┃computational complexity

ZEROS AND APPROXIMATIONS OF HOLANT POLYNOMIALS ON THE COMPLEX PLANE

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Abstract. We present fully polynomial time approximation schemes for a broad class of Holant problems with complex edge weights, which we call *Holant polynomials*. We transform these problems into partition functions of abstract combinatorial structures known as *polymers* in statistical physics. Our method involves establishing zero-free regions for the partition functions of polymer models and using the most significant terms of the *cluster expansion* to approximate them.
Results of our technique include new approximation and sampling algorithms for a diverse class of Holant polynomials in the low-temperature regime (i.e. small external field) and approximation algorithms for general Holant problems with small signature weights. Additionally, we give randomised approximation and sampling algorithms with faster running times for more restrictive classes. Finally, we improve the known zero-free regions for a perfect matching polynomial.

Keywords. Holant problems, approximate counting, partition functions, graph polynomials

Subject classification. 68Q25

1. Introduction

The ongoing effort to characterise the complexity of approximating partition functions that originate from statistical physics has

recently seen great progress. Such partition functions take as input a metric, usually a graph, that encodes how particles interact. Two kinds of such partition functions have been studied in the literature: vertex spin systems, where vertices assume some state (spin) and edges are functions encoding the energy of vertex interactions; and edge spin systems, where the edges assume spins and the vertices are functions encoding the energy of edge interactions. So far, the main body of literature focuses on the first category of vertex spin systems. Results include remarkable connections between the phase transitions spin systems undergo and the approximability of their partition function, see e.g. (Galanis *et al.* 2014; Peters & Regts 2019; Sly 2010; Weitz 2006).

 This article focuses on the second category of edge spin systems, which can be naturally encoded under the *Holant* framework of counting problems. Our results include approximation algorithms for *Holant polynomials* in the low energy regime and approximation algorithms for *Holant problems* with vertices encoding small weights. In particular, we identify new tractable cases for such Holants with respect to their approximability.

 The Holant framework originates in Valiant's "Holographic algorithms" (2008) to model perfect matching computations and was extended by Cai *et al.* (2011) to encode partition functions of edge spin systems such as edge covers and Eulerian orientations. A Holant problem is parametrised by a finite set of functions (often called *signatures*) $\mathcal{F}$ with domain D. For a graph $G = (V, E)$ and a mapping $\pi\colon V \to \mathcal{F}$, where $\pi(v) = f_v$ maps $v \in V$ to a function $f_v\colon D^{E(v)} \to \mathbb{C}$, the *Holant problem* is to compute the function

$$\mathrm{Hol}_{\mathcal{F}}(G, \pi) = \sum_{\sigma \in D^E} \prod_{v \in V} f_v(\sigma|_{E(v)})$$

with $E(v)$ denoting the set of edges incident to v.

 External conditions like fugacity are known in statistical physics as *external fields* and encoded in partition functions as weights in the system. In the Holant framework, this yields Holant problems with external fields, which we call *Holant polynomials*. For a signature set $\mathcal{F}$ and a domain $D = \{0, 1, \ldots, \kappa\}$ for some $\kappa \in \mathbb{Z}_{>0}$ the *Holant polynomial* maps a graph $G = (V, E)$ and a mapping $\pi\colon V \to \mathcal{F}$ to the function

$$Z_{\mathcal{F}}(G, \pi, \mathbf{z}) = \sum_{\sigma \in D^E} \prod_{v \in V} f_v(\sigma|_{E(v)}) \prod_{i=0}^{\kappa} z_i^{|\sigma|_i},$$

where $\mathbf{z} = (z_0, z_1, \ldots, z_\kappa)$ and $|\sigma|_i$ denotes the number of edges $e \in E$ with $\sigma(e) = i$. As an example, if $\mathbf{z} = (1, z)$ and the set of signatures $\mathcal{F}$ contains the functions taking the value 1 if at most one of the input variables is set to 1 and the value 0 otherwise, the Holant polynomial is the matching polynomial $Z_{\mathcal{M}}(G, \mathbf{z})$.

Our results restrict the signature sets to be subsets of $\mathcal{F}_0 = \{f \mid f(\mathbf{0}) \neq 0\}$ and to contain only polynomially computable signatures, i.e. $f \in \mathsf{FP}$. For $f \in \mathcal{F}_0$ with arity d we define $r(f) = \max_{x \in D^d \setminus \{\mathbf{0}\}}\{|f(x)|/|f(\mathbf{0})|\}$ and for a signature class $\mathcal{F} \subseteq \mathcal{F}_0$ we define $r(\mathcal{F}) = \max_{f \in \mathcal{F}}\{r(f)\}$. Our main theorem is the following.

THEOREM 1.1. *Let $\mathcal{F} \subseteq \mathcal{F}_0$. For all graphs G of maximum degree Δ and all $\pi \colon V \to \mathcal{F}$, the Holant polynomial admits an FPTAS for $\mathbf{z}$ in*

$$\left\{ (z_0, \ldots, z_\kappa) \in \mathbb{C}^{\kappa+1} \;\middle|\; z_0 \neq 0, \frac{|z_i|}{|z_0|} < (\Delta \kappa e^2 r_1(r_1 + 1))^{-1}, \; i \in [\kappa] \right\}$$

with $r_1 = \max\{1, r(\mathcal{F})\}$.

This result captures a very broad class of Holant polynomials. The only requirement in terms of the class of signatures is that the all zeros assignment σ_0 contributes a nonzero term in the sum. Essentially, this ensures the existence of a trivially computable solution for the related decision problem: the all zeros configuration. In a sense, an efficient way to show the existence of a solution is necessary since hardness of this decision problem immediately implies hardness of approximation as Dyer *et al.* (2004, Theorem 1) observe.

The region stated in Theorem 1.1 excludes the value $\mathbf{z} = \mathbf{1}$, therefore it does not apply to Holant problems directly. However, our technique also yields the following theorem.

THEOREM 1.2. *Let $\mathcal{F} \subseteq \mathcal{F}_0$, with $r(\mathcal{F}) < \max\{(2\sqrt{e})^{-1}(\Delta \kappa e)^{-\frac{\Delta}{2}},$ $0.2058(\kappa + 1)^{-\Delta}\}$. For all graphs G of maximum degree Δ and all $\pi \colon V \to \mathcal{F}$, the Holant problem $Z_{\mathcal{F}}(G, \pi)$ admits an FPTAS.*

Key to our technique is to translate the mappings σ as perturbations from a ground state σ_0, which results in a mathematical object called *abstract polymer model* (see Section 1.1). One of the advantages of polymer models is that they are *self-reducible*. A known implication of self-reducibility is the equivalence between approximate counting and sampling (Jerrum *et al.* 1986, Sinclair & Jerrum 1989). As Helmuth *et al.* (2019, Section 5) observe, counting algorithms for polymer models can be converted to algorithms that approximately sample from the *Gibbs distribution* μ_G, where in our case is defined as

$$\mu_G(\sigma) = \frac{\prod_{v \in V(G)} f_v(\sigma|_{E(v)}) \prod_{i=0}^{\kappa} z_i^{|\sigma|_i}}{Z_{\mathcal{F}}(G, \pi, \mathbf{z})}.$$

One of the downsides of the above algorithms is that the runtime is in $\mathcal{O}(n^\Delta)$. Under more restrictive conditions and for particular polymer models, Chen *et al.* (2021) showed how to obtain faster randomised algorithms. As we discuss in Section 5, we extend their technique to show that it also applies to polymer models for Holants.

The approach of our technique allows establishing improved regions of approximability when we restrict the set of signatures further. In Section 6.1.1, we illustrate this via the *perturbative perfect matching polynomial*, a holant polynomial defined as follows. For a graph G and a perfect matching M of G, let

$$Z_{\mathrm{pm}}(G, M, z) = \sum_{\sigma \in \{0,1\}^E} \prod_{v \in V} f(\sigma|_{E(v)}) z^{|\sigma \Delta \sigma_M|}.$$

Here, $\sigma_M \in \{0,1\}^E$ denotes the signature corresponding to M, $\sigma \Delta \bar{\sigma} = \{e \in E \mid \sigma(e) \neq \bar{\sigma}(e)\}$ for any two assignments $\sigma, \bar{\sigma} \in \{0,1\}^E$ and f is the "exactly one" function. This Holant polynomial was studied by Barvinok & Regts (2019), where they showed FPTAS for $|z| \leq (3.07438\Delta)^{-1}$, where Δ is the maximum degree of G. Using a polymer representation, we improve this region, even asymptomatically in terms of Δ.

THEOREM 1.3. *For all graphs G of maximum degree Δ, the polynomial $Z_{\mathrm{pm}}(G, M, z)$ admits an FPTAS for $z \in \mathbb{C}$ with $|z| \leq \left(\sqrt{4.85718(\Delta - 1)}\right)^{-1}$.*

1.1. Methodology.   The central part of our technical approach is to define a polymer model representation for Holant problems and Holant polynomials. Polymer models are an established tool for the study of partition functions in statistical physics (Friedli & Velenik 2017, Chapter 7) originating from the work of Gruber & Kunz (1971) and Kotecký & Preiss (1986). A polymer model consists of a finite set K of elements called *polymers* and a symmetric and reflexive binary *incompatibility* relation denoted by $\not\sim \subseteq K \times K$. Based on this relation, $\mathcal{I}(K)$ denotes the set of all subsets $\Gamma \subseteq K$ of pairwise compatible polymers, which we will call *families* of pairwise compatible polymers. Given an assignment of weights (*polymer functionals*) $\Phi \colon K \to \mathbb{C}$ to the polymers, we define the *polymer partition function*

$$Z(K, \Phi) = \sum_{\Gamma \in \mathcal{I}(K)} \prod_{\gamma \in \Gamma} \Phi(\gamma) \,.$$

Given a polymer model, we can construct the *polymer graph* $(K, \not\sim)$ where the polymers represent the vertices of this graph and the edges are given by the incompatibility relation. In this way, we observe that the families of compatible polymers are the independent sets of the polymer graph. Weighted sums of independent sets are naturally expressed by the independence polynomial of a graph G defined on $\mathbf{z} = (z_v)_{v \in V(G)}$ as

$$Z_{\mathcal{I}}(G, \mathbf{z}) = \sum_{I \in \mathcal{I}(G)} \prod_{v \in I} z_v,$$

where $\mathcal{I}(G)$ is the set of independent sets of G. From this definition observe that the partition function of a polymer system is the independence polynomial of the polymer graph, where each vertex γ in the polymer graph has weight $\Phi(\gamma)$.

As a simple example of how to translate a Holant polynomial to a polymer system, consider again the matching polynomial $Z_{\mathcal{M}}$. By converting G to its line graph G', observe that $Z_{\mathcal{M}}(G, (1, z)) = Z_{\mathcal{I}}(G', \mathbf{z})$, where $\mathbf{z} = (z)_{v \in V(G)}$. Our general method of Holant polynomials applied to the matching polynomial precisely captures this conversion: The polymer graph $(K, \not\sim)$ is the line graph G' of G, polymers are the edges of G and the weight function is $\Phi(\gamma) = z$.

In Section 3, we show how this translation can be extended to a general class of Holant polynomials.

Deterministic Algorithms   The strategy to derive a multiplicative approximation for $Z_{\mathcal{F}}$ is to obtain an additive approximation for $\log Z(G, \Phi)$. This idea originates from the work of Mayer & Montroll (1941), which gave a convenient infinite series representation of $\log Z$ called the *cluster expansion* and observed that one can obtain good evaluations of $\lim_{V(G) \to \infty} \frac{1}{V(G)} \log Z(G, \Phi)$ using the cluster expansion of $\log Z(G, \Phi)$.

There are two main advantages of translating a partition function to a polymer system. The first one is the convenient-to-use theorem of Kotecký & Preiss (1986, Theorem 1) that establishes conditions for zero-free regions of $Z(G, \Phi)$ and absolute convergence of the cluster expansion of $\log Z(G, \Phi)$. The second advantage is that if the cluster expansion of $\log Z(G, \Phi)$ converges absolutely then an additive approximation for $\log Z(G, \Phi)$ can be computed by enumerating small subgraphs of the polymer graph.

The first ones to derive approximation schemes employing polymer systems were Helmuth *et al.* (2019). In Theorem 2.2, they give conditions under which such a system can be used to obtain deterministic approximation algorithms. These results only apply to polymer systems for vertex spin systems and not to our polymer model. To this end, we extend their theorem and give conditions under which partition functions of general polymer systems can be efficiently approximated (Theorem 2.5). We note that Theorem 2.5 is not restricted to polymers for Holants and it might be of independent interest.

Randomised Algorithms   The fast randomised algorithms are based on the *Markov chain Monte Carlo method* (MCMC). Given a polymer system $(K, \not\sim)$ with weight function Φ we define a Markov chain with $\mathcal{I}(K)$ as state space and stationary distribution μ_K, where

$$\mu_K(\Gamma) = \frac{\prod_{\gamma \in \Gamma} \Phi(\gamma)}{Z(K, \Phi)}.$$

We identify the conditions that constitute this chain as *rapidly mixing*, i.e. the distribution of its state after polynomially many transitions is ε-close to its stationary distribution. A random sample Γ is obtained by running this chain starting with $\emptyset$ for $\mathcal{O}(\Delta n \log(n/\varepsilon))$ time. Our polymer representation for Holants yields a bijection between the families in $\mathcal{I}(K)$ and assignments σ of the edges; thus, a sampling algorithm for polymers implies a sampling algorithm for Holants.

Chen *et al.* (2021) studied a Markov chain for polymers representing a vertex spin system and established conditions to efficiently sample using this chain. We obtain our algorithms by adapting their approach to polymer models that originate from Holants. The sampling algorithms give fast randomised approximate counting algorithms. We discuss the technical details in Section 5.

1.2. Related literature and discussion of our results.

Holant polynomials   Most Holant polynomials considered in the literature study special cases of graph polynomials. Among them, the matching polynomial $Z_{\mathcal{M}}(G, \pi, (z, 1))$ of a graph G is perhaps the most studied from an algorithmic perspective. It was first studied in statistical physics as the partition function of the monomer–dimer model (Heilmann & Lieb 1972). The first approximation algorithm for the matching polynomial was the MCMC algorithm of Jerrum & Sinclair (1989). Barvinok (2016b) (see also 2016a, Section 5.1) was the first to connect the absence of zeros with approximation algorithms. He gave a quasi-polynomial algorithm for all $z \in \mathbb{C}$ that are not negative reals with $z \leq -1/(4(\Delta - 1))$ by computing $\mathcal{O}(\log|V(G)|)$ coefficients of the Taylor series expansion of the logarithm of the matching polynomial. Patel & Regts (2017) refined the computation of coefficients and gave an FPTAS for this region. On the other hand, Bezáková *et al.* (2021) showed that it is $\#\mathsf{P}$-hard to approximate $Z_{\mathcal{M}}(G, (1, z))$ when $z \in \mathbb{R}$ and $z < -1/(4(\Delta - 1))$.

Another graph polynomial studied in the literature is the edge cover polynomial. Translated to our framework, this is the Holant

polynomial $Z_{\mathcal{C}}(G, \pi, (1, z))$ where $\mathcal{C}$ contains the functions that evaluate to 1 if at least one of the inputs is 1. Liu *et al.* (2014) discovered an FPTAS for the edge cover polynomial for $z \in \mathbb{R}_{\geq 0}$. Csikvári & Oboudi (2011) showed that the roots of the edge cover polynomial—contrary to the matching polynomial—can take imaginary values and are contained in $\{z \in \mathbb{C} \mid |z| \leq 5.1\}$.

A different kind of Holant polynomial was studied by Lu *et al.* (2014). In their setting, each edge contributes its own individual weight instead of each domain element as in our case. Their results include approximation algorithms for real weighted Holants with a special type of signatures called Fibonacci gates.

Holant problems   There is an assiduous ongoing effort to characterise the computational complexity of Holant problems. The literature on exact computations of Holant problems is extensive and most results restrict the signatures to be of Boolean domain and symmetric, i.e. their value only depends on the Hamming weight of their input (Cai *et al.* 2016a). Due to the complexity of the problem, only few results go beyond symmetric signatures (Backens 2018; Cai *et al.* 2018; Lin & Wang 2017) or consider higher domain symmetric functions (Cai *et al.* 2016b, 2013).

Considering the complexity of approximating Holant problems, there are classical results targeting particular cases such as matchings (Jerrum & Sinclair 1989), weighted even subgraphs (Jerrum & Sinclair 1993), and edge covers (Bubley & Dyer 1997) and newer results on restricted classes of Holant problems (Cai *et al.* 2019; Huang *et al.* 2016; McQuillan 2013). Recently, Guo *et al.* (2021) have given a complexity characterisation for a subclass of Boolean symmetric functions called "generalised second-order recurrences." Their results rely on proving zero-free regions and apply to Holant problems where each vertex of the input graph is mapped to the same signature. They remark that it is not clear how to get approximation algorithms when the vertices are mapped to different signatures. Theorem 1.2 partially addresses this as it allows for mixed signature classes.

To our knowledge, the only result on zero-free regions of Holant problems with arbitrary domain size that includes non-symmetric

signatures and the possibility to assign mixed signatures to vertices is due to Regts (2018). As discussed by Patel & Regts (2017), this result can be used to derive FPTAS' for such Holant problems. The results of Regts (2018) require the signatures to output a complex value close to 1 on any input which makes them incomparable to Theorem 1.2, requiring our signatures to output only complex values close to 0. An advantage of Theorem 1.2 is that it allows for signatures to encode hard constraints, i.e. to take the value 0.

As an interesting side note, we mention possible implications for the problem of counting perfect matchings, a central problem in computational counting whose complexity remains unresolved. There is an expanding list of approximation problems that are equivalent to counting perfect matchings (Cai & Liu 2020; Guo et al. 2021; McQuillan 2013). In one of these results, Guo et al. (2021) show approximation equivalence between counting perfect matchings and some classes of Holant problems. These signature families are not included in Theorem 1.2 for the Holant problems but are captured by Theorem 1.1. Thus, if one could show a reduction to a Holant polynomial for a value of z within the ones in Theorem 1.1, then one would get an approximation algorithm for counting perfect matchings.

Further applications of our technique   The translation of a partition function to that of a polymer model has been particularly advantageous for vertex spin systems when the input graph is restricted to be a bipartite expander (Jenssen et al. 2020; Liao et al. 2019) or an unbalanced bipartite graph, in the sense that the maximum degree of one partition is much larger than the maximum degree of the other partition (Cannon & Perkins 2020). In the case of edge spin systems, it is not obvious if such properties can be helpful. We leave as future work to identify possible graph-theoretic properties that yield improved bounds for Holants.

As we already remarked, Theorem 2.5 applies to general polymer systems, that is the polymer system does not need to originate from a graph-theoretic problem. In Section 6, we discuss the potential extensions of our technique to the problem of counting weighted solutions to a system of sparse linear equations. This

problem was recently studied by Barvinok & Regts (2019) where they obtained zero-free regions and approximation algorithms. We show how to express this problem naturally as a polymer system and use the Kotecký–Preiss condition to obtain bounds for zero-free regions and deterministic algorithms. Although our bounds for the general case are weaker than the ones of Barvinok & Regts (2019), we can get improved bounds for some cases. In particular, one can define a univariate polynomial expressing perfect matchings in hypergraphs as deviations from a ground perfect matching. For this polynomial, we use our technique and improve the bounds of Barvinok & Regts (2019) (see Section 6.1.1 for details). It remains to be seen if, by refining the analysis, one can obtain better bounds for the general case.

2. Abstract polymer models and approximation algorithms

We develop a general tool to derive approximation schemes for polymer partition functions. Thereby, we will use the following definition of approximation.

DEFINITION 2.1 (Patel & Regts 2017). *Let q and ζ be nonzero complex numbers. We call ζ a multiplicative ε-approximation to q if $e^{-\varepsilon} \leq |q|/|\zeta| \leq e^{\varepsilon}$ and if the angle between ζ and q (as seen as vectors in $\mathbb{C} = \mathbb{R}^2$) is at most ε.*

The following observation follows immediately from the definition of the multiplicative ε-approximation.

OBSERVATION 2.2. *For any $\varepsilon, c > 0$, if ζ is a multiplicative ε-approximation to some value q, then we can also achieve a multiplicative ε-approximation for cq, namely $c\zeta$.*

A *fully polynomial time approximation scheme (FPTAS)* is an algorithm that, given a problem and some fixed parameter $\varepsilon > 0$, produces a multiplicative ε-approximation of its solution in time polynomial in n and $1/\varepsilon$.

Recall from Section 1.1 that a general polymer system consists of a finite set K of polymers and an incompatibility relation $\not\sim$

$\subseteq K \times K$. For a family of weight functionals $\{\Phi(\cdot, z) \colon K \to \mathbb{C} \mid z \in \mathbb{C}\}$, one can consider the corresponding partition functions as a mapping $Z(K, \Phi(\cdot, \cdot)) \colon \mathbb{C} \to \mathbb{C}$, with $z \mapsto Z(K, \Phi(\cdot, z))$. For each polymer $\gamma \in K$, its weight can then be seen as a function $\Phi(\gamma, \cdot) \colon \mathbb{C} \to \mathbb{C}$ with $z \mapsto \Phi(\gamma, z)$.

Recently, Helmuth *et al.* (2019) have also used a polymer representation to derive FPTAS' for some graph polynomials. We briefly explain their results before we adapt them to our setting. The polymer system defined by Helmuth *et al.* (2019) is used to model problems characterised by *edge*-constraints and assignments on the vertices of the input graph. Translated to our notation their system is defined as follows. A polymer γ_v for a graph G is a pair (γ, φ_γ), where γ is a connected subgraph of G and $\varphi_\gamma \colon V(\gamma) \to D$. Denote the collection of these polymers by $\mathcal{C}_v(G)$. In this edge-constraint system, polymers are already incompatible if they affect a common edge, which formally translates to $\gamma_v \nsim \gamma_v'$ if the graph distance of the respective subgraphs γ and γ' in G is less than 2. In their model, Helmuth *et al.* consider weight functions over one variable z. Additionally, they assume the weight functions $\Phi(\gamma_v, z)$ under study to be analytic functions of z in a neighbourhood of the origin of the complex plane and that there is an absolute constant $\rho > 0$ such that for each $\gamma_v \in \mathcal{C}_v(G)$ the first nonzero term in the Taylor series expansion of $\Phi(\gamma_v, z)$ around zero is of order $k \geq |\gamma|\rho$; this property is what they refer to as *Assumption 1*. For this polymer model, the conditions to derive an FPTAS for the resulting polymer partition function $Z(\mathcal{C}_v(G), \Phi(\cdot, z))$ are summarised in the following theorem.

THEOREM 2.3 (Helmuth *et al.* 2019). *Fix Δ and let $\mathfrak{G}$ be a set of graphs of degree at most Δ. Suppose:*

(i) *There is a constant c so that $Z(\mathcal{C}_v(G), \Phi(\cdot, z))$ is a polynomial in z of degree at most $c|G|$ for all $G \in \mathfrak{G}$.*

(ii) *The weight functions satisfy Assumption 1 and the Taylor coefficients up to order m of $\Phi(\gamma_v, z)$ can be computed in time $\exp(\mathcal{O}(m + \log|G|))$ for each $G \in \mathfrak{G}$ and $\gamma_v \in \mathcal{C}_v(G)$.*

(iii) *For every connected subgraph G' of every $G \in \mathfrak{G}$, we can list all polymers $\gamma_v \in \mathcal{C}_v(G)$ with $\gamma = G'$ in time $\exp(\mathcal{O}(|G'|))$.*

(iv) *There exists $\delta > 0$ so that for all $|z| < \delta$ and all $G \in \mathfrak{G}$, $Z(\mathcal{C}_v(G), \Phi(\cdot, z)) \neq 0$.*

Then for every z with $|z| < \delta$, there is an FPTAS for the partition function $Z(\mathcal{C}_v(G), \Phi(\cdot, z))$ for all $G \in \mathfrak{G}$.

The proof of this result is based on calculating the contribution of polymers of small size to the logarithm of the partition function. Assumption 1 ensures that only those small polymers contribute to the required first coefficients of the Taylor expansion. Enumerating all polymers up to a fixed size, however, is not enough to reproduce these coefficients as the polymers contribute within families and an enumeration of all small families would be too costly. To circumvent this problem the contribution of all small families can be computed by an inclusion–exclusion principle on sets of incompatible polymers. More formally, this yields a representation of $\log Z(\mathcal{C}_v(G), \Phi(\cdot, z))$ not over families of compatible polymers but instead over connected subgraphs of the polymer graph. An enumeration of trees and labellings with incompatible polymers then gives an efficient way to compute the low coefficients of the Taylor expansion of $\log Z(\mathcal{C}_v(G), \Phi(\cdot, z))$ via this representation.

The crucial step to consider the more convenient representation of $\log Z(\mathcal{C}_v(G), \Phi(\cdot, z))$ is the so-called *cluster expansion* for hard-core interactions (Friedli & Velenik 2017), which holds not only for the specific function $Z(\mathcal{C}_v(G), \Phi(\cdot, z))$ but for general polymer partition functions. In our notation, the cluster expansion of the partition function $Z(K, \Phi(\cdot, z))$ of a polymer system K with weights $\Phi(\cdot, z)$ is the following representation (which is always possible as soon as the Taylor expansion of $\log Z(K, \Phi(\cdot, z))$ around zero converges absolutely):

$$(2.4) \quad \log Z(K, \Phi(\cdot, z)) = \sum_{k \geq 1} \frac{1}{k!} \sum_{(\gamma_1, \ldots, \gamma_k)} \phi(\gamma_1, \ldots, \gamma_k) \prod_{i=1}^{k} \Phi(\gamma_i, z).$$

The sum in the above display equation is over ordered tuples of polymers. ϕ is the *Ursell* function of such a tuple, with

$$\phi(\gamma_1, \ldots, \gamma_k) = \sum_{G \in T(\gamma_1, \ldots, \gamma_k)} (-1)^{|E(G)|},$$

where $T(\gamma_1, \ldots, \gamma_k)$ denotes the set of all spanning connected subgraphs of the polymer incompatibility graph restricted to the polymers that appear in $(\gamma_1, \ldots, \gamma_k)$. Observe that the Ursell function assigns zero to all polymer sets S which are disconnected in the polymer graph, which yields the aforementioned representation of $\log Z(K, \Phi(\cdot, z))$ only requiring connected subgraphs of the polymer incompatibility graph.

In order to describe the properties required to approximate the partition function of a general polymer model $(K, \not\sim)$, we use the following notation. For $\gamma \in K$ the notion $|\gamma|$ denotes some fixed size function $|\cdot| \colon K \to \mathbb{R}_+$, which can be chosen suitably similar to the function a in Theorem 4.1. Similarly we use $|K|$ to denote a suitable size (not necessarily the cardinality) for the set of polymers K. With these notions we can lift (Helmuth *et al.* 2019, Theorem 2.2) to the general definition of a polymer model and derive the following set of conditions to efficiently compute approximations to a polymer partition function.

THEOREM 2.5. *Let $(K, \not\sim)$ be a polymer system and let $\{\Phi(\cdot, z) \colon K \to \mathbb{C} \mid z \in \mathbb{C}\}$ be a family of weight functions with the following conditions:*

(i) *The function $Z(K, \Phi(\cdot, z))$ is a polynomial of z of degree d.*

(ii) *Each function $\Phi(\gamma, z)$, $\gamma \in K$, is analytic in an open neighbourhood around zero such that the first nonzero term in its Taylor series expansion around zero is of order $k \geq |\gamma|\rho$ for some $\rho > 0$.*

(iii) *For each $m \in \mathbb{N}$ and $\gamma \in K$, the Taylor coefficients up to order m of $\Phi(\gamma, z)$ can be computed in time $\exp(\mathcal{O}(m + \log|K|))$.*

(iv) *All polymers $\gamma \in K$ with $|\gamma| \leq m$ can be enumerated in time $\exp(\mathcal{O}(m) + \log|K|)$.*

(v) *For each polymer $\gamma \in K$ all polymers $\gamma' \in K$ with $\gamma' \not\sim \gamma$ and $|\gamma'| \leq m$ can be enumerated in time $\exp(\mathcal{O}(m + \log|\gamma|))$.*

(vi) *There exists $\delta > 0$ so that for all $|z| < \delta$, the cluster expansion of $Z(K, \Phi(\cdot, \cdot))$ converges absolutely.*

Then for every z with $|z| < \delta$ and every $\varepsilon > 0$ an ε-approximation for $Z(K, \Phi(\cdot, z))$ can be computed in time

$$\exp(\mathcal{O}(\frac{1}{\rho}(1 - \frac{|z|}{\delta})^{-1} \log(\frac{d}{\varepsilon}) + \log(|K|))).$$

PROOF.   First assume $Z(K, \Phi(\cdot, z))$ is a polynomial of degree d in z. Absolute convergence of $\log Z(K, \Phi(\cdot, z))$ for all z with $|z| < \delta$ implies that $Z(K, \Phi(\cdot, z))$ has no roots in the open disc of radius δ around zero. By (Patel & Regts 2017, Lemma 2.2) exponentiating the value of the Taylor series of $\log Z(K, \Phi(\cdot, z))$ truncated at $m = (1 - \frac{|z|}{\delta})^{-1} \log(\frac{d}{\varepsilon})$ yields a multiplicative ε-approximation for $Z(K, \Phi(\cdot, z))$, for each z with $|z| < \delta$.

Due to the representation in (2.4) and the absolute convergence of this series, the k-th Taylor coefficient of $\log Z(K, \Phi(\cdot, z))$ can be computed with the Taylor coefficients of order k of the products of functions $\Phi(\gamma, z)$ for $\gamma \in S \subseteq K$ (here the subsets S contain the elements of the corresponding k-tuple in (2.4)). By condition 2, the k-th Taylor coefficient of $\Phi(\gamma, z)$ is nonzero only for polymers of size at most $\frac{k}{\rho}$. All $S \subseteq K$ which play a role in computing the k-th Taylor coefficient of $\log Z(K, \Phi(\cdot, z))$ are connected subgraphs of the polymer graph (otherwise the Ursell function is zero) which only contain at most k polymers of size at most $\frac{k}{\rho}$.

Enumerating all these sets S can be done as in the proof of Helmuth *et al.* (2019, Theorem 2.2) by enumerating all trees with at most k vertices (to be spanning trees that ensure connectivity) and assigning them polymers of size at most $\frac{k}{\rho}$ such that only incompatible polymers are assigned to adjacent vertices to create all subsets $S \subseteq K$ such that $G(S)$ is connected. Property 3 ensures that it is possible to efficiently enumerate the at most $\exp(\mathcal{O}(k) + \log |K|)$ polymers to choose for the root vertex, and moving downward in the tree, property 4 restricts and efficiently computes the choices to pick an incompatible neighbouring polymer. Regardless of the underlying polymer structure, the Ursell function of a graph H (subgraph $G(S)$ of the polymer graph of the general polymer system) can be computed in time $\exp(\mathcal{O}(|V(H)|))$ as described by

Helmuth *et al.* (2019, Lemma 2.6). This enumeration of the relevant sets $S \subseteq K$ and the computation of their contribution to the k-th Taylor coefficient of $\log Z(K, \Phi(\cdot, z))$ can be done in time $\exp(\mathcal{O}(k) + \log|K|)$. Overall, an ε-approximation for $Z(K, \Phi(\cdot, \cdot))$ can hence be computed by computing the k-th Taylor coefficient of $\log Z(K, \Phi(\cdot, z))$ for all $k \leq m$ which yields a total running time in $\exp(\mathcal{O}((1 - \frac{|z|}{\delta})^{-1} \log(\frac{d}{\varepsilon})) + \log|K|)$. $\qquad\square$

3. Holants as polymer models

In this section, we explain how to express a Holant polynomial as the partition function of a polymer system. Recall the definition of a Holant polynomial

$$Z_{\mathcal{F}}(G, \pi, \mathbf{z}) = \sum_{\sigma \in D^E} \prod_{v \in V(G)} f_v(\sigma|_{E(v)}) \prod_{i=0}^{\kappa} z_i^{|\sigma|_i},$$

where $|\sigma|_i$ denotes the number of edges for which σ assigns the value i. We implicitly assume a fixed total order on the edges in G, which gives a well-defined mapping of a subset of edges to a vector: in the above definition $\sigma|_{E(v)}$ represents the vector $(\sigma(e_1), \ldots, \sigma(e_d))$, where $(e_1, \ldots, e_d)$ is the ordered set of edges adjacent to v.

To represent a general Holant polynomial as a polymer partition function, we restrict the class of signatures to $\mathcal{F}_0 = \{f \mid f(\mathbf{0}) \neq 0\}$. We further require that $z_0 \neq 0$. If we are interested in approximating Holants with $\mathbf{z}$ that contains 0 values, we can retranslate the Holant to reduce the domain and exclude these elements as any assignment that maps to them will not contribute to the partition function. These requirements ensure that the assignment σ_0, which maps every edge to 0, contributes a nonzero weight to the partition function. The families of compatible polymers will express assignments in terms of their "deviations" from the ground state σ_0.

Given $Z_{\mathcal{F}_0}(G, \pi, \mathbf{z})$ over domain $D = \{0, 1, \ldots, \kappa\}$, we define the following polymer model. Let $\mathcal{C}(G)$ be the set of connected subgraphs of G containing at least one edge. A polymer γ_ϕ for G is a pair (γ, ϕ_γ), where $\gamma \in \mathcal{C}(G)$ and $\phi_\gamma \colon E(\gamma) \to [\kappa]$. Let $\mathcal{C}_\kappa(G)$ denote the set of all such polymers for G. For $\gamma_\phi, \gamma'_\phi \in \mathcal{C}_\kappa(G)$, we

say that two polymers are incompatible $\gamma_\phi \not\sim \gamma'_\phi$, if $V(\gamma) \cap V(\gamma') \neq \emptyset$. Finally, we write $\mathcal{I}_\kappa(G)$ to denote the collection of finite subsets of pairwise compatible polymers of $\mathcal{C}_\kappa(G)$.

For $\pi \colon V \to \mathcal{F}_0$, we define the weight function Φ_π for each $\gamma_\phi \in \mathcal{C}_\kappa(G)$ and $\mathbf{z} \in \mathbb{C}^{\kappa+1}$ by

$$\Phi_\pi(\gamma_\phi, \mathbf{z}) = \left(\prod_{i=1}^{\kappa} \left(\frac{z_i}{z_0} \right)^{|E^\kappa(\gamma_\phi)|_i} \right) \prod_{v \in V(\gamma)} f_v(E^\kappa(\gamma_\phi)) \frac{1}{f_v(\mathbf{0})}$$

for each polymer γ_ϕ. We denote $(\varphi_\gamma(e_1), \ldots, \varphi_\gamma(e_d))$ by $E^\kappa(\gamma_\phi)$ with $E(v) = \{e_1, \ldots, e_d\}$ (listed in the implicitly assumed fixed total order on the edges), where $\varphi_\gamma(e) = \phi_\gamma(e)$, if $e \in \gamma$ and $\varphi_\gamma(e) = 0$, otherwise. Further, $|E^\kappa(\gamma_\phi)|_i$ denotes the number of occurrences of the value i in $E^\kappa(\gamma_\phi)$.

The partition function for this graph polymer model then translates to:

$$Z(\mathcal{C}_\kappa(G), \Phi_\pi(\cdot, \mathbf{z})) = \sum_{\Gamma \in \mathcal{I}_\kappa(G)} \prod_{\gamma_\phi \in \Gamma} \Phi_\pi(\gamma_\phi, \mathbf{z})$$

$$= \sum_{\Gamma \in \mathcal{I}_\kappa(G)} \prod_{\gamma_\phi \in \Gamma} \left(\prod_{i=1}^{\kappa} \left(\frac{z_i}{z_0} \right)^{|E^\kappa(\gamma_\phi)|_i} \right) \prod_{v \in V(\gamma)} f_v(E^\kappa(\gamma_\phi)) \frac{1}{f_v(\mathbf{0})}.$$

Now we show that our polymer model encodes the Holant as intended, i.e. an ε-approximation for the polymer partition function yields a ε-approximation for the Holant polynomial.

LEMMA 3.1. *For all finite graphs $G = (V, E)$, all $\mathcal{F} \subseteq \mathcal{F}_0$, all $\pi \colon V \to \mathcal{F}_0$ and all $\mathbf{z} \in \mathbb{C}^{\kappa+1}$ with $z_0 \neq 0$,*

$$Z_\mathcal{F}(G, \pi, \mathbf{z}) = z_0^{|E(G)|} \left(\prod_{v \in V} f_v(\mathbf{0}) \right) Z(\mathcal{C}_\kappa(G), \Phi_\pi(\cdot, \mathbf{z})).$$

PROOF.   Every assignment σ uniquely corresponds to the set of κ-edge-coloured connected subgraphs which are induced by the edges $e \in E$ with $\sigma(e) \neq 0$ together with the colouring given by σ. More formally, let $G[\sigma]$ be the subgraph of G induced by the edges

e with $\sigma(e) \neq 0$. By definition, each maximal connected component γ in $G[\sigma]$ is a polymer in $\mathcal{C}(G)$, so $(\gamma, \sigma|_{E(\gamma)})$ is a polymer in $\mathcal{C}_\kappa(G)$; observe that by definition σ only assigns the colours in $[\kappa]$ to such a component. Furthermore, the collection of all maximal connected components in $G[\sigma]$ is a set of pairwise compatible polymers in $\mathcal{C}(G)$, so their coloured versions are pairwise compatible in $\mathcal{C}_\kappa(G)$. Consequently, the set of maximal connected components in $G[\sigma]$ together with their colourings assigned by σ is a set in $\mathcal{I}_\kappa(G)$.

Conversely, every set $\bar{\Gamma} \in \mathcal{I}_\kappa(G)$ uniquely corresponds to the assignment $\sigma_{\bar{\Gamma}}$ defined by $\sigma_{\bar{\Gamma}}(e) = \phi_\gamma(e)$ if $e \in E(\gamma)$, for some $\gamma_\phi = (\gamma, \phi_\gamma) \in \bar{\Gamma}$ and $\sigma_{\bar{\Gamma}}(e) = 0$ otherwise. Observe that in the former case, $e \in E(\gamma)$, there is only one $\gamma_\phi \in \Gamma$ which covers this edge by the compatibility condition, so this is well defined.

We abuse notation and denote families $\bar{\Gamma} \in \mathcal{I}_\kappa(G)$ with "bar" to use Γ to refer to the corresponding collection of subgraphs $\gamma \in \mathcal{C}(G)$ with $(\gamma, \phi) \in \bar{\Gamma}$ for some colouring function ϕ. Such an uncoloured collection Γ can then be seen as a subgraph of G. These observations yield

$$z_0^{|E(G)|} \left(\prod_{v \in V} f_v(\mathbf{0}) \right) Z(\mathcal{C}_\kappa(G), \Phi_\pi(\cdot, \mathbf{z}))$$

$$= z_0^{|E(G)|} \left(\prod_{v \in V} f_v(\mathbf{0}) \right)$$

$$\cdot \sum_{\bar{\Gamma} \in \mathcal{I}_\kappa(G)} \prod_{\gamma_\phi \in \bar{\Gamma}} \left(\prod_{i=1}^{\kappa} \left(\frac{z_i}{z_0} \right)^{|E^\kappa(\gamma_\phi)|_i} \right) \prod_{v \in V(\gamma)} f_v(E^\kappa(\gamma_\phi)) \frac{1}{f_v(\mathbf{0})}$$

$$= z_0^{|E(G)|} \sum_{\bar{\Gamma} \in \mathcal{I}_\kappa(G)} \prod_{v \notin V(G[\Gamma])} f_v(\mathbf{0}) \prod_{v \in V(G[\Gamma])} f_v(E^\kappa(\bar{\Gamma})) \left(\prod_{i=1}^{\kappa} \left(\frac{z_i}{z_0} \right)^{|E^\kappa(\bar{\Gamma})|_i} \right)$$

$$= z_0^{|E(G)|} \sum_{\bar{\Gamma} \in \mathcal{I}_\kappa(G)} \prod_{v \in V} f_v(E^\kappa(\bar{\Gamma})) \left(\prod_{i=1}^{\kappa} \left(\frac{z_i}{z_0} \right)^{|E^\kappa(\bar{\Gamma})|_i} \right)$$

$$= z_0^{|E(G)|} \sum_{\bar{\Gamma} \in \mathcal{I}_\kappa(G)} \prod_{v \in V} f_v(\sigma_{\bar{\Gamma}}|_{E(v)}) \left(\prod_{i=1}^{\kappa} \left(\frac{z_i}{z_0} \right)^{|\sigma_{\bar{\Gamma}}|_i} \right)$$

$$= z_0^{|E(G)|} \sum_{\sigma \in D^E} \prod_{v \in V(G)} f_v(\sigma|_{E(v)}) \prod_{i=1}^{\kappa} \left(\frac{z_i}{z_0} \right)^{|\sigma|_i}$$

$$= \sum_{\sigma \in D^E} \prod_{v \in V(G)} f_v(\sigma|_{E(v)}) \left(z_0^{|E(G)| - \sum_{i=1}^{k} |\sigma|_i} \right) \prod_{i=1}^{\kappa} z_i^{|\sigma|_i}$$

$$= \sum_{\sigma \in D^E} \prod_{v \in V(G)} f_v(\sigma|_{E(v)}) \prod_{i=0}^{\kappa} z_i^{|\sigma|_i}$$

$$= Z_{\mathcal{F}}(G, \pi, \mathbf{z}).$$

This concludes the lemma. $\square$

We remark that the choice to use colour 0 as a ground state is only for convenience. If there exists $c \in D$ with $z_c \neq 0$ and the all c configuration σ_c evaluating a nonzero term in the Holant partition function, we can use a polymer model whose compatible families express deviations from σ_c. In fact, as we will see in Section 6, we can define polymer systems as deviations from any ground state assignment σ with nonzero weight.

4. Deterministic algorithms

We have already explained how to translate a Holant partition function $Z_{\mathcal{F}_0}(G, \pi, \mathbf{z})$ into $Z(\mathcal{C}(G), \Phi_\pi(\cdot, \mathbf{z}))$, for $\mathbf{z}$ with $z_0 \neq 0$. In this section, we will first identify the combinations of signature families and values of $\mathbf{z}$ for which the Taylor expansion of the Holants converges absolutely via the Kotecký–Preiss condition and then show how Theorem 2.5 applies.

4.1. Holant polynomials. We begin by establishing absolute convergence for the logarithm of Holant polynomials. A crucial component is the following theorem of Kotecký & Preiss.

THEOREM 4.1 (Kotecký & Preiss 1986, Theorem 1). *If there exists a function* $a \colon K \to [0, \infty)$ *such that for all* $\gamma \in K$,

$$\sum_{\gamma' \not\sim \gamma} |\Phi(\gamma')| e^{a(\gamma')} \leq a(\gamma),$$

where the sum is over all polymers γ' incompatible with γ, then the cluster expansion for $\log Z(K, \Phi)$ converges absolutely and, in particular, $Z(K, \Phi) \neq 0$.

To apply the above theorem, we use an upper bound of Borgs et al. (2013, Lemma 2.1(b)) on the number of connected subgraphs of the input graph G that contain a fixed vertex, which is based on a well-known formula for bounding the number of subtrees (Stanley 1999, Theorem 5.3.10) (also see Bollobás 2006, Equation 7 for a bound based on the number of vertices).

LEMMA 4.2. *In any graph G of maximum degree Δ, the number of connected subgraphs of G with m edges containing a fixed vertex is at most $\frac{1}{m+1}\binom{(m+1)\Delta}{m} < \frac{(e\Delta)^m}{2}$.*

As Holant polynomials have a domain of arbitrary size, we will use the following generalisation of Lemma 4.2.

COROLLARY 4.3. *In any graph G of maximum degree Δ, the number of connected κ-edge-coloured subgraphs of G with m edges containing a fixed vertex is at most $\frac{(\Delta\kappa e)^m}{2}$.*

PROOF.   Considering the κ^m different colourings that can be assigned to a graph with m edges and using Lemma 4.2, the claimed bound follows immediately. $\square$

Recall that for $f \in \mathcal{F}_0$ with arity d we defined the value $r(f) = \max_{x \in D^d \setminus \{\mathbf{0}\}}\{|f(x)|/|f(\mathbf{0})|\}$ and that for a function class $\mathcal{F} \subseteq \mathcal{F}_0$ we defined $r(\mathcal{F}) = \max_{f \in \mathcal{F}}\{r(f)\}$.

LEMMA 4.4. *Let $\mathcal{F} \subseteq \mathcal{F}_0$. For all graphs G of maximum degree Δ and all $\pi \colon V \to \mathcal{F}$, the Taylor expansion of $\log Z_{\mathcal{F}}(G, \pi, \mathbf{z})$ converges absolutely in*

$$\left\{ (z_0, \ldots, z_\kappa) \in \mathbb{C}^{\kappa+1} \;\middle|\; z_0 \neq 0, \frac{|z_i|}{|z_0|} \leq (\Delta\kappa e^2 r_1(r_1+1))^{-1}, \; i \in [\kappa] \right\}$$

with $r_1 = \max\{1, r((\mathcal{F}))\}$.

PROOF.   We aim to apply Theorem 4.1 on the polymer representation $Z(\mathcal{C}_\kappa(G), \Phi_\pi(\cdot, \mathbf{z}))$. Consider a fixed polymer $\gamma_\phi \in \mathcal{C}_\kappa(G)$. Each polymer γ'_ϕ incompatible with γ_ϕ contributes to the sum that has to be bounded by $a(\gamma_\phi)$ the term

$$
\begin{aligned}
|\Phi_\pi(\gamma'_\phi, \mathbf{z})| \, e^{a(\gamma'_\phi)} &= \\
&= \left(\prod_{i=1}^{\kappa} \left(\frac{|z_i|}{|z_0|} \right)^{|E^\kappa(\gamma'_\phi)|_i} \prod_{v \in V(\gamma')} |f_v(E^\kappa(\gamma'_\phi))| \frac{1}{|f_v(\mathbf{0})|} \right) e^{a(\gamma'_\phi)} \\
&\leq \left(\max_{1 \leq i \leq \kappa} \left\{ \frac{|z_i|}{|z_0|} \right\} \right)^{|E(\gamma')|} r_1^{|V(\gamma')|} \, e^{a(\gamma'_\phi)}.
\end{aligned}
$$

In the following, we will estimate the number of polymers γ'_ϕ incompatible with γ_ϕ with respect to their number of edges. To this end, denote by $\mathcal{C}_\kappa^{\gamma_\phi}(i)$ the set of polymers $\gamma'_\phi \in \mathcal{C}_\kappa(G)$ with $\gamma'_\phi \nsim \gamma_\phi$ and $i = |E(\gamma')|$, for each $1 \leq i \leq |E(G)|$. First, observe that by the definition of the polymers in $\mathcal{C}_\kappa(G)$ the incompatibility $\gamma'_\phi \nsim \gamma_\phi$ implies that the corresponding subgraphs γ' and γ share at least one vertex. Further, γ' has to be a connected subgraph of G. By Corollary 4.3 we conclude that $\mathcal{C}_\kappa^{\gamma_\phi}(i)$ has cardinality at most $|V(\gamma)|(\frac{(\Delta\kappa e)^i}{2})$.

Consider $a(\gamma_\phi) = \alpha|E(\gamma)|$ for some constant $\alpha > 0$ to be assigned optimally later. This choice of a with the bounds on the cardinality of $\mathcal{C}_\kappa^{\gamma_\phi}(i)$, and the fact that a connected subgraph with i edges contains at most $i + 1$ vertices, yields

$$
\begin{aligned}
\sum_{\gamma'_\phi \nsim \gamma_\phi} |\Phi_\pi(\gamma'_\phi, \mathbf{z})| e^{a(\gamma'_\phi)} &\leq \sum_{i=1}^{|E(G)|} |\mathcal{C}_\kappa^{\gamma_\phi}(i)| \left(\max_{1 \leq i \leq \kappa} \left\{ \frac{|z_i|}{|z_0|} \right\} \right)^i r_1^{i+1} \, e^{\alpha i} \\
&\leq \sum_{i=1}^{|E(G)|} |V(\gamma)| \frac{(\Delta\kappa e)^i}{2} \left(\max_{1 \leq i \leq \kappa} \left\{ \frac{|z_i|}{|z_0|} \right\} \right)^i r_1^{i+1} e^{\alpha i}.
\end{aligned}
$$

With β as shorthand on the upper bound on $\max_{1 \leq i \leq \kappa} \left\{ \frac{|z_i|}{|z_0|} \right\}$ in order to describe the region for $\mathbf{z}$, we can reformulate the condition of Theorem 4.1 to

$$\sum_{i=1}^{|E(G)|} |V(\gamma)| \frac{(\Delta \kappa e)^i}{2} \beta^i \, r_1^{i+1} \, e^{\alpha i} \quad \leq \quad \alpha |E(\gamma)|$$

$$\Leftrightarrow \quad \sum_{i=1}^{|E(G)|} (\Delta \kappa e^{\alpha+1} \beta r_1)^i \quad \leq \quad 2\alpha \frac{|E(\gamma)|}{|V(\gamma)| r_1}$$

$$\Leftarrow \quad \frac{1}{1 - \Delta \kappa e^{\alpha+1} \beta r_1} - 1 \quad \leq \quad \frac{\alpha}{r_1}$$

$$\Leftrightarrow \quad \Delta \kappa e^{\alpha+1} \beta r_1 \quad \leq \quad \frac{\alpha}{\alpha + r_1}$$

$$\Leftrightarrow \quad \beta \quad \leq \quad \frac{\alpha}{r_1 \Delta \kappa e^{\alpha+1}(\alpha + r_1)}.$$

Maximising the region for $\mathbf{z}$ for which approximation is possible means choosing α depending on r_1 to maximise $\frac{\alpha}{r_1 e^{\alpha+1}(\alpha+r_1)}$. The first derivative of this expression with respect to α is

$$\frac{r_1 e^{\alpha+1}(\alpha + r_1) - \alpha(r_1 e^{\alpha+1}(\alpha + r_1) + r_1 e^{\alpha+1})}{(r_1 e^{\alpha+1}(\alpha + r_1))^2} = \frac{r_1 - r_1 \alpha - \alpha^2}{r_1 e^{\alpha+1}(\alpha + r_1)^2}.$$

The only positive value for α that sets the derivative to zero is $\alpha = \frac{1}{2}(\sqrt{r_1}\sqrt{r_1 + 4} - r_1)$, and furthermore, the second derivative is negative at this point.
Plugging this into the bound on β gives

$$\beta \leq \frac{\sqrt{r_1}\sqrt{r_1 + 4} - r_1}{r_1 \Delta \kappa (\sqrt{r_1}\sqrt{r_1 + 4} + r_1) e^{\frac{1}{2}(\sqrt{r_1}\sqrt{r_1+4} - r_1)+1}}.$$

Note that any value of $\alpha > 0$ gives a bound. As r_1 goes to infinity, α goes to 1. Setting $\alpha = 1$ gives the simpler bound

$$\beta \leq \frac{1}{\Delta \kappa e^2 r_1(r_1 + 1)}$$

stated in the lemma. □

What remains to obtain an FPTAS is to show how to apply Theorem 2.5 to the polymer partition function $Z(\mathcal{C}_\kappa(G), \Phi_\pi(\cdot, \mathbf{z}))$. Observe that from the definition of the weights $\Phi_\pi(\gamma_\phi, \mathbf{z})$, the partition function $Z(\mathcal{C}_\kappa(G), \Phi_\pi(\cdot, \mathbf{z}))$ can be a multivariate polynomial,

so not necessarily univariate. This introduces a catalogue of issues when attempting to apply Theorem 2.5 on $Z(\mathcal{C}_\kappa(G), \Phi_\pi(\cdot, \mathbf{z}))$ directly. To circumvent these issues, we introduce an additional variable x and transform the weights $\Phi_\pi(\gamma_\phi, \mathbf{z})$ to univariate polynomials of x where we assume the variables $\mathbf{z}$ to be fixed.

For a given weight $\Phi_\pi(\gamma_\phi, \mathbf{z})$, we define the univariate weight

$$
\Phi_\pi^x(\gamma_\phi, \mathbf{z}, x) = \left(\prod_{i=1}^{\kappa} \left(\frac{z_i}{z_0} \right)^{|E^\kappa(\gamma_\phi)|_i} \right) x^{|E(\gamma)|} \prod_{v \in V(\gamma)} f_v(E^\kappa(\gamma_\phi)) \frac{1}{f_v(\mathbf{0})},
$$

which serves as input for $Z(\mathcal{C}_\kappa(G), \Phi_\pi^x(\cdot, \mathbf{z}, x))$. In particular, setting $x = 1$ yields the original weight $\Phi_\pi^x(\gamma_\phi, \mathbf{z}, 1) = \Phi_\pi(\gamma_\phi, \mathbf{z})$ and, interpreted as this univariate polynomial weight function, the degree of $\Phi_\pi^x(\cdot, \mathbf{z}, \cdot)$ corresponds to the number of edges γ_ϕ which enables the application of Theorem 2.5.

THEOREM 4.5. *Let $\mathcal{F} \subseteq \mathcal{F}_0$. For all graphs G of maximum degree Δ and all $\pi \colon V \to \mathcal{F}$, the Holant polynomial admits an FPTAS for $\mathbf{z}$ in*

$$
\left\{ (z_0, \ldots, z_\kappa) \in \mathbb{C}^{\kappa+1} \;\middle|\; z_0 \neq 0, \frac{|z_i|}{|z_0|} < (\Delta \kappa e^2 r_1 (r_1 + 1))^{-1}, \; i \in [\kappa] \right\}
$$

with $r_1 = \max\{1, r(\mathcal{F})\}$.

PROOF.   Due to the definition of $\mathcal{F}_0$ and Lemma 3.1, we obtain

$$
Z_\mathcal{F}(G, \pi, \mathbf{z}) = z_0^{|E(G)|} \left(\prod_{v \in V} f_v(\mathbf{0}) \right) Z(\mathcal{C}_\kappa(G), \Phi_\pi(\cdot, \mathbf{z}));
$$

thus, it suffices to approximate $Z(\mathcal{C}_\kappa(G), \Phi_\pi(\cdot, \mathbf{z}))$. We use the above defined representation of $Z_\mathcal{F}(G, \pi, \mathbf{z})$ as a univariate polynomial $Z(\mathcal{C}_\kappa(G), \Phi_\pi^x(\cdot, \mathbf{z}, x))$ to apply Theorem 2.5 and show how $Z(\mathcal{C}_\kappa(G), \Phi_\pi^x(\cdot, \mathbf{z}, x))$ satisfies the theorem's conditions. As size functions, we choose $|\mathcal{C}_\kappa(G)|$ the cardinality of G, i.e. the number of vertices, and as $|\gamma_\phi|$ the number of edges of the support graph.

1. The partition function $Z(\mathcal{C}_\kappa(G), \Phi_\pi^x(\cdot, \mathbf{z}, x))$ is a polynomial of x of maximum degree $|E(G)|$.

2. For each polymer γ_ϕ, its weight $\Phi_\pi^x(\gamma_\phi, \mathbf{z}, x)$ is a monomial in x of degree $|E(\gamma)| = |\gamma_\phi|$; thus, condition 2 holds with $\rho = 1$.

3. For each polymer γ_ϕ, its weight $\Phi_\pi^x(\gamma_\phi, \mathbf{z}, x)$ can be computed exactly, not just its first m Taylor coefficients, which can be done in time $\mathcal{O}(G) = \mathcal{O}(|\mathcal{C}_\kappa(G)|)$. Recall here that we only consider constraint functions that can be computed efficiently for the general ground class $\mathcal{F}_0$.

4. The support γ of a polymer γ_ϕ is a connected subgraph of G and adjoined with the edge-colouring ϕ_γ we obtain, using Corollary 4.3, that there are at most $\frac{(\Delta\kappa e)^m}{2}$ such edge-coloured connected subgraphs with at most m edges containing a fixed vertex. There are $|V(G)|$ many choices for a fixed vertex and thus there are at most $|V(G)|m(\Delta\kappa e)^m \in \exp(\mathcal{O}(m + \log|\mathcal{C}_\kappa(G)|))$ polymers of size m. We can enumerate these as Patel & Regts (2017, Lemma 3.7.) by enumerating all connected subgraphs $S \subseteq G$ of size $|S| \leq m$, which requires a run-time in $\mathcal{O}(|V(G)|^2 m^7)$. Afterwards, for every such subgraph S we add the $\kappa^{|S|} \leq \kappa^m$ different edge-colourings and obtain a run-time in $\exp(\mathcal{O}(m + \log|V(G)|))$.

5. For $\gamma_\phi \in \mathcal{C}_\kappa(G)$ with $|\gamma| = m$, we have that $\gamma'_\phi \in \mathcal{C}_\kappa(G)$ is incompatible with γ_ϕ if their supports γ and γ' share at least one vertex v. Hence, we enumerate for all $v \in V(\gamma)$ all polymers γ'_ϕ of size at most m containing v and then remove duplicates. There are at most $\frac{(\Delta\kappa e)^m}{2}$ such edge-coloured connected subgraphs of size m containing a fixed vertex due to Corollary 4.3. For each $v \in V(\gamma)$, we can then enumerate all connected subgraphs $\gamma' \subseteq G$ containing v and of size at most m as Patel & Regts (2017, Lemma 3.7.), which takes time $\mathcal{O}(|\gamma|^2 m^7) \subseteq \exp(\mathcal{O}(m + \log|\gamma|))$.

6. From Lemma 4.4, we have that $\log(Z(\mathcal{C}_\kappa(G), \Phi_\pi(\cdot, \mathbf{z})))$ converges absolutely for $\mathbf{z}$ with $\frac{|z_i|}{|z_0|} \leq (\Delta\kappa e^2 r_1(r_1 + 1))^{-1}$ for all $1 \leq i \leq \kappa$. For a fixed $\mathbf{z}$ in the region defined by the statement of the theorem, denote $q = \min\{\frac{|z_0|}{|z_i|}(\Delta\kappa e^2 r_1(r_1+1))^{-1} \mid 1 \leq i \leq \kappa\} > 1$. Adding x with $|x| \leq q$ to the calculations

in Lemma 4.4 shows that $\log(Z(\mathcal{C}_\kappa(G), \Phi_\pi^x(\cdot, \mathbf{z}, x)))$ converges absolutely for $|x| \leq q$ and $\mathbf{z}$ in the region defined in the statement of the theorem.

In summary, the conditions of Theorem 2.5 are satisfied with $K = \mathcal{C}_\kappa(G)$, $\rho = 1$ and $d = E(G)$ and for all x with $|x| \leq q$. This shows that a $(1 + \varepsilon)$-approximation for $Z(\mathcal{C}_\kappa(G), \Phi_\pi^x(\cdot, \mathbf{z}, x)$ can be computed in time $\exp(\mathcal{O}((1 - \frac{|x|}{q})^{-1} \log(\frac{E(G)}{\varepsilon}) + \log(|\mathcal{C}_\kappa(G)|)))$. With our choice of $|\mathcal{C}_\kappa(G)| = |V(G)|$ and with x chosen to be 1, to approximate the original partition function $Z(\mathcal{C}_\kappa(G), \Phi_\pi(\cdot, \mathbf{z}))$, this yields an overall running time in $\exp(\mathcal{O}((1 - \frac{1}{q})^{-1} \log(\frac{E(G)}{\varepsilon}) + \log |V(G)|))$ which is in $\exp(\mathcal{O}(\log(\frac{1}{\varepsilon}) + \log |V(G)|))$ for any fixed $\mathbf{z}$. $\square$

4.2. Holant problems. The partition function $Z_\mathcal{F}(G, \pi)$ of a Holant problem can be viewed as the value of a Holant polynomial $Z_\mathcal{F}(G, \pi, \mathbf{1})$ at $\mathbf{z} = (1, 1, \ldots, 1)$. This immediately gives a polymer representation for Holant problems. The polymer partition function is simply $Z(\mathcal{C}_\kappa(G), \Phi_\pi(\cdot, \mathbf{1}))$. In this section, we derive bounds that depend only on the functions of $\mathcal{F}$ that target Holant problems in particular. This gives the analogue of Lemma 4.4 for Holant problems.

LEMMA 4.6. *Let $\mathcal{F} \subseteq \mathcal{F}_0$, with $r(\mathcal{F}) \leq \max\{(2\sqrt{e})^{-1}(\Delta\kappa e)^{-\frac{\Delta}{2}}, 0.2058(\kappa + 1)^{-\Delta}\}$. For all graphs G of maximum degree Δ and all $\pi\colon V \to \mathcal{F}$, the Taylor expansion of $\log Z_\mathcal{F}(G, \pi)$ converges absolutely.*

PROOF.   We again aim to apply Theorem 4.1 on the polymer representation $Z(\mathcal{C}_\kappa(G), \Phi_\pi(\cdot, \mathbf{1}))$. Consider a fixed polymer $\gamma_\phi \in \mathcal{C}_\kappa(G)$. With $\mathbf{z}$ fixed to $\mathbf{1}$, each polymer γ'_ϕ incompatible with γ_ϕ contributes to the sum that has to be bounded by $a(\gamma_\phi)$ the term

$$|\Phi_\pi(\gamma'_\phi, \mathbf{1})| \, e^{a(\gamma'_\phi)} = \left(\prod_{v \in V(\gamma')} |f_v(E^\kappa(\gamma'_\phi))| \frac{1}{|f_v(\mathbf{0})|} \right) e^{a(\gamma'_\phi)}$$
$$\leq r(\mathcal{F})^{|V(\gamma')|} \, e^{a(\gamma'_\phi)}.$$

As in the proof of [Lemma 4.4](#), we use $\mathcal{C}_\kappa^{\gamma_\phi}(i)$ to denote the set of polymers with i edges and incompatible with γ_ϕ, and use the estimate $|\mathcal{C}_\kappa^{\gamma_\phi}(i)| \leq |V(\gamma)|(\frac{(\Delta\kappa e)^i}{2})$.

Since now $r(\mathcal{F}) < 1$, we need to consider a lower bound on the number of vertices in a polymer in $\mathcal{C}_\kappa^{\gamma_\phi}(i)$ to upper bound its weight. A connected subgraph of maximum degree Δ with i vertices contains at most $\frac{\Delta i}{2}$ edges. This bound together with the choice $a(\gamma_\phi) = \alpha|V(\gamma)|$ for some $\alpha > 0$ to be fixed later and $r = r(\mathcal{F})$ yields

$$\sum_{\gamma'_\phi \not\sim \gamma_\phi} |\Phi_\pi(\gamma'_\phi, \mathbf{1})|e^{a(\gamma'_\phi)} \leq \sum_{i=1}^{|V(G)|} |\mathcal{C}_\kappa^{\gamma_\phi}(\tfrac{\Delta i}{2})|\, r^i\, e^{i\alpha}$$

$$\leq \sum_{i=1}^{|V(G)|} |V(\gamma)|\frac{1}{2}((\Delta\kappa e)^{\frac{\Delta}{2}}\, r\, e^\alpha)^i.$$

With geometric series estimate for this sum, bounding this by $a(\gamma_\phi) = \alpha|V(\gamma)|$ yields the inequality

$$|V(\gamma)|\frac{1}{2}\left(\frac{1}{1 - (\Delta\kappa e)^{\frac{\Delta}{2}}\, r\, e^\alpha} - 1\right) \leq \alpha|V(\gamma)|$$

$$1 - (\Delta\kappa e)^{\frac{\Delta}{2}}\, r\, e^\alpha \geq \frac{1}{2\alpha + 1}$$

$$(\Delta\kappa e)^{\frac{\Delta}{2}}\, r\, e^\alpha \leq 1 - \frac{1}{2\alpha + 1}$$

$$r \leq \frac{2\alpha}{(2\alpha + 1)(\Delta\kappa e)^{\frac{\Delta}{2}}\, e^\alpha}.$$

The best bound for α maximises the function $\frac{2\alpha}{(2\alpha+1)e^\alpha}$. The first derivative for α is $\frac{-4\alpha^2 - 2\alpha + 2}{(2\alpha+1)^2 e^\alpha}$. This expression is zero when $\alpha = \frac{1}{2}$ and the second derivative is negative at this point. This yields the bound

$$r \leq \frac{1}{2(\Delta\kappa e)^{\frac{\Delta}{2}}\, \sqrt{e}}.$$

To obtain the second bound of the lemma, we use $\mathcal{V}_\kappa^{\gamma_\phi}(j)$ to denote the set of polymers with j *vertices* that are incompatible

with γ_ϕ. As Borgs *et al.* (2013), we bound $|\mathcal{V}_\kappa^{\gamma_\phi}(j)| \leq |V(\gamma)|(\kappa + 1)^{j\Delta}$. This bound together with the choice $a(\gamma_\phi) = \alpha|V(\gamma)|$ for some $\alpha > 0$ yields the bound

$$\sum_{\gamma_\phi' \not\sim \gamma_\phi} |\Phi_\pi(\gamma_\phi', \mathbf{1})| e^{a(\gamma_\phi')} \leq \sum_{j=1}^{|V(G)|} |\mathcal{V}_\kappa^{\gamma_\phi}(j)| \, r^j \, e^{\alpha j}$$

$$\leq \sum_{j=1}^{|V(G)|} |V(\gamma)|(\kappa + 1)^{j\Delta} \, r^j \, e^{\alpha j}.$$

The Kotecký–Preiss condition is hence satisfied for α and r such that the inequality

$$\sum_{j=1}^{|V(G)|} |V(\gamma)|(\kappa + 1)^{j\Delta} \, r^j \, e^{\alpha j} \leq \alpha|V(\gamma)|$$

$$\Leftrightarrow \qquad \sum_{j=1}^{|V(G)|} ((\kappa + 1)^\Delta r \, e^\alpha)^j \leq \alpha$$

$$\Leftarrow \qquad \frac{1}{1 - (\kappa + 1)^\Delta r \, e^\alpha} \leq \alpha + 1$$

$$\Leftrightarrow \qquad 1 - (\kappa + 1)^\Delta r \, e^\alpha \geq \frac{1}{\alpha + 1}$$

$$\Leftrightarrow \qquad (\kappa + 1)^\Delta r \, e^\alpha \leq 1 - \frac{1}{\alpha + 1}$$

$$\Leftrightarrow \qquad r \leq \frac{\alpha}{(\alpha + 1)(\kappa + 1)^\Delta e^\alpha}$$

holds. To find the best α to maximise the function $\frac{\alpha}{(\alpha+1)e^\alpha}$, we again find the positive root of the derivative.

This gives $\alpha = \frac{\sqrt{5}-1}{2}$, and the second derivative is negative at this point. We obtain the bound

$$r \leq \frac{\sqrt{5} - 1}{(\sqrt{5} + 1)(\kappa + 1)^\Delta e^{\frac{\sqrt{5}-1}{2}}} \approx 0.2058(\kappa + 1)^{-\Delta}.$$

Together the two bounds give the lemma.   □

As in the case for Holant polynomials, the above lemma gives rise to FPTAS' for the following Holant problems.

THEOREM 4.7. *Let $\mathcal{F} \subseteq \mathcal{F}_0$, with $r(\mathcal{F}) < \max\{(2\sqrt{e})^{-1}(\Delta\kappa e)^{-\frac{\Delta}{2}},$ $0.2058(\kappa+1)^{-\Delta}\}$. For all graphs G of maximum degree Δ and all $\pi\colon V \to \mathcal{F}$, the Holant problem $Z_{\mathcal{F}}(G, \pi)$ admits an FPTAS.*

PROOF.   Since a Holant problem is a Holant polynomial at $\mathbf{z} = \mathbf{1}$, the proof is identical to the proof of Theorem 1.1 by using Lemma 4.6 instead of Lemma 4.4. The only difference is that q is now defined by $(\max\{\frac{(2\sqrt{e})^{-1}(\Delta\kappa e)^{-\frac{\Delta}{2}}}{r(\mathcal{F})}, \frac{0.2058(\kappa+1)^{-\Delta}}{r(\mathcal{F})}\})^{\frac{1}{\Delta}}$, where the exponent $\frac{1}{\Delta}$ ensures that in the calculations of Lemma 4.6 the term $r^{|V(\gamma')|}$ cancels out the $|x|^{|E(\gamma')|}$ term. $\square$

5. Fast randomised algorithms

Recently, Chen *et al.* (2021) have studied Markov chains on vertex spin polymer models. Their results establish conditions yielding fast randomised sampling and counting algorithms with polynomial run-time and linear dependency on the maximum degree Δ of the input graph. We follow their approach and show how their algorithms can be adapted to Holant problems and Holant polynomials exploiting the respective polymer models.

Consider a Holant polynomial $Z_{\mathcal{F}}(G, \pi, \mathbf{z})$, where for the rest of this section we restrict the values of the signatures in $\mathcal{F}$ to be nonnegative reals and we further restrict $\mathbf{z} \in (\mathbb{R}_{\geq 0})^{\kappa+1}$. We aim to design fast algorithms that sample from the distribution μ_G with

$$\mu_G(\sigma) = \frac{\prod_{v \in V(G)} f_v(\sigma|_{E(v)}) \prod_{i=0}^{\kappa} z_i^{|\sigma|_i}}{Z_{\mathcal{F}}(G, \pi, \mathbf{z})}.$$

To do so, we will use polymer models. Recall our definition of the polymer partition function $Z(\mathcal{C}_\kappa(G), \Phi_\pi(\cdot, \mathbf{z}))$ from Section 3. The restrictions to the nonnegative reals imply $\Phi_\pi(\cdot, \mathbf{z}) \in \mathbb{R}_{\geq 0}$. We will design a Markov chain with the families of $\mathcal{I}_\kappa(G)$ as state space with stationary distribution $\mu_{\mathcal{C}_\kappa(G)}$, where

$$\mu_{\mathcal{C}_\kappa(G)}(\Gamma) = \frac{\sum_{\gamma_\phi \in \Gamma} \Phi_\pi(\gamma_\phi, \mathbf{z})}{Z(\mathcal{C}_\kappa(G), \Phi_\pi(\cdot, \mathbf{z}))}.$$

To ensure that the Markov chain converges to its stationary distribution in polynomial time, we require the following condition.

DEFINITION 5.1. *Let G be a graph. The polymer model $(\mathcal{C}_\kappa(G),$ $\Phi_\pi(\cdot, \mathbf{z}))$ satisfies the* mixing condition *if there exists a constant $\xi \in (0, 1)$ such that for each $\gamma_\phi \in \mathcal{C}_\kappa(G)$,*

$$\sum_{\gamma'_\phi \not\sim \gamma_\phi} |E(\gamma'_\phi)| \Phi_\pi(\gamma'_\phi, \mathbf{z}) \le \xi |E(\gamma_\phi)| .$$

For every $e_0 \in E(G)$, let $\mathcal{C}_\kappa(e_0) = \{\gamma_\phi \in \mathcal{C}_\kappa(G) \mid e_0 \in \gamma\}$ be the set of polymers whose underlying graph contains the edge e_0 and let $\alpha(e_0) = \sum_{\gamma \in \mathcal{C}_\kappa(e_0)} \Phi_\pi(\gamma_\phi, \mathbf{z})$. We define the probability distribution μ_0 on $\mathcal{C}(e_0) \cup \{\emptyset\}$ by $\mu_0(\gamma_\phi) = \Phi_\pi(\gamma_\phi, \mathbf{z})$ and $\mu_0(\emptyset) = 1 - \alpha(e_0)$. Definition 5.1 ensures that $\alpha(e_0) < 1$, for every $e_0 \in E(G)$ (by choosing any γ_ϕ with $\gamma = e_0$); hence, μ_0 is a valid probability distribution. We are now ready to define the transition of the Holant polymer Markov chain $(\Gamma_t)_{t \in \mathbb{N}}$.

- ○ Choose $e_0 \in E(G)$ uniformly at random.

- ○ If there exists $\gamma_\phi \in \Gamma_t$ with $e_0 \in E(\gamma_\phi)$, then $\Gamma_{t+1} \leftarrow \Gamma_t \setminus \{\gamma_\phi\}$ with probability $1/2$.

- ○ Otherwise, sample γ_ϕ from μ_0 and if $X_t \cup \{\gamma_\phi\} \in \mathcal{I}(G)$, then $\Gamma_{t+1} \leftarrow \Gamma_t \cup \{\gamma_\phi\}$ with probability $1/2$.

In all other cases, we set $\Gamma_{t+1} \leftarrow \Gamma_t$.

Let P be the transition matrix of the above chain and let $T(\varepsilon) = \max_{\Gamma \in \mathcal{I}_\kappa(G)} \min\{t \mid \|P^t(\Gamma, \cdot) - \mu_{\mathcal{C}_\kappa(G)}(\cdot)\|_T V \le \varepsilon\}$ be its mixing time. We have the following lemma.

LEMMA 5.2. *Let $\mathcal{F} \subseteq \mathcal{F}_0$ and G be a graph of maximum degree Δ and let $\pi \colon V(G) \to \mathcal{F}$. When the mixing condition applies, the Holant polymer Markov chain has stationary distribution $\mu_{\mathcal{C}_\kappa(G)}$ and mixes in $T(\varepsilon) \in O(\Delta n \log(n/\varepsilon))$ many iterations.*

PROOF.   The Markov chain $(\Gamma_t)_{t \in \mathbb{N}}$ is ergodic and thus it has a unique stationary distribution, which is the limit distribution. We first show that $\mu_{\mathcal{C}_\kappa(G)}$ is the unique stationary distribution of the above Markov chain. Let $\Gamma, \Gamma' \in \mathcal{I}_\kappa(G)$ such that there exists $\gamma_\phi \in \mathcal{C}_\kappa(G)$ with $\Gamma \cup \{\gamma_\phi\} = \Gamma'$. It suffices to show that

$\mu_{\mathcal{C}_\kappa(G)}(\Gamma)P(\Gamma,\Gamma') = \mu_{\mathcal{C}_\kappa(G)}(\Gamma')P(\Gamma',\Gamma)$. The latter holds, since

$$\mu_{\mathcal{C}_\kappa(G)}(\Gamma)P(\Gamma,\Gamma') = \frac{\prod_{\gamma'_\phi \in \Gamma} \Phi_\pi(\gamma'_\phi, \mathbf{z})}{Z_\mathcal{F}(G, \pi, \mathbf{z})} \frac{|E(\gamma)|}{|E(G)|} \frac{1}{2} \Phi_\pi(\gamma_\phi)$$

$$= \frac{\prod_{\gamma'_\phi \in \Gamma'} \Phi_\pi(\gamma'_\phi, \mathbf{z})}{Z_\mathcal{F}(G, \pi, \mathbf{z})} \frac{|E(\gamma)|}{|E(G)|} \frac{1}{2}$$

$$= \mu_{\mathcal{C}_\kappa(G)}(\Gamma')P(\Gamma',\Gamma).$$

To upper bound the mixing time of this Markov chain, we will use path coupling as Dyer & Greenhill (1999). To this end, we define a metric $\mathrm{dist}(\cdot, \cdot)$ on Ω by setting $\mathrm{dist}(\Gamma, \Gamma') = 1$ if for some $\gamma_\phi \in \mathcal{C}_\kappa(G)$, $\Gamma \cup \{\gamma_\phi\} = \Gamma'$ or $\Gamma' \cup \{\gamma_\phi\} = \Gamma$. This function dist can be naturally extended to all pairs Γ, Γ' in Ω by shortest paths. Formally let $\Gamma = \Gamma_0, \Gamma_1, \ldots, \Gamma_\ell = \Gamma'$ be a shortest path between Γ and Γ' in Ω, then $\mathrm{dist}(\Gamma, \Gamma') = \sum_{i=1}^{\ell} \mathrm{dist}(\Gamma_{i-1}, \Gamma)$. We can now observe that the diameter $W = \max_{(\Gamma,\Gamma')}\{\mathrm{dist}(\Gamma, \Gamma')\}$ of Ω is at most n, since no family in $\mathcal{I}_\kappa(G)$ can contain more than $\frac{n}{2}$ polymers.

We define our coupling to be the chain denoted by (X_t, Y_t) as follows. First observe that as we are using path coupling, we only need to define how the chain progresses for pairs that only differ in one polymer. Let $\gamma_\phi = (\gamma, \phi_\gamma) \in \mathcal{C}_\kappa(G)$ be such that $X_t \cup \{\gamma_\phi\} = Y_t$, then (X_t, Y_t) progresses as follows.

○ For both X_t and Y_t, choose the same $e_0 \in E(G)$ uniformly at random.

○ If $e_0 \in \gamma$, let $X_{t+1} \leftarrow X_t$ and $Y_{t+1} \leftarrow Y_t \backslash \{\gamma_\phi\}$ with probability $1/2$. With remaining probability $1/2$, sample γ'_ϕ from μ_0 and let $X_{t+1} \leftarrow X_t \cup \{\gamma'_\phi\}$ and $Y_{t+1} \leftarrow Y_t$.

○ If $e_0 \notin \gamma$, then X_t behaves as the original chain Γ_t and Y_t copies X_t if possible, otherwise Y_t remains at the same state.

We will now show that the distance of adjacent states reduces in expectation. We have that $\mathbb{E}[\mathrm{dist}(X_{t+1}, Y_{t+1}) \mid X_t, Y_t]$ is at most

$$1 + \frac{1}{2|E(G)|}\left(-|E(\gamma)| + \sum_{\gamma'_\phi \not\sim \gamma_\phi} |E(\gamma'_\phi)|\Phi_\pi(\gamma'_\phi, \mathbf{z})\right),$$

since the distance decreases by 1 with probability $1/2$ if we choose an edge in γ and it increases by 1 with probability $1/2$ if we sample a polymer that is incompatible with γ_ϕ. The latter occurs with probability $|E(G)|^{-1} \sum_{\gamma'_\phi \not\sim \gamma_\phi} |E(\gamma')| \Phi_\pi(\gamma'_\phi, \mathbf{z})$. From the statement of the lemma, the mixing condition applies, which yields

$$\mathbb{E}[\text{dist}(X_{t+1}, Y_{t+1}) \mid X_t, Y_t] \leq 1 - |E(\gamma)|\frac{1-\xi}{2|E(G)|} \leq 1 - \frac{1-\xi}{2|E(G)|}.$$

Now we can use the path coupling lemma (Dyer & Greenhill 1999, (17) in Section 6) which yields $T(\varepsilon) \leq \log(W/\varepsilon)2|E(G)|/(1-\xi) \in O(\Delta n \log(n/\varepsilon))$. $\qquad\square$

To obtain a fast sampling algorithm, we have to show that each iteration of the polymer Markov chain only requires constant time in expectation. To do so, as Chen *et al.* (2021, Definition 4), we need to identify under which condition this holds.

DEFINITION 5.3. *Given a graph G of maximum degree Δ, we say that a polymer model $(\mathcal{C}_\kappa(G), \Phi(\cdot, \mathbf{z}))$ satisfies the polymer sampling condition with constant $\tau \geq 5 + 3\ln(\kappa\Delta)$ if $\Phi(\gamma_\phi, \mathbf{z}) \leq e^{-\tau|E(\gamma)|}$ for all $\gamma_\phi \in \mathcal{C}_\kappa(G)$.*

Mimicking Chen *et al.* (2021), we consider the following algorithm to sample from μ_0 in constant time in expectation. Let $\varrho = \tau - 2 - \ln(\kappa\Delta) \geq 3 + 2\ln(\kappa\Delta)$.

- ◦ Choose k according to the geometric distribution with parameter $1 - e^{-\varrho}$, that is $\mathbb{P}(k = i) = (1 - e^{-\varrho})e^{-\varrho i}$. Note that $\mathbb{P}(k \geq i) = e^{-\varrho i}$.

- ◦ List all polymers in $\mathcal{C}_\kappa(e_0, k) = \{\gamma_\phi \in \mathcal{C}_\kappa(e_0) \mid |E(\gamma)| \leq k\}$ and compute their weight functions $\Phi(\cdot, \mathbf{z})$. Recall that $\mathbf{z}$ is considered to be fixed.

- ◦ Mutually exclusively output $\gamma_\phi \in \mathcal{C}_\kappa(e_0, k)$ with probability $\Phi(\gamma_\phi, \mathbf{z})e^{\varrho|E(\gamma)|}$ and with all remaining probability output $\emptyset$. Observe that if $k = 0$ then we output $\emptyset$ with probability 1.

LEMMA 5.4. *The above sampling algorithm under the polymer sampling condition (Definition 5.3) outputs a polymer γ from the distribution μ_0 in constant time in expectation.*

PROOF.   The proof follows that of Chen *et al.* (2021, Lemma 16). We first show that the algorithm is well defined, i.e. the probabilities $\Phi(\gamma_\phi, \mathbf{z})e^{\varrho|E(\gamma)|}$ sum to less than 1. Using Lemma 4.2 we have

$$
\begin{aligned}
\sum_{\gamma \in \mathcal{C}_\kappa(e_0)} \Phi(\gamma_\phi, \mathbf{z})e^{\varrho|E(\gamma)|} &\leq \frac{1}{2} \sum_{k \geq 1} e^{\tau k - \varrho k}(e\kappa\Delta)^k \\
&= \frac{1}{2} \sum_{k \geq 1} e^{-k(2+\ln(\kappa\Delta))}(e\kappa\Delta)^k \\
&= \frac{1}{2} \sum_{k \geq 1} e^{-k} < 1.
\end{aligned}
$$

Next, we will show that the output of the sampler has distribution μ_0. Let $\gamma_\phi \in \mathcal{C}_\kappa(e_0)$. In order to have nonzero probability to output γ_ϕ we must choose $k \geq |E(\gamma)|$. This happens with probability $e^{-\varrho|E(\gamma)|}$ by the distribution of k. Conditioned on the choice of an appropriate k, the probability of the sampler to output γ_ϕ is then $\Phi(\gamma_\phi, \mathbf{z})e^{\varrho|E(\gamma)|}$. Thus, the probability of choosing any $\gamma_\phi \in \mathcal{C}_\kappa(e_0)$ is $\Phi(\gamma_\phi, \mathbf{z})$, showing that the outputs of our sampler are distributed according to μ_0.

Finally, we analyse the expected run-time of the sampler. Note that as Patel & Regts (2017, Lemma 3.5) we can enumerate all polymers in $\mathcal{C}_\kappa(e_0, k)$ in time $\mathcal{O}(k^5(e\Delta)^{2k})$. From Corollary 4.3, the number of weights we have to consider are at most $k(\kappa e\Delta)^k/2$. Given a polymer with k edges, we can compute its weight in polynomial time; hence, we can compute all weights in time $\mathcal{O}(k^c(\kappa e\Delta)^k)$ for some constant c. Following the calculations of Chen *et al.* (2021, Lemma 16), we can show that the expected run-time is constant. $\square$

COROLLARY 5.5. *Let G be a graph of maximum degree Δ, let $\mathcal{F} \subseteq \mathcal{F}_0$ and let $\pi\colon V(G) \to \mathcal{F}$. Let $(\mathcal{C}_\kappa(G), \Phi_\pi(\cdot, \mathbf{z}))$ be a polymer model satisfying the sampling condition. There is an ε-approximate sampling algorithm for $\mu_{\mathcal{C}_\kappa(G)}$ with run-time in $\mathcal{O}(\Delta n \log(n/\varepsilon))$.*

PROOF.   The proof is identical to the proof of Chen *et al.* (2021, Theorem 5).   □

Chen *et al.* (2021, Section 3) show how to use a sampler with simulated annealing in order to obtain a fast randomised algorithm. The run-time of this algorithm can be upper-bounded by the $\mathcal{O}(n/\varepsilon^2 \log(\Delta n/\varepsilon))$ calls to the randomised sampler. This approach can be used with the randomised sampler we describe above to get a randomised algorithm with run-time in $\mathcal{O}(\Delta n^2/\varepsilon^2 \log^2(\Delta n/\varepsilon))$.

By randomised approximation algorithm, we mean a *fully polynomial time randomised approximation scheme (FPRAS)*. The latter is an algorithm that, given a problem and some fixed parameter $\varepsilon > 0$, produces with probability at least $3/4$ a multiplicative ε-approximation of its solution in time polynomial in n and $1/\varepsilon$.

THEOREM 5.6. *Let G be a graph of maximum degree Δ, $\mathcal{F} \subseteq \mathcal{F}_0$ and $\pi \colon V(G) \to \mathcal{F}$. For the Holant polynomial $Z_{\mathcal{F}}(G, \pi, \mathbf{z})$, there exists an ε-sampling algorithm from the distribution μ_G with run-time in $\mathcal{O}(\Delta n \log(n/\varepsilon))$ for $\mathbf{z}$ in*

$$\left\{ (z_0, \ldots, z_\kappa) \in (\mathbb{R}_{\geq 0})^{\kappa+1} \mid z_0 \neq 0, \frac{z_i}{z_0} \leq ((\Delta\kappa)^3 e^5 r_1^2)^{-1}, \ i \in [\kappa] \right\}$$

with $r_1 = \max\{1, r(\mathcal{F})\}$. Furthermore, $Z_{\mathcal{F}}(G, \pi, \mathbf{z})$ admits an FPRAS with run-time $\mathcal{O}(\Delta n^2/\varepsilon^2 \log^2(\Delta n/\varepsilon))$ for these values of $\mathbf{z}$.

PROOF.   Recall from the proof of Lemma 3.1 that there is a bijection between the assignments σ for the Holant polynomial and the families of polymers $\Gamma \in \mathcal{I}_\kappa(G)$. Using this bijection, it suffices to sample from the equivalent distribution $\mu_{\mathcal{C}_\kappa(G)}$. It remains to show that the mixing and the sampling conditions apply for our polymer model.

From the statement of the lemma, for any $\gamma_\phi \in \mathcal{C}_\kappa(G)$, we have

$$\Phi_\pi(\gamma_\phi, \mathbf{z}) = \left(\prod_{i=1}^{\kappa} \left(\frac{z_i}{z_0} \right)^{|E^\kappa(\gamma_\phi)|_i} \right) \prod_{v \in V(\gamma)} f_v(E^\kappa(\gamma_\phi)) \frac{1}{f_v(\mathbf{0})}$$

$$\leq ((\Delta\kappa)^3 e^5 r_1^2)^{-|E(\gamma)|} r(\mathcal{F})^{|V(\gamma)|}.$$

The graphs of our polymers are connected; hence, for each $\gamma_\phi \in \mathcal{C}_\kappa(G)$, $|V(\gamma)| \leq |E(\gamma)| + 1$. Together with the fact that $r_1 = \max\{1, r(\mathcal{F})\}$, this gives

(5.7) $$\Phi_\pi(\gamma_\phi, \mathbf{z}) \leq ((\Delta\kappa)^3 \mathrm{e}^5)^{-|E(\gamma)|}.$$

Thus, this polymer system satisfies the sampling condition (Definition 5.3).

Regarding the mixing condition, recall that for any polymer γ_ϕ, $|\mathcal{C}_\kappa^{\gamma_\phi}(i)| \leq |V(\gamma)|(\frac{(\Delta\kappa\mathrm{e})^i}{2})$. Using the latter and (5.7), we have

$$\sum_{\gamma'_\phi \not\sim \gamma_\phi} |E(\gamma'_\phi)| \Phi_\pi(\gamma'_\phi, \mathbf{z}) \leq \sum_{i=1}^m i|V(\gamma)|(\frac{(\Delta\kappa\mathrm{e})^i}{2})((\Delta\kappa)^3 \mathrm{e}^5)^{-i}$$
$$\leq \sum_{i=1}^m \frac{|V(\gamma)|}{2}((\Delta\kappa)^2 \mathrm{e}^3)^{-i}$$
$$< \frac{|V(\gamma)|}{2}.$$

Since for any connected graph γ, $|V(\gamma)| \leq E(\gamma) + 1$, the mixing condition (Definition 5.1) holds. $\square$

Similar to the Holant polynomials, we prove the following theorem for Holant problems.

THEOREM 5.8. *Let G be a graph of maximum degree Δ, $\mathcal{F} \subseteq \mathcal{F}_0$ such that $r(\mathcal{F}) \leq ((\Delta\kappa)^{-\frac{3\Delta}{2}} \mathrm{e}^{-\frac{5\Delta}{2}})$ and $\pi\colon V(G) \to \mathcal{F}$. There exists an ε-sampling algorithm from the distribution μ_G for $Z_\mathcal{F}(G, \pi)$ with run-time in $\mathcal{O}(\Delta n \log(n/\varepsilon))$. Furthermore, $Z_\mathcal{F}(G, \pi)$ admits an FPRAS with run-time $\mathcal{O}(\Delta n^2/\varepsilon^2 \log^2(\Delta n/\varepsilon))$.*

PROOF.   Following the proof of Theorem 5.6, we only have to show that the sampling and the mixing condition hold.

From the statement of the lemma, for any $\gamma_\phi \in \mathcal{C}_\kappa(G)$, we have

$$\Phi_\pi(\gamma_\phi, \mathbf{z}) = \prod_{v \in V(\gamma)} f_v(E^\kappa(\gamma_\phi)) \frac{1}{f_v(\mathbf{0})} \leq r(\mathcal{F})^{|V(\gamma)|}.$$

From the conditions of the lemma, we have $r(\mathcal{F}) < 1$. Recall that G has maximum degree Δ, thus for each $\gamma_\phi \in \gamma$, we have $|V(\gamma)| \geq (2|E(\gamma)|)/\Delta$ yielding

$$\Phi_\pi(\gamma_\phi, \mathbf{z}) \leq (r(\mathcal{F}))^{-\frac{2|E(\gamma)|}{\Delta}} \leq ((\Delta\kappa)^3 \mathrm{e}^5)^{-|E(\gamma)|},$$

which implies the sampling condition (Definition 5.3).

The proof for the mixing condition (Definition 5.1) is identical to the proof Theorem 5.6. □

6. Further applications of abstract polymers

In this section, we will show how the problem of counting weighted solutions to a system of sparse equations as studied by Barvinok & Regts (2019) can be modelled as a polymer system and derive zero-free regions for this problem. The parameter of this problem is a set of complex numbers $w_1, w_2, \ldots, w_m \in \mathbb{C}$. We define the weight of a vector $\mathbf{x} \in \mathbb{Z}_{\geq 0}^m$ with $\mathbf{x} = (x_1, x_2, \ldots, x_m)$ as $w(\mathbf{x}) = w_1^{x_1} w_2^{x_2} \ldots w_m^{x_m}$. Given a finite set $X \subset \mathbb{Z}_{\geq 0}^m$, we define its weight,

$$w(X) = \sum_{\mathbf{x} \in X} w(\mathbf{x}).$$

Given an $n \times m$ matrix $A = (a_{i,j})$ with $a_{i,j} \in \mathbb{Z}$ and positive integers $\kappa_1, \ldots, \kappa_m \in \mathbb{Z}_{>0}$ the task is to approximate $w(X)$ with

$$(6.1) \quad X = \left\{ \mathbf{x} \in \mathbb{Z}_{\geq 0}^m \mid Ax = \mathbf{0} \text{ and for all } j \in [m], x_j \leq \kappa_j \right\}.$$

We view the above as a Holant problem where the input is a hypergraph. Here, the vectors correspond to edge assignments and the constraints given by each row of the matrix correspond to the vertex functions. We are going to model this problem as a polymer system.

First, we explain the underlying hypergraph H_A of the matrix A. Given an $n \times m$ integer matrix $A = (a_{i,j})$, we define the hypergraph H_A with n vertices and m edges, where vertex i is in edge j if $a_{i,j} \neq 0$. Hence computing $w(X)$ is a Holant problem on the hypergraph H_A, where edge j can take an assignment in $[\kappa_j]$ and the signature of vertex i outputs the value 1 if the constraint $\sum_{j=1}^m a_{i,j} x_j = 0$ is satisfied. A vector $\mathbf{x} \in X$ corresponds to an assignment to the set of hyperedges of H.

Given a vector $\mathbf{x}$, its support $\mathrm{supp}(\mathbf{x}) = \{j \in [m] \mid x_j \neq 0\}$ is the set of indices of its nonzero entries. Given a hypergraph H

and a hyperedge set $S \subseteq E(H)$, let $H[S]$ be the subhypergraph induced by the hyperedge set S. A hypergraph H is connected if its underlying bipartite graph G_H is connected, where $G_H = (V_1, V_2, E)$ with $V_1 = V(H)$, $V_2 = E(H)$ and $E = \{\{u, v\} \mid u \in V_1, v \in V_2 \text{ and } v \in u\}$. We say that a vector $\mathbf{x} \in \mathbb{Z}_{\geq 0}^m$ is connected if the subhypergraph $H[\mathrm{supp}(\mathbf{x})]$ induced by the hyperedge set in the support of $\mathbf{x}$ is connected.

The idea of translating the system into a polymer model is to express the solutions in terms of their distance from $\mathbf{0}$, which is a solution to the system, and to represent this distance by a sum of connected vectors. Hence, we define the set of polymers $\mathcal{C}(X)$ to contain the connected (with respect to H_A) vectors of $X \setminus \{\mathbf{0}\}$ and the weight of a polymer $\gamma \in \mathcal{C}(X)$ to be $\Phi(\gamma) = w(\gamma)$. The reason we exclude $\mathbf{0}$ from our polymer set is that this will be the ground state in our polymer representation. Two polymers $\gamma_1, \gamma_2 \in \mathcal{C}(X)$ are defined to be incompatible, $\gamma_1 \nsim \gamma_2$, if their underlying hypergraphs share vertices, i.e. $V(H_A[\mathrm{supp}(\gamma_1)]) \cap V(H_A[\mathrm{supp}(\gamma_2)]) \neq \emptyset$. The resulting families of pairwise compatible polymers denoted by $\mathcal{I}(X)$ contain then vectors with pairwise disjoint support. This is crucial to show that the sum over all vectors in such a family yields a vector in X.

LEMMA 6.2. *For the polymer system $\mathcal{C}(X)$, we have*

$$Z(\mathcal{C}(X), \Phi(\cdot)) = w(X).$$

PROOF.   We define the function $\sigma \colon \mathcal{I}(X) \to \mathbb{Z}_{\geq 0}^m$ with $\sigma(\emptyset) = \mathbf{0}$ and, for each $\Gamma \in \mathcal{I}(X)$, $\sigma(\Gamma) = \sum_{\gamma \in \Gamma} \gamma$, where the summation of vectors is done element-wise. As we defined above, two compatible polymers $\gamma_1 \sim \gamma_2$ cannot share vertices in the underlying hypergraph H_A, which implies that $\mathrm{supp}(\gamma_1) \cap \mathrm{supp}(\gamma_2) = \emptyset$. Thus, for a family of compatible polymers Γ we have that $\sigma(\Gamma) \in X$ since there is no $j \in [m]$ with $\sigma(\Gamma)_j > \kappa_j$, and $A\sigma(\Gamma) = \mathbf{0}$ as for each polymer $\gamma \in \Gamma$ we have $A\gamma = \mathbf{0}$. We now show that σ is bijective.

For injectivity consider two families of compatible polymers $\Gamma_1 \neq \Gamma_2$. Let $\gamma_1 \in \Gamma_1 \Delta \Gamma_2$ be a polymer with maximum support cardinality and assume without loss of generality that $\gamma_1 \in \Gamma_1 \setminus \Gamma_2$. First assume the existence of $j \in \mathrm{supp}(\gamma_1)$ that is not in the

support of any polymer in Γ_2. The latter assumption implies $\sigma(\Gamma_1) \neq \sigma(\Gamma_2)$, since $(\sigma(\Gamma_1))_j \neq 0 = (\sigma(\Gamma_2))_j$.

Now assume the contrary, i.e. $\mathrm{supp}(\gamma_1) \subseteq \bigcup_{\gamma \in \Gamma_2} \mathrm{supp}(\gamma)$. Since γ_1 is connected in H_A, the support of γ_1, which represents a set of connected hyperedges in H_A, cannot be partitioned into pairwise compatible sets. Hence, Γ_2 can contain at most one polymer γ_2 with $\mathrm{supp}(\gamma_1) \subseteq \mathrm{supp}(\gamma_2)$. Due to the maximality of the support cardinality in the choice of γ_1, we have $\mathrm{supp}(\gamma_1) = \mathrm{supp}(\gamma_2)$. Since $\gamma_1 \notin \Gamma_2$, this means that $\gamma_1 \neq \gamma_2$ which means that there is at least one index j in which γ_1 and γ_2 differ. By the definition of incompatibility, no other polymer in Γ_1 or Γ_2 can affect this index j and it follows that $(\sigma(\Gamma_1))_j = (\sigma(\{\gamma_1\}))_j \neq (\sigma(\{\gamma_2\}))_j = (\sigma(\Gamma_2))_j$. This implies $\sigma(\Gamma_1) \neq \sigma(\Gamma_2)$ and concludes the proof that σ is injective.

For surjectivity, we will argue that, given a vector $x \in X$, there is always a family of polymers $\Gamma \in \mathcal{I}(X)$ with $\sigma(\Gamma) = x$. Assume that the hypergraph $H_A[\mathrm{supp}(x)]$ induced by the support of x has k connected components induced by the sets of edges $C_1 \ldots C_k$ for some $k \geq 0$. We deduce that the vectors γ_i with $(\gamma_i)_j = x_j$ for all $j \in C_i$ and $(\gamma_i)_j = 0$ otherwise are in $\mathcal{C}(X)$ since by definition their support induces connected subhypergraphs of H_A. Hence, for the family $\Gamma = \{\gamma_1, \ldots \gamma_k\}$ we have $\sigma(\Gamma) = x$.

Finally, observe that for any family $\Gamma \in \mathcal{I}(X)$ we have that $\prod_{\gamma \in \Gamma} w(\gamma) = w(\sigma(\Gamma))$. The latter yields

$$
\begin{aligned}
Z(\mathcal{C}(X), \Phi(\cdot)) &= \sum_{\Gamma \in \mathcal{I}(X)} \prod_{\gamma \in \Gamma} w(\gamma) \\
&= \sum_{\Gamma \in \mathcal{I}(X)} w(\sigma(\Gamma)) = \sum_{x \in X} w(x) = w(X),
\end{aligned}
$$

where the last equality comes from the bijectivity of σ. $\square$

By this polymer representation, we can now apply Theorem 4.1 to prove absolute convergence of $\log w(X)$ which yields the following.

LEMMA 6.3. *Let A be an $n \times m$ integer matrix, let $\kappa_1, \ldots, \kappa_m \in \mathbb{Z}_{>0}$ and X as in (6.1). Assume the number of nonzero entries in*

every row of A does not exceed r for some $r \geq 2$ and the number of nonzero entries in every column of A does not exceed c for some $c \geq 1$. Let $w = \max\{|w_1|, \ldots, |w_m|\}$ and $\kappa = \max\{\kappa_1, \ldots, \kappa_m\}$. If $w \leq ((re+1)c\kappa e^{1/2})^{-1}$, then $\log w(X)$ converges absolutely.

PROOF. Consider the polymer representation of $w(X)$ appearing in Lemma 6.2. Based on the definition of w and $w \leq 1$ we deduce that for every $\gamma \in \mathcal{C}(X)$ it holds $w_j^{x_j} \leq w$ for all $j \in \text{supp}(\gamma)$. Thus, $\Phi(\gamma) = w(\gamma) \leq w^{|E(\gamma)|}$. To apply Theorem 4.1 consider an arbitrary fixed polymer $\gamma \in \mathcal{C}(X)$ and denote by $\mathcal{C}^\gamma(i) = |\{\gamma' \in \mathcal{C}(X) \mid \gamma' \nsim \gamma, |E(\gamma)| = i\}|$ the number of polymers of size i incompatible with γ. As in the previous bounds, we choose $a(\gamma') = \alpha|E(\gamma')|$ where $\alpha \in \mathbb{R}_{>0}$ will be chosen later in order to optimise the bound.

$$\sum_{\gamma' \nsim \gamma} |\Phi(\gamma')| e^{a(\gamma')} \leq \sum_{\gamma' \nsim \gamma} w^{|E(\gamma')|} e^{a(\gamma')}$$
$$\leq \sum_{i=1}^m \mathcal{C}^\gamma(i) w^i e^{\alpha i}.$$

Observe that in the hypergraph representation r denotes the maximum degree of H_A and c denotes the maximum hyperedge size of H_A. Further observe that a hypergraph $H = (V, E)$ is also a hypergraph $H' = (E, V)$ with the same underlying bipartite graph representation, i.e. $G_H = G_{H'}$. Now we use (Liu *et al.* 2018, Corollary 3.8) to deduce that there are at most $\frac{(erc)^{i-1}}{2}\kappa^i$ many hyperedge-coloured connected hyperedge-induced subhypergraphs of H_A with i hyperedges that contain a fixed hyperedge. The latter corollary applies as coloured hypergraphs fall into the definition of *insects* (Liu *et al.* 2018, Definition 3.8). This bound implies $\mathcal{C}^\gamma(i) \leq \frac{(erc)^{i-1}}{2}\kappa^i|V(\gamma)|$, which gives

$$\sum_{\gamma' \nsim \gamma} |\Phi(\gamma')| e^{a(\gamma')} \leq \sum_{i=1}^m \frac{(erc)^{i-1}}{2}\kappa^i|V(\gamma)| w^i e^{\alpha i}$$
$$\leq \frac{|V(\gamma)|}{2rce} \sum_{i=1}^m (e^{\alpha+1} rc\kappa w)^i.$$

We apply Theorem 4.1 and it remains to identify the values of w for which the following holds,

$$\frac{|V(\gamma)|}{2rce}\sum_{i=1}^{m}(\mathrm{e}^{\alpha+1}rc\kappa w)^i \leq \alpha|E(\gamma)|.$$

Since m can be arbitrarily large, we use the geometric series formula for the sum on the left-hand side of the above inequality, hence the above equation is implied by

$$\sum_{i=0}^{\infty}(\mathrm{e}^{\alpha+1}rc\kappa w)^i - 1 \leq 2rce\alpha\frac{|E(\gamma)|}{|V(\gamma)|}$$

$$\Leftarrow \qquad \frac{1}{1-\mathrm{e}^{\alpha+1}rc\kappa w} - 1 \leq 2rce\alpha\frac{|E(\gamma)|}{|V(\gamma)|}.$$

We know that in H each hyperedge contains at most c vertices, therefore for any polymer γ we have $|V(\gamma)| \leq c|E(\gamma)|$. Using this, the above inequality is implied by

$$\frac{1}{1-\mathrm{e}^{\alpha+1}rc\kappa w} - 1 \leq 2re\alpha$$

$$\Leftrightarrow \qquad \mathrm{e}^{\alpha+1}rc\kappa w \leq \frac{2re\alpha}{2re\alpha + 1}$$

$$\Leftrightarrow \qquad w \leq \frac{2\alpha}{(2re\alpha + 1)c\kappa\mathrm{e}^{\alpha}}.$$

Through derivative analysis, we find this is maximal for $2er\alpha^2 + \alpha - 1 = 0$, which resolves to $\alpha = \frac{\sqrt{8er+1}-1}{4er}$. This brings the final bound to

$$w \leq \frac{\sqrt{8er+1}-1}{(\sqrt{8er+1}+1)rc\kappa\mathrm{e}^{(\sqrt{8er+1}-1)/(4er)+1}}.$$

Choosing $\alpha = \frac{1}{2}$ for simplicity instead yields the bound given in the statement

$$w \leq \frac{1}{(re+1)c\kappa\mathrm{e}^{1/2}}.$$

$\square$

When X is restricted to vectors in $\{0,1\}^m$ Barvinok & Regts (2019, Theorem 1.1) using a different technique were able to obtain the improved bound of $w \leq \frac{0.46}{r\sqrt{c}}$. Furthermore given an integer $\kappa > 1$ for $X \subseteq (\mathbb{Z}/\kappa\mathbb{Z})^m$, Barvinok & Regts (2019, Theorem 1.2) showed the bound $w \leq \frac{0.46}{(\kappa-1)r\sqrt{c}}$. The bounds for $w(X)$ yield smaller regions than the theorems of Barvinok & Regts but are applicable to a broader class of sets X. As a possible application of their theorem, they give a polynomial expressing perfect matchings in terms of their distance from a given perfect matching. As we show in the next section, we can utilise the type of constraints perfect matchings impose and obtain a better bound by using our polymer approach.

6.1. Improved zero-free regions for a perfect matching polynomial. Given a k-hypergraph $H = (V, E)$ and a perfect matching $M \subseteq E$, as we discussed in the introduction for graphs, we define the *perturbative perfect matching polynomial* expressing the distance to M in the following way

$$Z_{\mathrm{pm}}(H, M, z) = \sum_{\sigma \in \{0,1\}^E} \prod_{v \in V} f(\sigma|_{E(v)}) z^{|\sigma \Delta \sigma_M|}.$$

Here, $\sigma_M \in \{0,1\}^E$ denotes the signature corresponding to M, $\sigma \Delta \bar{\sigma} = \{e \in E \mid \sigma(e) \neq \bar{\sigma}(e)\}$ for any two assignments $\sigma, \bar{\sigma} \in \{0,1\}^E$ and f is the "exactly one" function. Note that finding a perfect matching on a k-hypergraph with $k \geq 3$ is NP-complete (see e.g. Ausiello *et al.* 1999), therefore we assume that M is given. Barvinok & Regts (2019) prove that for $|z| \leq \frac{0.46}{\Delta\sqrt{k}}$ this polynomial has no roots. When the k-hypergraph is k-partite, this can be improved to $|z| \leq \frac{1}{\sqrt{\Delta-1}}$ (Barvinok 2019). By using our technique, we improve the general bound to $|z| \leq ((\Delta - 1 + k)e)^{-1}$ for any k-hypergraph of maximum degree Δ.

Let $H = (V, E)$ be a k-hypergraph of maximum degree Δ. Let $G = (V_L, V_R, E)$ be the corresponding bipartite graph, where $V_L = V(H)$, $V_R = E(H)$ and $E(G) = \{(u, e) \mid u \in V(H), e \in E(H) \text{ and } u \in e\}$. Let $\Delta_L = \Delta$ be the maximum degree of the vertices in V_L and $\Delta_R = k$ be the maximum degree of the vertices in V_R. Any perfect matching M' in H can be seen as an assignment

$\sigma_{M'} : V_R \to \{0, 1\}$, with $\sigma_{M'}(v) = 1$ if and only if $v \in M'$. Let M be the "ground" perfect matching for H. Hence, $M \subseteq V_R$ in the bipartite graph G.

Given a perfect matching M', let $E_{M'} = \{v \in V_R \mid \sigma_M(v) \neq \sigma_{M'}(v)\}$ and consider the subgraph $G[S_{M'}]$ induced by the set $S_{M'} = E_{M'} \cup \bigcup_{v \in E_{M'}} \Gamma_G(v)$. We rewrite Z_{pm} in terms of the bipartite graph G as

$$Z_{\mathrm{pm}}(G, M, z) = \sum_{M' \in \mathcal{PM}(H)} z^{|V_R(G[S_{M'}])|},$$

where $\mathcal{PM}(H)$ denotes the set of perfect matchings of H. Observe that for each $M' \in \mathcal{PM}(H)$, $G[S_{M'}]$ has the property that each vertex $v \in V(G[S_{M'}]) \cap V_L$ has exactly one neighbour in M and one neighbour in $V_R \setminus M$.

We are now ready to define a polymer model for $Z_{\mathrm{pm}}(G, M, z)$. The set of polymers $\mathcal{C}(G)$ contains the connected subgraphs of G such that every vertex in V_L has exactly one neighbour in M and exactly one neighbour in $V_R \setminus M$ and that for every $v \in V_R$, $\Gamma_G(v) \subseteq V(\gamma)$. We say that two polymers $\gamma \nsim \gamma'$ are incompatible if $V(\gamma) \cap V(\gamma') \neq \emptyset$. Given a polymer γ and $z \in \mathbb{C}$, we define $\Phi_{\mathrm{pm}}(\gamma, z) = z^{|V_R(\gamma)|}$.

LEMMA 6.4. *Let $H = (V, E)$ be a finite hypergraph and let G be the corresponding bipartite graph. For all $z \in \mathbb{C}$, $Z_{\mathrm{pm}}(H, M, z) = Z(\mathcal{C}(G), \Phi_{\mathrm{pm}}(\cdot, z))$.*

PROOF.   Since $Z_{\mathrm{pm}}(H, M, z) = Z_{\mathrm{pm}}(G, M, z)$, it suffices to show that $Z_{\mathrm{pm}}(G, M, z) = Z(\mathcal{C}(G), \Phi_{\mathrm{pm}}(\cdot, z))$. We now give a bijection between the perfect matchings M' and the families of polymers Γ, such that $z^{|V_R(G[S_{M'}])|} = \prod_{\gamma \in \Gamma} \Phi_{\mathrm{pm}}(\gamma, z)$.

The ground matching M corresponds to the empty set. Given a perfect matching M' observe that the connected components of $G[S_{M'}]$ are in fact polymers in $\mathcal{C}(G)$, say $\gamma_1, \gamma_2, \ldots, \gamma_j$, where $j \geq 0$. Since $\gamma_1, \gamma_2, \ldots, \gamma_j$ are the connected components of $G[S_{M'}]$, they are pairwise compatible. From the definition of $\Phi_{\mathrm{pm}}(\gamma, z)$, it follows that $\prod_{i=1}^{j} \Phi_{\mathrm{pm}}(\gamma_i, z) = \prod_{i=1}^{j} z^{|V_R(\gamma_i)|} = z^{|V_R(G[S_{M'}])|}$. $\square$

In order to apply Theorem 4.1, we will use the following lemma.

LEMMA 6.5. *Let $G = (V_L, V_R, E)$ be a bipartite graph, where Δ_L is the maximum degree of the vertices in V_L, such that the vertices in V_R have degree at least 2. Let $M \subseteq V_R$, such that every vertex $v \in V_L$ has exactly one neighbour in M. Given a vertex $u \in V_L$, the number of connected induced subgraphs G' of G such that the following hold:*

(i) $u \in V(G')$;

(ii) $|V(G') \cap V_R| = k$;

(iii) for each $v \in V_R$, $\Gamma_G(v) \subseteq V(G')$; and

(iv) each $v \in (V(G') \cap V_L)$ has exactly one neighbour in $V(G') \cap M$ and exactly one neighbour in $V(G') \cap (V_R \setminus M)$

is at most $(\Delta_L - 1)^{k-1}$.

PROOF.   Let $V_L' = V(G') \cap V_L$ and $V_R' = V(G') \cap V_R$. Since $u \in V_L$, we have $u \in V_L'$. Condition 4 implies that in G' the vertex u has exactly two neighbours $v_M \in M$ and $v_{\bar{M}} \notin M$. By the definition of M the choice of v_M is fixed and there are at most $\Delta_L - 1$ choices for $v_{\bar{M}} \in V_R \setminus M$. Since G' is connected, either $k = 2$ and the lemma is proved, or there must exist at least one other vertex $u_1 \in \Gamma_{G'}(v_M) \cup \Gamma_{G'}(v_{\bar{M}})$. As in the case of u, Condition 4 implies the existence of a fixed neighbour of u_1 in M and at most $\Delta_L - 1$ choices for a neighbour of u_1 in $V_R \setminus M$. Proceeding with this argumentation for each vertex in V_L' we observe that each vertex in $V_R' \setminus M$ is a result of one of the up to $\Delta_L - 1$ choices for each vertex in V_L'. Since there must be at least one vertex $v \in M$ whose choice is fixed, the number of the induced subgraphs G' is at most $(\Delta_L - 1)^{k-1}$.   □

LEMMA 6.6. *For all k-hypergraphs H with maximum degree Δ and a given ground perfect matching M, $Z_{\mathrm{pm}}(H, M, z)$ has no roots in $|z| \leq ((\Delta - 1 + k)e)^{-1}$.*

PROOF.   Let H be a k-hypergraph with $G = (V_L, V_R, E)$ its corresponding bipartite graph, where $\Delta_L = \Delta$ and $\Delta_R = k$. Consider

the polymer model with $Z(\mathcal{C}(G), \Phi_{\mathrm{pm}}(\cdot, z)) = Z_{\mathrm{pm}}(H, M, z)$. As in the previous absolute convergence proofs, we apply Theorem 4.1 for $Z(\mathcal{C}(G), \Phi_{\mathrm{pm}}(\cdot, z))$ by choosing $a(\gamma) = \alpha |V_R(\gamma)|$, where $\alpha \in \mathbb{R}_{\geq 0}$ to be chosen later. Let $\mathcal{C}_{\mathrm{pm}}^{\gamma}(i)$ be the number of polymers $\gamma' \not\sim \gamma$ with $|V_R(\gamma')| = i$. We have

$$\sum_{\gamma' \sim \gamma} |\Phi(\gamma')| \mathrm{e}^{a(\gamma')} \leq \sum_{\gamma' \sim \gamma} |z|^{|V_R(\gamma')|} \mathrm{e}^{\alpha |V_R(\gamma')|}$$

$$\leq \sum_{i=1}^{|V_R|} \mathcal{C}_{\mathrm{pm}}^{\gamma}(i) |z|^i \mathrm{e}^{\alpha i}.$$

We observe that each polymer γ is a connected induced subgraph of G that fulfils Conditions 3 and 4 of the statement of Lemma 6.5, with $M = M_0$. Therefore, by Lemma 6.5 we have $\mathcal{C}_{\mathrm{pm}}^{\gamma}(i) \leq |V_L(\gamma)|(\Delta_L - 1)^{i-1}$. In order to prove the lemma, it suffices to show that

$$\sum_{i=1}^{|V_R|} |V_L(\gamma)|(\Delta_L - 1)^{i-1} |z|^i \mathrm{e}^{\alpha i} \leq \alpha |V_R(\gamma)|$$

$$\Leftrightarrow \quad \frac{|V_L(\gamma)|}{\Delta_L - 1} \sum_{i=1}^{|V_R|} (\Delta_L - 1)^i |z|^i \mathrm{e}^{\alpha i} \leq \alpha |V_R(\gamma)|.$$

Since Δ_R is the maximum degree of each vertex in V_R, for each polymer γ, $\frac{1}{\Delta_R} \leq \frac{|V_R(\gamma)|}{|V_L(\gamma)|}$. It remains to show

$$\sum_{i=0}^{|V_R|} (\Delta_L - 1)^i |z|^i \mathrm{e}^{\alpha i} \leq \frac{\alpha(\Delta_L - 1) + \Delta_R}{\Delta_R}.$$

Since $|V_R|$ might be arbitrarily large, using the formula for geometric series, the above inequality is implied by

$$\frac{1}{1 - (\Delta_L - 1)\mathrm{e}^{\alpha}|z|} \leq \frac{\alpha(\Delta_L - 1) + \Delta_R}{\Delta_R}$$

$$\Leftrightarrow \quad (\Delta_L - 1)\mathrm{e}^{\alpha}|z| \leq 1 - \frac{\Delta_R}{\alpha(\Delta_L - 1) + \Delta_R}$$

$$\Leftrightarrow \quad (\Delta_L - 1)e^\alpha|z| \le \frac{\alpha(\Delta_L - 1)}{\alpha(\Delta_L - 1) + \Delta_R}$$

$$\Leftrightarrow \quad |z| \le \frac{\alpha}{(\alpha(\Delta_L - 1) + \Delta_R)e^\alpha}.$$

Substituting $\Delta = \Delta_L$ and $k = \Delta_R$, we obtain

$$|z| \le \frac{\alpha}{(\alpha(\Delta - 1) + k)e^\alpha}.$$

The optimal bound can be found by maximising the function $f(\alpha) = \frac{\alpha}{(\alpha(\Delta-1)+k)e^\alpha}$. We observe that

$$f'(\alpha) = \frac{(\alpha(\Delta - 1) + k)e^\alpha - \alpha((\Delta - 1)e^\alpha + (\alpha(\Delta - 1) + k)e^\alpha)}{((\alpha(\Delta - 1) + k)e^\alpha)^2}.$$

Solving $f'(\alpha) = 0$ for $\alpha > 0$ yields $\alpha = \frac{\sqrt{k^2+4(\Delta-1)k}-k}{2(\Delta-1)}$ and, furthermore, $f''(\alpha) < 0$ at this value.

Substituting we obtain the bound

$$|z| \le \frac{\sqrt{k^2 + 4(\Delta - 1)k} - k}{(\Delta - 1)(\sqrt{k^2 + 4(\Delta - 1)k} + k)e^{\frac{\sqrt{k^2+4(\Delta-1)k}-k}{2(\Delta-1)}}}.$$

Setting $\alpha = 1$ for simplicity yields the bound $|z| \le ((\Delta - 1 + k)e)^{-1}$ given in the statement of the lemma. $\qquad\square$

6.1.1. Perfect matchings on graphs.   When $H = G$ is a graph of maximum degree Δ, instead of a hypergraph, we obtain even better bounds for $Z_{\mathrm{pm}}(G, M, z)$. Since perfect matchings on graphs G are Holants, we recall the definition of our polymer system we employed for the study of the Holant framework. That is, $\mathcal{C}(G)$ is the set of connected subgraphs containing at least one edge and for two polymers $\gamma, \gamma' \in \mathcal{C}(G)$ we defined $\gamma \nsim \gamma'$ if and only if $V(\gamma) \cap V(\gamma') \ne \emptyset$. Furthermore, we identified an assignment $\sigma \in \{0, 1\}^E$ of edges with a vector in $\{0, 1\}^{|E|}$ by assuming an inherent enumeration of the edges. In fact, we can use this model to consider the distance to a ground state different from the empty set. To this end, for $v \in V$ we define the vertex constraints f_v to pick only assignments corresponding to cycles alternating between the

perfect matching M and the assigned edgeset, where we also allow an empty cycle. Formally, f_v assigns 1 to $\mathbf{0}$ as well as to vectors $\mathbb{1}_{e_M} + \mathbb{1}_e$ for $e_M \in M$ and $e \in E(G) \setminus M$ with $v \in e_M \cap e$, and 0 otherwise. We define the weight function for a polymer $\gamma \in \mathcal{C}(G)$ and $z \in \mathbb{C}$ by

$$\Phi_{\mathrm{pm}}(\gamma, z) = \prod_{v \in V(\gamma)} f_v(\mathbb{1}_{E(\gamma)}) z^{|E(\gamma)|}.$$

LEMMA 6.7. $Z_{\mathrm{pm}}(G, M, z) = Z(\mathcal{C}(G), \Phi_{\mathrm{pm}}(\cdot, z))$ for all $z \in \mathbb{C}$ and all finite graphs $G = (V, E)$.

PROOF.   Every perfect matching corresponds to an assignment $\sigma \in \{0, 1\}^E$ with $f(\sigma) = 1$ that contributes $z^{\sigma \Delta \sigma_M}$ to the partition function $Z_{\mathrm{pm}}(G, M, z)$. The difference $\sigma \Delta \sigma_M$ corresponds to a set of disjoint cycles, alternating with respect to M. In this way, any perfect matching σ translates to a set of polymers, each of nonzero weight, which together yield the value $z^{\sigma \Delta \sigma_M}$.

Conversely, an incompatible set of polymers $\Gamma \in \mathcal{I}(G)$ of nonzero weight assigned by Φ_{pm} translates to a perfect matching by editing the ground matching M according to the edges altered by the polymer as follows. The set Γ corresponds to the perfect matching $M_\Gamma = (M \setminus (M \cap E(\Gamma))) \cup (E(\Gamma) \setminus M)$ which differs from M by $|M \cap E(\Gamma))| + |E(\Gamma) \setminus M| = |E(\Gamma)|$ edges, so $\prod_{\gamma \in \Gamma} \Phi_{\mathrm{pm}}(\gamma, z) = z^{|E(\Gamma)|} = z^{\sigma_M \Delta \sigma_{M_\Gamma}}$.

In both cases, the empty family $\{\emptyset\} \in \mathcal{I}(G)$ corresponds to the assignment $\sigma = \mathbf{0}$ which counts 1 to represent the contribution of the ground polymer. $\square$

We will now show the following bound, which matches asymptotically the bound of Barvinok (2019) for bipartite graphs; however, our bound applies to all graphs.

THEOREM 6.8. *For all graphs G of maximum degree Δ, the polynomial $Z_{\mathrm{pm}}(G, M, z)$ has no roots in the region $\{z \in \mathbb{C} \mid |z| \leq \left(\sqrt{4.85718\,(\Delta - 1)}\right)^{-1}\}$ and the cluster expansion of its logarithm converges absolutely.*

PROOF.   We will again apply Theorem 4.1 to the polymer representation $Z(\mathcal{C}(G), \Phi_{\mathrm{pm}}(\cdot, z))$. For the sake of simplicity, we now restrict this polymer definition to the set of polymers with nonzero contribution to the partition function. Hence, let

$$\mathcal{C}_{\mathrm{pm}}(G) = \{\gamma \in \mathcal{C}(G) \mid \prod_{v \in V(\gamma)} f_v(\mathbb{1}_{E(\gamma)}) = 1\}$$

and, therefore, $Z(\mathcal{C}(G), \Phi_{\mathrm{pm}}(\cdot, z)) = Z(\mathcal{C}_{\mathrm{pm}}(G), \Phi_{\mathrm{pm}}(\cdot, z))$.

We fix a polymer $\gamma \in \mathcal{C}_{\mathrm{pm}}(G)$ and in order to bound the number of polymers incompatible with γ we denote by $\mathcal{C}_{\mathrm{pm}}^{\gamma}(i)$ the number of polymers $\gamma' \nsim \gamma$ with $|E(\gamma')| = i$. First, observe that each polymer in $\mathcal{C}_{\mathrm{pm}}(G)$ has an even number of edges, and more precisely, $|E(\gamma') \cap M| = \frac{1}{2}|E(\gamma')|$. Further, by the special structure of polymers in $\mathcal{C}_{\mathrm{pm}}(G)$ we can estimate $|\mathcal{C}_{\mathrm{pm}}^{\gamma}(i)|$ better than with the general Lemma 4.2.

Any $\gamma' \in \mathcal{C}_{\mathrm{pm}}(G)$ with $\gamma' \nsim \gamma$ has to intersect with γ on at least one of the edges from M. There are exactly $\frac{1}{2}|E(\gamma)|$ choices for such a common edge in $M \cap E(\gamma) \cap E(\gamma')$. Starting with such a fixed edge from M, γ' builds a cycle alternating between edges from $E(G) \setminus M$ and M. As M is a perfect matching, the choice of edges from $E(G) \setminus M$ completely determines the edges from $M \cap E(\gamma')$. Moreover, in a graph of maximum degree Δ there are only $\Delta - 1$ choices to continue from a fixed vertex with edges from $E(G) \setminus M$. This yields a total of at most $\frac{1}{2}|E(\gamma)|(\Delta - 1)^{i/2}$ polymers in $\mathcal{C}_{\mathrm{pm}}^{\gamma}(i)$.

We now set $a(\gamma) = \alpha|E(\gamma)|$, where we will choose $\alpha > 0$ later in order to improve the bound on the region. By this choice of $a(\gamma)$ and with $j = \frac{i}{2}$, we obtain

$$\sum_{\gamma' \nsim \gamma} |\Phi_{\mathrm{pm}}(\gamma', z)| e^{a(\gamma')} \leq \sum_{j=2}^{\frac{1}{2}|V(G)|} |\mathcal{C}_{\mathrm{pm}}^{\gamma}(2j)| \, |z|^{2j} \, e^{2\alpha j}$$

$$\leq \sum_{j=2}^{\frac{1}{2}|V(G)|} \frac{1}{2}|E(\gamma)|(\Delta - 1)^j \, |z|^{2j} \, e^{2\alpha j}.$$

In order to apply Theorem 4.1, we are going to choose a bound on $|z|$ such that

$$\sum_{j=2}^{\frac{1}{2}|V(G)|} \frac{1}{2}|E(\gamma)|(\Delta-1)^j |z|^{2j} e^{2\alpha j} \leq a(\gamma) = \alpha|E(\gamma)|,$$

which is equivalent to

$$\sum_{j=2}^{\frac{1}{2}|V(G)|} (\Delta-1)^j |z|^{2j} e^{2\alpha j} \leq 2\alpha.$$

We now set $q = (\Delta-1)|z|^2 e^{2\alpha}$, which is equivalent to $|z| = \sqrt{\frac{q}{(\Delta-1)e^{2\alpha}}}$, and by this choice and the geometric series, we obtain

$$\sum_{j=2}^{\frac{1}{2}|V(G)|} (\Delta-1)^j |z|^{2j} e^{2\alpha j} = \sum_{j=2}^{\frac{1}{2}|V(G)|} q^j < \frac{1}{1-q} - 1$$

assuming that $q \in (0,1)$. Hence, we have to choose α such that $\frac{1}{1-q} - 1 \leq 2\alpha$, which holds exactly if $q \leq \frac{2\alpha}{1+2\alpha}$. We insert this choice of q into the chosen bound on $|z|$ and obtain

$$(6.9) \qquad |z| \leq \sqrt{\frac{2\alpha}{1+2\alpha} \frac{1}{(\Delta-1)e^{2\alpha}}}.$$

Define $g(\alpha) = \sqrt{\frac{2\alpha}{1+2\alpha} \frac{1}{(\Delta-1)e^{2\alpha}}}$. The derivative of g has a positive root at $\alpha = \frac{-1+\sqrt{5}}{4}$ and, furthermore, $f''(\alpha) < 0$ at this point.

Therefore, choosing $\alpha = \frac{-1+\sqrt{5}}{4}$ maximises the bound of (6.9) to

$$|z| \leq \sqrt{\frac{3-\sqrt{5}}{2(\Delta-1)\left(e^{\frac{\sqrt{5}-1}{2}}\right)}} \approx \left(\sqrt{4.85718\,(\Delta-1)}\right)^{-1}.$$

□

Theorem 1.3 is an immediate corollary of the above theorem together with Theorem 2.5.

Acknowledgements

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Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

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