AUTOMATED POSITIVE PART EXTRACTION FOR LATTICE PATH GENERATING FUNCTIONS IN THE OCTANT

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ABSTRACT. The question of classifying the nature of the generating functions of restricted lattice walks has enjoyed much attention in past years. We prove that a certain class of octant walks have a D-finite generating function using the theory of multivariate formal Laurent series.

1. Introduction

We focus our attention in this paper to the positive octant, i.e., the three-dimensional integer lattice, restricted so that all coordinates are nonnegative. Let \( L = (\mathbb{Z}_{\geq 0})^3 \). Fix a model (also called stepset) \( S \subset \{-1, 0, 1\}^3 \setminus \{(0, 0, 0)\} \). A length \( m \) \( S \)-walk is any walk which starts at \((0, 0, 0)\) and takes \( m \) steps from \( S \). Let \( f(i, j, k; n) \) denote the number of \( S \)-walks of length \( n \) ending at point \((i, j, k) \in L\).

We form the generating function

\[
F(x, y, z; t) = \sum_{i,j,k,n \geq 0} f(i, j, k; n) x^i y^j z^k t^n
\]

and ask whether \( F(x, y, z; t) \) is D-finite over \( \mathbb{Q}(x, y, z, t) \) in each variable. In other words, does there exist a nontrivial linear differential equation in each variable with coefficients in \( \mathbb{Q}[x, y, z, t] \)?

There are \( 2^{3^3} - 1 = 67,108,864 \) models in the octant. After choosing a canonical representative for models that are in bijection to each other for simple reasons and removing all cases that are equivalent to lower-dimensional problems, we are still left with \( 10,908,263 \) models [2]. In [3], these remaining models were sorted according to properties that sometimes help establish whether the corresponding generating function is D-finite. One of these properties is the order of a certain group of rational transformations associated to the model. If the group of the model is finite, then it may be possible to establish the D-finite nature of the generating function via the orbit sum argument of [6] (summarized in the next section). There are altogether \( 2,430 \) models with a finite group [2, 8]. For 108 of them, it was shown in [3] that their corresponding generating functions are D-finite. We show in the present paper that the orbit sum argument applies to 1,964 additional models, and that they are therefore also D-finite. The remaining 358 models are the zero orbit sum cases, for which different methods are needed.

2. The Orbit Sum Method

For a fixed model \( S \), we define the stepset (Laurent) polynomial to be \( P_S = \sum_{(u,v,w) \in S} x^u y^v z^w \). The rational transformation \( \phi_x : \mathbb{Q}(x, y, z) \to \mathbb{Q}(x, y, z) \) given...
by \( \phi(x, y, z) := \left( x^{-1} \sum_{(i, v, w) \in S} y^i z^w, y, z \right) \) fixes \( P_S \) as well as \( y \) and \( z \), and is idempotent. The transformations \( \phi_y \) and \( \phi_z \) are defined similarly. Then, the group \( G_S \) generated by \( \phi_x, \phi_y, \phi_z \) via composition is called the group of the model \( [10] \). For \( g \in G_S \), \( \text{sgn}(g) = 1 \) if \( g \) is a composition of an even number of generators, and \(-1\) otherwise.

Most models in the octant have an infinite group, but for the 2,430 cases in the octant with a finite group, we can attempt to use the orbit sum method to prove that their corresponding generating functions are D-finite. The details of this technique for the octant appear in \([3]\); we reproduce a brief sketch here.

The starting point of the technique is the \textit{functional equation}, which can be obtained using an inclusion-exclusion argument. The left-hand side of this equation only involves \( F(x, y, z; t) \), but the right-hand side involves sections or specializations of \( F(x, y, z; t) \) such as \( F(x, y, 0; t) \) and \( F(x, 0, 0; t) \) \([3]\) Eqn. 7]. Using the group of the model, we form the \textit{orbit sum}, which allows us to eliminate the sections on the right-hand side and leaves us with:

\[
\sum_{g \in G} \text{sgn}(g) g(xyz)(F(g(x), g(y), g(z); t)) = \frac{1}{1 - tP_S} \sum_{g \in G} \text{sgn}(g) g(xyz) \tag{1}
\]

The generating function \( F(x, y, z; t) \) is an element of \( \mathbb{Q}[x, y, z][[t]] \). Thus, \( F_g := F(g(x), g(y), g(z); t) \in \mathbb{Q}[x, y, z][[t]] \) is a power series in \( t \) with coefficients \( a_i \in \mathbb{Q}(x, y, z) \). We regard each of these \( a_i \) as a \textit{multivariate formal Laurent series} rather than a rational function (see Section \([10]\)). Then, the positive part extraction \( [x^0 y^0 z^0] \) is well-defined, and we apply it to obtain an expression with only \( F(x, y, z; t) \) on the right-hand side

\[
xyzF(x, y, z; t) = [x^0 y^0 z^0] \frac{1}{1 - tP_S(x, y, z)} \sum_{g \in G} \text{sgn}(g) g(xyz) \tag{2}
\]

The above equation holds if every monomial in \( F_g \) has at least one negative component in its exponent for each non-identity element \( g \in G_S \). Then, \( F(x, y, z; t) \) can be written as the diagonal of a rational series, and is therefore D-finite \([3, 10]\).

The orbit sum technique gives a uniform method for proving that some octant models have D-finite generating functions. However, it is not without its limitations. If there are one or more non-identity \( g \in G_S \) such that \( F(g(x), g(y), g(z); t) \) contributes to the positive part on the left-hand side, we do not obtain an expression for \( xyzF(x, y, z; t) \) alone, and therefore cannot conclude that \( F(x, y, z; t) \) is D-finite. For such models, a different proof technique is needed. Included among these models are the so-called \textit{zero orbit sum} cases, for which the right-hand side of Equation \([1]\) is 0. In the quadrant, these models correspond exactly to the cases where the generating function is algebraic \([4, 5]\). In the octant, there are two subclasses among the zero orbit sum cases: \textit{Hadamard} and \textit{“mysterious”}. Bostan et al provide an alternative proof technique for octant Hadamard cases in \([3]\): all of the zero orbit sum Hadamard models they consider have D-finite generating functions. The remaining 170 models are those which were deemed \textit{“mysterious”} in \([2]\). These cases have yet to be definitively classified, but there is strong computational evidence that at least some of them have non-D-finite generating functions \([2]\).

In this paper, we identify models for which \( xyzF(x, y, z; t) \) is the only surviving term on the left-hand side of Equation \([1]\) after the positive part extraction, and
prove automatically that their generating functions are D-finite via the orbit sum argument.

3. Multivariate formal Laurent series

We recall here the bare essentials of the theory of multivariate formal Laurent series, as formalized by Aparicio-Monforte and Kauers [1]. In order to ensure that multiplication of series is well-defined, we consider multivariate series with support contained in a line-free cone.

Let \( k \) be a field, \( x_1, \ldots, x_n \) be \( n \) indeterminates, and \( C \subset \mathbb{R}^n \) be a line-free cone. \( k_C([x_1, \ldots, x_n]) := \{ f(x) = \sum_k a_k x^k \mid \text{supp } f(x) \subseteq C \} \) with the usual addition and Cauchy product multiplication is an integral domain. If, on the other hand, we fix a specific additive order on \( \mathbb{Z}^n \), we can form the sets \( k_\leq([x]) := \bigcup_{C \in C} k_C([x]) \) and \( k_\leq((x)) := \bigcup_{v \in \mathbb{Z}^n} x^v k_\leq([x]) \), where \( x = (x_1, \ldots, x_p) \) with \( x_i \) indeterminate for every \( i \), and \( C \) is the set of all cones \( C \subset \mathbb{R}^p \) compatible with \( \leq \). The condition that \( \leq \) be additive ensures that \( k_\leq([x]) \) is a ring and that \( k_\leq((x)) \) is a field [1, Thm. 15]. We call \( k_\leq([x]) \) a multivariate formal Laurent series ring and \( k_\leq((x)) \) the field of the multivariate formal Laurent series ring. We define the leading exponent of an element \( f(x) \) to be \( \text{lexp}_\leq f(x) = \min_\leq(\text{supp } f(x)) \in \mathbb{Z}^p \), and the leading term \( \text{lt}_\leq f(x) = x^{\text{lexp}_\leq f(x)} \).

The following theorem is essential for the automatic positive part extraction we will describe in the next section:

**Theorem 1** ([1, Thm. 17]). Let \( C \subset \mathbb{R}^q \) be a line-free cone and \( f(y) \in k_C([y]) \). Let \( \leq \) be an additive order on \( \mathbb{Z}^p \) and \( a_1(x), \ldots, a_q(x) \in k_\leq((x)) \setminus \{0\} \). Let \( M \in \mathbb{Z}^{p \times q} \) be the matrix whose \( i \)-th column consists of the leading exponent \( \text{lexp}(a_i(x)) \). Let \( C' \subset \mathbb{R} \) be a cone containing \( MC := \{ Mx \mid x \in C \} \subset \mathbb{R}^p \) as well as \( \text{supp } (a(x)/\text{lt}(a_i(X))) \) for every \( i \in \{1, \ldots, q\} \). Suppose that \( C \cap \ker M = \{0\} \) and that \( C' \) is line-free. Then, \( f(a_1(x), \ldots, a_q(x)) \) is well-defined and belongs to the ring \( k_{C'}([x]) \).

After the positive part extraction is applied with the help of this theorem, the next step is to find a differential equation for \( F(x, y, z; t) \) and possibly an expression for \( F(x, y, z; t) \) itself. The theory of multivariate formal Laurent series is also useful for this step: in [4], for example, this theory is used to prove computationally guessed annihilating differential operators for the sections \( F(x, 0; t) \) and \( F(0, y; t) \) of certain quadrant models. These operators lead to an annihilating differential operator for \( F(x, y; t) \), as well as explicit expressions for \( F(x, y; t) \) in terms of hypergeometric functions.

4. Application to Lattice Paths

For a given \( S \), we apply Theorem [1] \( |G_S| \) times. The support of \( F(x, y, z; t) \) can be shown to be contained in \( C = \langle \{(0, 0, 0, 1), (0, 1, 0, 1), (0, 0, 1, 1), (0, 1, 0, 1), (1, 0, 0, 1), (1, 0, 1, 1), (0, 1, 1, 1), (1, 1, 1, 1)\} \rangle \). Fix a non-identity \( g \in G_S \). We set \( f(y) = F(x, y, z; t), a_1(x) := g(x), a_2(x) := g(y), a_3(x) := g(z), \) and \( a_4(x) = t \). To create an additive order on \( \mathbb{Z}^p \), we collect all polynomials \( q_i \) that appear in the numerator or denominator of the \( a_i \). For each of these polynomials \( q_i \) we choose a leading term, and check that this choice of leading term is compatible with the cone. If so, we check the conditions of Theorem [1] are fulfilled. If they are, we conclude that the composition \( F_g = F(g(x), g(y), g(z); t) \) is valid, and also obtain a cone \( C'_g \) with the property that \( F_g \in k_{C'_g}([x]) \). Next, define \( B \) to be the smallest cone
containing $C$ and $C'_g$. We check that $B$ is line-free, and that $\text{supp}(g(xyz)F_g)\cap C = \emptyset$. Then, we have proven that $[x>0 y>0 z>0]g(xyz)F_g = 0$.

If we experience a failure at any of the above steps, we simply choose different leading terms for the $q_i$ and try again. The properties of $G_S$ ensure that there are not many polynomials $q_i$ for which we can choose leading terms, and that each $q_i$ can only contain a small number of monomials. Thus, it is computationally feasible to check every combination of leading terms that is compatible with $C$.

We repeat this process for every non-identity $g \in G$, setting $B$ to be equal to the smallest cone containing the previous cone $B$ and the cone $C'_g$. If the process terminates successfully, we obtain a cone $B$ with the property that $g(xyz)F_g \in k_\prec((x))$ for every $g$. We also know that the only contribution to the left-hand side of the orbit sum with support intersecting $C$ is the element $xyzF(x, y, z)$. That is, the positive part extraction step yields an expression for $xyzF(x, y, z; t)$ alone that allows us to conclude that $F(x, y, z; t)$ is D-finite.

**Example 1.** Let $S = \{(-1, -1, 0), (-1, 0, 1), (-1, 1, -1), (0, -1, 1), (0, 0, -1), (0, 1, 0), (1, 0, 0)\}$. $G_S = \{\phi_x, \phi_y, \phi_z\} \cong D_{12}$, with $\phi_x = \left(\frac{yz^2 + y^2 + z}{xyz}, y, z\right)$, $\phi_y = \left(x, \frac{x}{y}, z\right)$, $\phi_z = \left(x, y, \frac{y}{z}\right)$. For this example, the only polynomial that appears as a term in a rational transformation is $p = yz^2 + y^2 + z$. Choose $\text{lexp}_\prec(p) = (0, 1, 2, 0)$. For each $g \in G$ we now attempt to apply Theorem [4]. Consider for example the element $\phi_x \in G_S$. $M = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$.

We have that $C \cap \ker(M) = \{0\}$. Additionally, $C'_{\phi_x} = \langle(0, -2, 1, 0), (0, -1, 2, 0), (0, 0, 0, 1)\rangle$. Thus, $F_{\phi_x} = \frac{yz^2 + y^2 + z}{xyz}yF\left(\frac{yz^2 + y^2 + z}{xyz}, y, z; t\right)$ is well-defined, and additionally $\text{supp}(\phi_x(xyz)F_{\phi_x})\cap C = \emptyset$. Moreover, the smallest cone $B$ containing both $C$ and $C'_{\phi_x}$ is line-free. Continuing this process for each $g \in G_S$, we obtain the cone $C_G = \langle(1, 1, 1, 1), (1, -1, 2, 1), (0, 1, -2, 0), (-1, -1, 3, 1), (0, -1, 1, 0), (-1, -1, 2, 1)\rangle$, which is line-free. The left-hand side of the orbit sum equation is well-defined in $kC_G[[x]]$, and $F(x, y, z; t)$ is the only term that survives the operation $\text{supp}(g(xyz) \cdot F(g(x), g(y), g(z); t)) \cap C$ for $g \in G_S$, and $F(x, y, z; t)$ is D-finite.

**Example 2.** Next we consider a case for which the right-hand side of Equation [3] is equal to zero. Let $S = \{(-1, -1, -1), (-1, 0, 0), (-1, 0, 1), (-1, 1, 0), (1, -1, 0), (1, 0, -1), (1, 1, 1)\}$. $G_S \cong D_{12}$ as before, but is generated by different rational transformations $\phi_x, \phi_y, \phi_z$ than in the previous example. In particular, we have $\phi_x\phi_y\phi_z = (x, z, y)$. Since $\text{lt}_\prec(x) = x$, $\text{lt}_\prec(y) = y$ and $\text{lt}_\prec(z) = z$ for any choice of $\prec$, we have $M_{\phi_x\phi_y\phi_z} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$. Since $C'_{\phi_x\phi_y\phi_z} = C$, the term $xyzF(x, z, y)$ on the left-hand side of Equation [3] survives the positive part extraction, and we cannot proceed.
5. Octant cases with finite group

Using the technique outlined in the previous section, we obtain the following theorem.

**Theorem 2.** All 2,072 three-dimensional octant models with finite group and nonzero orbit sum are D-finite.

We say that a model is three-dimensional if the condition that \( \sum_{s \in S} a_s s \geq (0, 0, 0) \) is a truly three-constraint problem. A model defined in the octant need not be three-dimensional; see [3, §2.1, §7.1] for a more extended discussion.

Theorem 2 includes the 108 cases that were already proven in [3]. In [2], it was conjectured that the 1,964 models covered in Theorem 2 could be proved D-finite by the orbit sum method. The contribution of the current work is to confirm this conjecture. The proof is fully automatic: our implementation of the process outlined in Section 4 uses Sage [7] and requires only the model \( S \) as input.

The remaining 358 models not covered by Theorem 2 are exactly those for which Equation 1 has a vanishing right-hand side. This shows that the only cases for which the orbit sum technique fails at the positive part extraction step are those that are equivalent to two-dimensional cases with multiplicities, which are discussed in [3, 9].

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