of this technique - maybe by more raw computing power or better ways to manipulate algebraic expressions.
Let us briefly explain the troubles in the specific case of partially directed walks. The recursions leading to the functional equation are essentially the same, as outlined above. However, the problem lies in the infinite sequence of the roots of the Kernel. Here we have seen that it was essential to simplify them significantly, in order to be able to work with the results from the iterated substitutions. In the case of boundary lines with general slope α this is not easily possible. Therefore, while carrying out the iterative scheme, the new solutions to $K(u, v) = 0$ get more and more complicated until they reach a point where it is not feasible to work with them anymore. This marks the limits of the Kernel methods, in a way - our methods of working with such complex expressions are simply not sophisticated enough to produce results with it for very difficult problems.

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