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Transfer-matrix methods meet Ehrhart theory

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ABSTRACT

Transfer-matrix methods originated in physics where they were used to count the number of allowed particle states on a structure whose width n is a parameter. Typically, the number of states is exponential in n. One mathematical instance of this methodology is to enumerate the proper vertex colorings of a graph of growing size by a fixed number of colors.

In Ehrhart theory, lattice points in the dilation of a fixed polytope by a factor k are enumerated. By inclusion–exclusion, relevant conditions on how the lattice points interact with hyperplanes are enforced. Typically, the number of points are (quasi-) polynomial in k. The text-book example is that for a fixed graph, the number of proper vertex colorings with k colors is polynomial in k.

This paper investigates the joint enumeration problem with both parameters n and k free. We start off with the classical graph colorings and then explore common situations in combinatorics related to Ehrhart theory. We show how symmetries can be explored to reduce calculations and explain the interactions with Discrete Geometry.

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1. Introduction

Graph colorings have been intriguing mathematicians and computer scientists for decades. Historically, graph colorings first appeared in the context of the 4-color conjecture. Birkhoff — trying to prove said conjecture — introduced what is now called the chromatic polynomial. Whitney later generalized this notion from planar graphs to arbitrary graphs, see [24]. Chromatic polynomials are one of the fundamental objects in algebraic graph theory with many questions about them still unanswered. For instance, in 1968 Read asked which polynomials arise as chromatic polynomials of some graph. This question remains wide open to this day. However, some progress has been made. In 2012, June Huh showed that the absolute values of the coefficients form a log-concave sequence, see [13, Thm. 3], thus proving a conjecture by Rota, Heron, and Welsh. Not only classifying chromatic polynomials is extremely challenging, but also explicitly computing the coefficients turns out be $\#P$-hard, see [14].

In the first part of this article, we examine proper k-colorings of Cartesian graph products of the form $G \times P_n$ and $G \times C_n$, where G is an arbitrary graph and P_n (C_n) is the path (cycle) graph on n nodes, respectively. The motivation for this problem is twofold.

First, it lies at the intersection of transfer-matrix methods and Ehrhart theory, both areas being interesting in their own right. Classically, transfer-matrix methods have been used to count the number of (possibly closed) walks on weighted graphs. However, transfer-matrix methods also made an appearance in seemingly unrelated areas such as calculating DNA-protein-drug binding in gene regulation [23], the 3-dimensional dimer problem [7], counting graph homomorphisms [15], computing the partition function for some statistical physical models [11], and determining the entropy in physical systems [12]. One of the big problems in these applications is that the size of the transfer matrices increases extremely fast as the size of the system increases. Therefore, one needs to either limit the size of the system or find a way of "compactifying" these transfer matrices. In [7], Ciucu uses symmetry to reduce the size of the matrix. We follow and expand these ideas. Similar techniques have also been used by [15]. Ehrhart theory is the study of integer points in polytopes and as such it appears in various disguises anytime someone tries to examine/count/find Diophantine solutions to a system of linear inequalities with bounded solution set. Moreover, it is related to algebraic geometry and commutative algebra [6,8,20], optimization [3,22], number theory [1,2,17], combinatorics [4,20], and — for this article most importantly — to proper graph colorings [5].

Second, this problem also has direct applications to physics: If G represents a molecular structure, then $G \times P_n$ corresponds to several connected layers of that molecular structure. The k colors correspond to k different states of the atoms. Counting the number of possible combinations is the same as counting the number of colorings. If we furthermore assume that two adjacent atoms are not allowed to be in the same state, we arrive at a classical proper coloring problem. Since n is very large in physical systems and also k may vary, the (doubly or single) asymptotic behavior is of interest.