The complexity of approximating the complex-valued Ising model on bounded degree graphs

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Workshop on

Interplay between statistical mechanics, graph theory, computational complexity and holomorphic dynamics

Overview

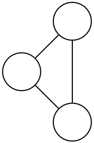
- The Ising model on bounded-degree graphs (no external field)
- A novel zero-free region for the Ising model
- Hardness of approximation in the complex plane
- Connection between zeros and hardness in the Ising model

Galanis, Goldberg, Herrera-Poyatos, *The complexity of approximating the complex-valued Ising model on bounded degree graphs*, arXiv:2105.00287, 2021.

Brackground: the Ising Model

Parameters: $\beta \in \mathbb{C}$ (edge interaction), $\lambda \in \mathbb{C}$ (external field), graph $G = (V, E)$.

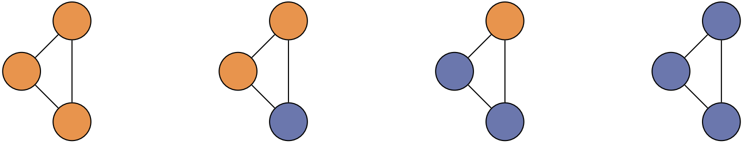
Configurations: $\sigma : V \to \{0, 1\}$.



Probability of a configuration σ: $\mathbb{P}(\sigma) \propto w(\sigma) = \beta^{m(\sigma)} \lambda^{|\sigma|}$

where $m(\sigma)$ is the number of monochromatic edges in σ.

Ising partition function: $Z_{\text{Ising}}(G; \beta, \lambda) = \sum_{\sigma} w(\sigma)$



$\lambda^3 \beta^3$ $\qquad$ $\lambda^2 \beta$ $\qquad$ $\lambda \beta$ $\qquad$ β^3

$$Z = (\lambda^3 + 1)\beta^3 + 3(\lambda^2 + \lambda)\beta$$

- Real $\beta > 1$: Ferromagnetic (prefer many monochromatic edges)
- Real $\beta \in (0, 1)$: Antiferromagnetic (prefer few monochromatic edges)

Computing the partition function

#Ising(β, λ): On input $G = (V, E)$, compute the value $Z_{\text{Ising}}(G; \beta, \lambda)$.

Exact computation of $Z_{\text{Ising}}(G; \beta, \lambda)$ is #P-hard for almost every $\beta, \lambda \in \mathbb{C}\backslash\{0\}$ [Dyer, Greenhill '00; Bulatov, Grohe '05; Goldberg, Grohe, Jerrum, Thurley '08; Cai, Chen, Lu '11].

Problem: Can we approximate #Ising(β, λ)?

- FPTAS for real-valued $Z(G)$:
  For $\varepsilon > 0$, compute $\hat{Z}$ in time $\text{poly}(\text{size}(G), 1/\varepsilon)$ s.t. $\hat{Z} = e^z Z(G)$ for some $z \in [-\varepsilon, \varepsilon]$.
- FPTAS for complex-valued $Z(G)$:
  For $\varepsilon > 0$, compute $\hat{Z}$ in time $\text{poly}(\text{size}(G), 1/\varepsilon)$ s.t. $\hat{Z} = e^z Z(G)$ for some $z \in \mathbb{C}$ with $|z| \leq \varepsilon$.

Why complex parameters?

[Barvinok '17]

Absence of zeros in the complex plane $\Rightarrow$ Approximation algorithm for $Z(G;\lambda)$, even for real values of λ

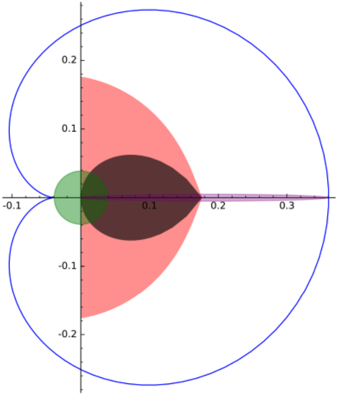
Main Idea:

- Assume $Z(G;\lambda) \neq 0$ for all λ in a "region" around the origin.
- Taylor series expansion of $\log Z(G;\lambda)$ converges.
- Compute truncated Taylor series.

Answering the question:

1. [Patel-Regts '17] On bounded-degree graphs this gives poly-time algorithms.
2. Complex zeros vs approximability: how critical is the absence of zeros?
3. Connections with classical statistical physics/combinatorics results: phase transitions, quantum computation (IQP circuits), exact counting.

Approx. algorithms for the independent set polynomial



Zero-free regions for $\Delta = 10$.

$\Delta :=$ maximum degree of input graph G.

Notation:

$$Z_G(\lambda) = \sum_{I \text{ independent set}} \lambda^{|I|}.$$

Cardioid:

$\Lambda_\Delta = \{\lambda : |z| \leq 1/(\Delta - 1), \lambda = z/(1-z)^{\Delta-1}\}$.

Zero-free regions:

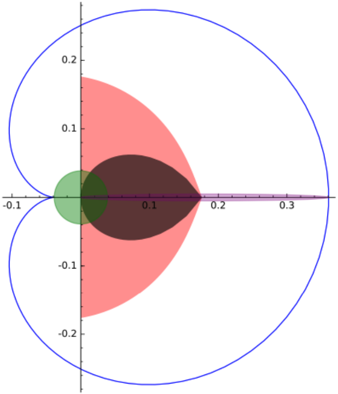
[Patel, Regts '16;
Harvey, Srivastava, Vondrák '16]:
FPTAS when $|\lambda| < \lambda^*(\Delta) = (\Delta-1)^{\Delta-1}/\Delta^\Delta$.

[Peters, Regts '19]: FPTAS in the strip around $[0, \lambda_c)$, where $\lambda_c = (\Delta-1)^{\Delta-1}/(\Delta-2)^\Delta$.

[Peters, Regts '19]: FPTAS when $|\lambda| \leq \varepsilon_{\Delta,\epsilon} \sim \frac{\pi}{(2+\epsilon)(\Delta-1)}$ and $|\arg(\lambda)| \leq \frac{\varepsilon\pi}{2(2+\varepsilon)}$.

[Bencs, Csikvári '18]: FPTAS when $\mathrm{Re}(\lambda) \geq 0$ and $|\lambda| < \delta_\Delta \sim \frac{1.374}{\Delta}$.

Hardness for the independent set polynomial



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Cardioid:

$\Lambda_\Delta = \{\lambda : |z| \leq 1/(\Delta - 1), \lambda = z/(1-z)^{\Delta-1}\}$.

[Bezáková, Galanis, Goldberg, Štefankovič '18]:
Approximation problem is #P-hard for non-real $\lambda \notin \Lambda_\Delta$ on bipartite graphs.

[Buys '19, Rivera-Leterier '19]:
There exist $\lambda \in \mathrm{Int}(\Lambda_\Delta)$ and G with max. degree Δ such that $Z_G(\lambda) = 0$.

[de Boer, Buys, Guerini, Peters, Regts '21]:
Zeros $\Rightarrow$ #P-Hardness of approximation.

Approximation algorithms for Ising

Notation:

Δ maximum degree of input graph G.

$\beta_c := \frac{\Delta}{\Delta-2}$ and $(1/\beta_c, \beta_c)$ is the uniqueness region of the Δ-regular infinite tree (more on β_c later).

Setting 1: Ferromagnetic Ising (real $\beta > 1$ and $\lambda \in \mathbb{C}$):

Lee-Yang zeros: zeros are on the unit circle $|\lambda| = 1$.

[Liu, Sinclair, Srivastava '19]: FPTAS when $\beta > 1$ and $|\lambda| \neq 1$.

[Peters, Regts '20]: FPTAS when $\beta < \beta_c$ and λ is on the "zero-free" arc of the unit circle.

[Buys, Galanis Patel, Regts '20]: #P-hard when:

- $\beta \geq \beta_c$ and $\lambda \neq \pm 1$;
- $\beta < \beta_c$ and λ is not on the "zero-free" arc of the unit circle.

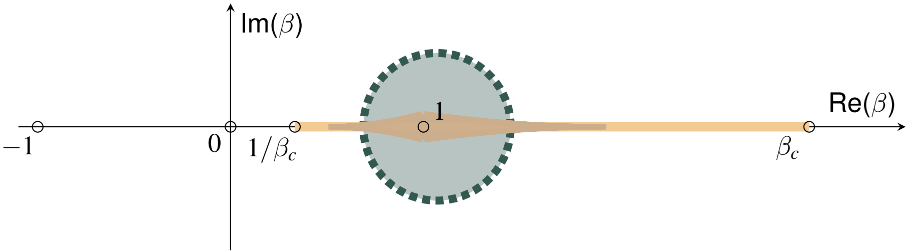
This setting is well understood.

Approximation algorithms for Ising

Setting 2: No external field ($\beta \in \mathbb{C}$ and $\lambda = 1$):

- [Liu-Sinclair-Srivastava '19]: FPTAS in a strip around $(1/\beta_c, \beta_c)$.
- [Barvinok '17, Mann-Bremner '19]: FPTAS in the disc $|\frac{\beta-1}{\beta+1}| \leq \delta_\Delta \sim \frac{0.561}{\Delta}$.
- [Barvinok-Barvinok 21']: FPTAS in a "diamond" around some of $(1/\beta_c, \beta_c)$.

Hardness and zeros on non-real edge interactions: nothing known outside these regions.



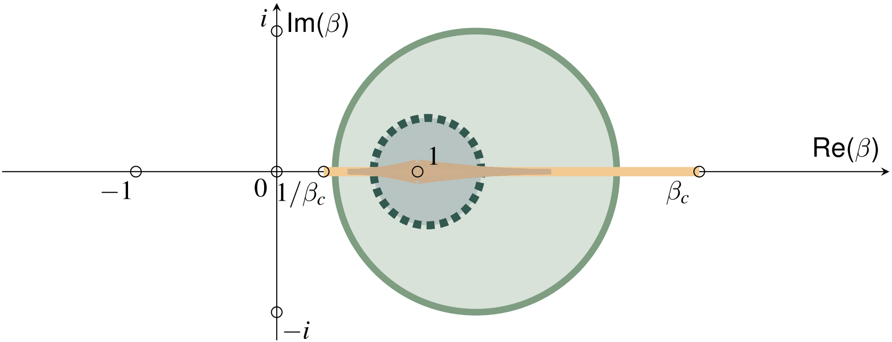
Zero-free regions for $\Delta = 3$.

This talk: [Galanis, Goldberg, Herrera-Poyatos '21] new work on this case.

A novel zero-free region

Theorem 1: Let $\Delta \geq 3$ and $\varepsilon_\Delta = \tan(\frac{\pi}{4(\Delta-1)}) \in (0,1)$.

Then $Z_{\text{Ising}}(G;\beta) \neq 0$ for all $\beta \in \mathbb{C}$ with $|\frac{\beta-1}{\beta+1}| \leq \varepsilon_\Delta$ and all graphs G with maximum degree Δ.



Zero-free regions for $\Delta = 3$. New region is in large circle.

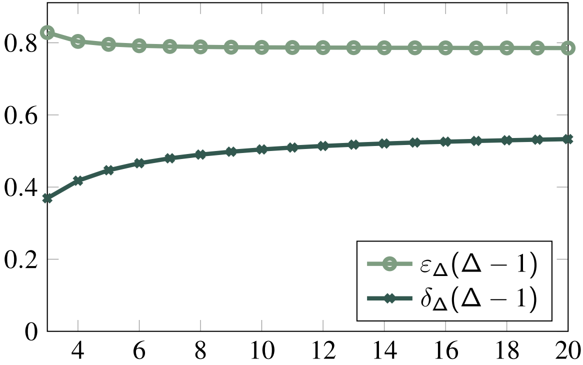
Comparison with Barvinok-Mann-Bremner

- [Barvinok '17, Mann-Bremner '19]: FPTAS in the disc $|\frac{\beta-1}{\beta+1}| \leq \delta_\Delta$.

$$\delta_\Delta = \max\left\{\sin\left(\frac{\alpha}{2}\right)\cos\left(\Delta\frac{\alpha}{2}\right) : 0 < \alpha < \frac{2\pi}{3\Delta}\right\}$$

- Our region: FPTAS in the disc $|\frac{\beta-1}{\beta+1}| \leq \varepsilon_\Delta$.

$$\varepsilon_\Delta = \tan\left(\frac{\pi}{4(\Delta-1)}\right)$$



- Limit of $\delta_\Delta(\Delta-1)$: $0.561...$
- Limit of $\varepsilon_\Delta(\Delta-1)$: $\pi/4 = 0.785...$

Comparison with Barvinok-Barvinok and Liu-Sinclair-Srivastava

$\mathcal{E}_\Delta :=$ maximal zero-free region containing 1.

- [Liu-Sinclair-Srivastava '19]:

For any $\beta \in (1/\beta_c, \beta_c) = (\frac{\Delta-2}{\Delta}, \frac{\Delta}{\Delta-2})$, there exists a $\delta > 0$ such that $B(\beta, \delta) \subseteq \mathcal{E}_\Delta$.

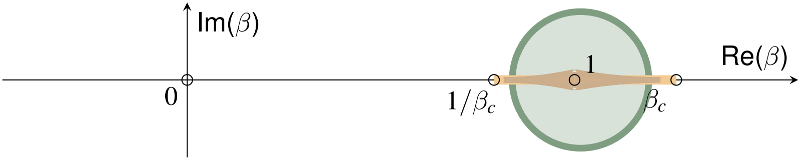
Proof is not constructive, δ is unknown.

- [Barvinok-Barvinok 21']:

Let $0 < \delta < 1$. If $|\mathrm{Re}(a)| < \dfrac{1-\delta}{\Delta}$ and $|\mathrm{Im}(a)| \le \dfrac{\delta^2}{10\Delta}$, then $e^{2a} \in \mathcal{E}_\Delta$.

Multivariate Ising, can include field close to 1.

- Our region: If $|\frac{\beta-1}{\beta+1}| \le \varepsilon_\Delta \sim \frac{0.785\ldots}{\Delta-1}$, then $\beta \in \mathcal{E}_\Delta$.



Zero-free regions for $\Delta = 10$. These regions are incomparable for general Δ.

Computational problems

Fix $\beta \in \mathbb{C}$, $\Delta \geq 3$, $K > 1$ real, $\rho \in (0, \pi/2)$.

$\textsc{IsingNorm}(\beta, \Delta, K)$

Instance: A (multi)graph G with maximum degree at most Δ.
Output: A rational number $\hat{N}$ such that

$$\hat{N}/K \leq |Z_{\text{Ising}}(G; \beta)| \leq K\hat{N}.$$

$\textsc{IsingArg}(\beta, \Delta, \rho)$

Instance: A (multi)graph G with maximum degree at most Δ.
Output: A rational $\hat{A}$ such that $|\hat{A} - a| \leq \rho$ for some $a \in \arg(Z_{\text{Ising}}(G; \beta))$, where $\arg(z) = \{a \in \mathbb{R} : \exp(ai) = z/|z|\}$.

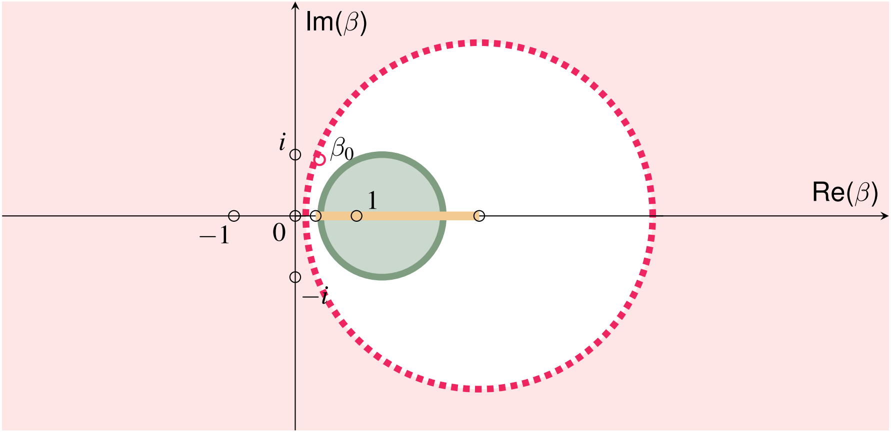
Remark: we can amplify any constant approximation into an FPTAS.

Corollary: $\textsc{IsingNorm}(\beta, \Delta, 1.01)$ and $\textsc{IsingArg}(\beta, \Delta, \pi/3)$ have a poly-time algorithm when $|\frac{\beta-1}{\beta+1}| < \varepsilon_\Delta \sim \frac{0.785\ldots}{\Delta-1}$.

Our hardness result

Theorem 2: Let $\Delta \geq 3$ and $\beta \in \mathbb{C}_{\mathbb{A}} \setminus (\mathbb{R} \cup \{i, -i\})$ with $\left|\frac{\beta-1}{\beta+1}\right| > \frac{1}{\sqrt{\Delta-1}}$. Then $\textsc{IsingNorm}(\beta, \Delta, 1.01)$ and $\textsc{IsingArg}(\beta, \Delta, \pi/3)$ are #P-hard.

Remark: There are zeros β_0 inside this region that imply hardness.



Results for $\Delta = 3$.

The tree of self-avoiding walks

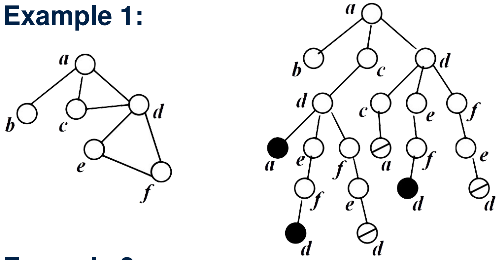
Pinning: conditioning on $\sigma(v) = j$.

SAW tree: Self-avoiding walks starting at vertex a. Leaves for cycles are added and pinned.

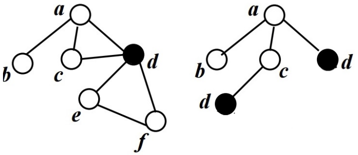
$$Z_v^j(G;\beta) = \sum_{\sigma \text{ s.t. } \sigma(v)=j} \beta^{m(\sigma)}$$

$$R(G,v;\beta) = \frac{Z_v^1(G;\beta)}{Z_v^0(G;\beta)}.$$

Example 1:



Example 2:



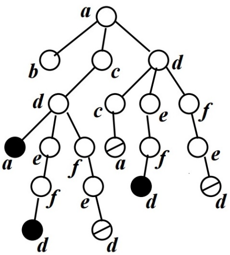
Idea: reducing the study of Z on graphs to its study on trees.

[Weitz '06]: $R(G,a;\beta) = R(T,a;\beta)$.

[Liu, Sinclair, Srivastava '19]:

- $Z_{\text{Ising}}(G;\beta)$ divides $Z_{\text{Ising}}(T;\beta)$.
- $Z_{\text{Ising}}(T;\beta) \neq 0 \Rightarrow Z_{\text{Ising}}(G;\beta) \neq 0$.

Trees and multivariate complex dynamics



$$h_\beta(z) := \frac{\beta z + 1}{\beta + z}, \qquad F_{\beta,k}(z_1, \ldots, z_k) := \prod_{j=1}^{k} h_\beta(z_j)$$

- If T is a node,

$$R(T, v; \beta) = \begin{cases} 1 & \text{if vertex unpinned;} \\ \infty & \text{if vertex pinned to 1;} \\ 0 & \text{if vertex pinned to 0.} \end{cases}$$

- $(T_1, v_1), \ldots, (T_d, v_d)$: trees hanging from (T, a), $r_j = R(T_j, v_j; \beta)$. Then $R(T, v; \beta) = F_{\beta,d}(r_1, \ldots, r_d)$.

Finding zero-free regions: prove $F_{\beta,k}$ is closed on $S \subset \mathbb{C} \cup \{\infty\}$ with $-1 \notin S$.

$$Z_{\text{Ising}}(T; \beta) = Z_v^0(T, v; \beta) \left(1 + \frac{Z_v^1(T, v; \beta)}{Z_v^0(T, v; \beta)}\right) = Z_v^0(T, v; \beta)\,(1 + R(T, v; \beta)) \neq 0$$

Proof-sketch of zero-free region

Our region: $\Delta \geq 3$ and $|\frac{\beta-1}{\beta+1}| \leq \varepsilon_\Delta = \tan\left(\frac{\pi}{4(\Delta-1)}\right)$.

Reminder: $$h_\beta(z) := \frac{\beta z + 1}{\beta + z}, \qquad F_{\beta,k}(z_1, \ldots, z_k) := \prod_{j=1}^{k} h_\beta(z_j).$$

Observation: $$\frac{h_\beta(z) - 1}{h_\beta(z) + 1} = \frac{(\beta - 1)(z - 1)}{(\beta + 1)(z + 1)}$$

Proof - Induction on height of tree - $S = \{z \in \mathbb{C} : \mathrm{Re}(z) \geq 0\} \cup \{\infty\}$

Claim 1: $\mathrm{Re}(z) \geq 0$ if and only if $|\frac{z-1}{z+1}| \leq 1$.

Claim 2: If $\mathrm{Re}(z) \geq 0$, then $|\frac{h_\beta(z)-1}{h_\beta(z)+1}| \leq \varepsilon_\Delta$.

Claim 3: If $|\frac{y-1}{y+1}| \leq \varepsilon_\Delta$, then $\mathrm{Arg}(y) \in \left[-\frac{\pi}{2(\Delta-1)}, \frac{\pi}{2(\Delta-1)}\right]$.

Claim 4: If $\mathrm{Re}(z_j) \geq 0$ for all j, then $\mathrm{Re}(F_{\beta,k}(z_1, \ldots, z_k)) \geq 0$. ■

The importance of pinnings in the Ising model

Trees with no pinnings are trivial in the Ising model (with no external field)!

T tree with no pinnings:

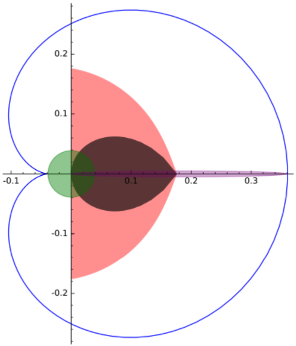
- $R(T, v; \beta) = 1$ for all β;
- $Z_{\text{Ising}}(T; \beta) = 0$ if and only if $\beta = -1$.

[Bencs '18] Updated divisibility result for the independent set polynomial
$T' \leftarrow$ subtree of SAW tree without pinnings,
$Z_G(\lambda)$ divides $Z_{T'}(\lambda)$.

No such result can exist for the Ising model!

Trees without pinnings capture *ratios / implementations* in the Hard-core model.

The ideas of Bezáková-Galanis-Goldberg-Štefankovič



Zero-free regions for $\Delta = 10$.

Independent set polynomial:

$$Z_G(\lambda) = \sum_{I \text{ independent set}} \lambda^{|I|}.$$

Easiness: Ratios (with pinnings) bounded away from -1.

Hardness: Ratios (no pinnings) dense around -1.

Cardioid:
$\Lambda_\Delta = \{\lambda : |z| \leq 1/(\Delta - 1), \lambda = z/(1-z)^{\Delta-1}\}$.

Implementation result:

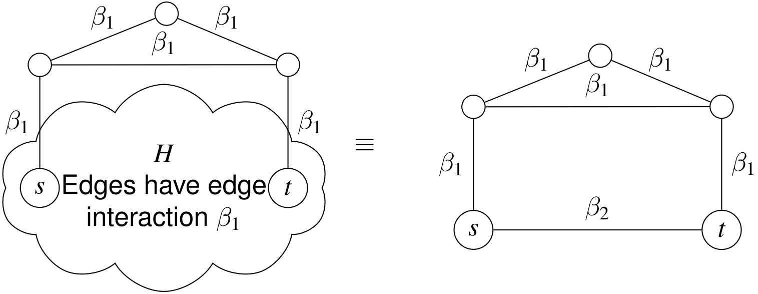
$\lambda \notin \Lambda_\Delta \implies \{R(T, v; \lambda) : T \text{ tree max. deg. } \Delta\}$ is dense in the complex plane.

Proof idea : Complex dynamics on univariate tree recurrence $f(z) = \dfrac{1}{1 + \lambda z^d}$.

Implementations when there is no external field

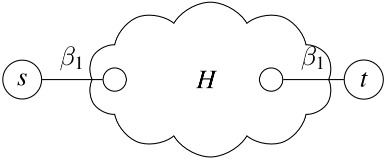
Definition idea: Let $\beta_1, \beta_2 \in \mathbb{C}^2$ and let H be a graph.

- H β_1-*implements* β_2 with terminals $s, t \in V(H)$ if (H, s, t) with edge interaction β_1 "behaves" as an edge with edge interaction β_2.



$$\beta_2 = Z_{st}^{11}(H; \beta_1)/Z_{st}^{01}(H; \beta_1).$$

- H (Δ, β_1)-*implements* $\beta_2 \in \mathbb{C}$:
  - H has maximum degree at most Δ,
  - distinct vertices s and t of degree 1.



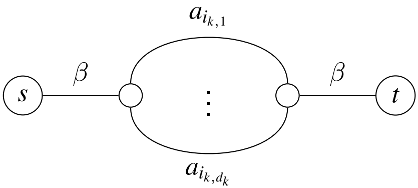
A recursive gadget

$$h_\beta(x) = \frac{\beta x + 1}{\beta + x}, \qquad g_\beta(x) = h_\beta(h_\beta(x)) = \frac{x + 2\beta + x\beta^2}{1 + 2x\beta + \beta^2}$$

Ising program: Sequence $a_0, a_1, \ldots$, starting with $a_0 = \beta$ and satisfying

$$a_k = g_\beta(a_{i_{k,1}} \cdots a_{i_{k,d_k}}) \quad \text{for } k \geq 1,$$

where $d_k \in [d]$ and $i_{k,1}, \ldots, i_{k,d} \in \{0, \ldots, k-1\}$.



- Ising program generates $a_k \iff \exists H_k$ that (Δ, β)-implements a_k.

Study the recurrence $f(z) = g_\beta(z^d)$.

Complex dynamics: implementing the complex plane

$$h_\beta(x) = \frac{\beta x + 1}{\beta + x}, \qquad g_\beta(x) = h_\beta(h_\beta(x)) = \frac{x + 2\beta + x\beta^2}{1 + 2x\beta + \beta^2}$$

Ising model

∘ $f(z) = g_\beta(z^d)$

∘ Starting value: β (one edge)

∘ Fixed point ω: 1

∘ ω repelling when $|\frac{\beta-1}{\beta+1}| > \frac{1}{\sqrt{\Delta-1}}$.

Independent set polynomial

$f(z) = (1 + \lambda z^d)^{-1}$

∘ Starting value: λ (vertex unpinned)

∘ Fixed point ω: choose fixed point with smallest norm.

∘ ω repelling when $\lambda \notin \Lambda_\Delta$.

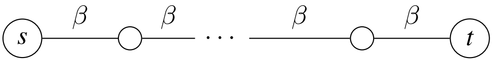
Observation: $f(z) = g(z^d)$ where g is Mobius map.

Strategy resembles [BGGS '18].

Complex dynamics: implementing the complex plane

Steps in the proof

1. Get arbitrary close to ω (program-approximable fixed point). Specific to g.



   Ising: Implements $g^n(\beta)$, which converges to 1 or -1.

2. Implement dense subset of open set U containing ω. General proof.

3. When ω is repelling,

$$\bigcup_{n=0}^{\infty} f^n(U) = \widehat{\mathbb{C}} \setminus E_f.$$

   Use this to implement complex plane. General proof.

Implementation result: We can implement a dense subset of $\mathbb{C}$.

Zeros imply hardness?

Let $\beta \in \mathbb{C}_{\mathbb{A}} \setminus (\mathbb{R} \cup \{i, -i\})$.

Lemma 6: (Δ, β) implements $-1 \implies$ hardness of approximation.

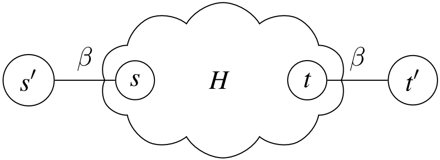
Idea: use zeros to (Δ, β)-implement -1.

Assumptions:

- $Z_{\text{Ising}}(H; \beta) = 0$
- $\max\{\deg(s), \deg(t)\} \leq \Delta - 1$

Implementing -1:

$Z^{11}_{s't'}(H;\beta)/Z^{01}_{s't'}(H;\beta) = -1$



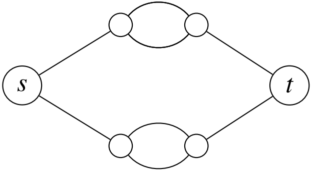
Example: Graph G with max. degree $\Delta = 3$.

$Z^{01}_{st}(G; x) = (1 + x^2 + 2x^3)^2$

$Z^{11}_{st}(G; x) = x^2(2 + x + x^3)^2$

Zero β inside disc: $\left|\frac{\beta-1}{\beta+1}\right| < \frac{1}{\sqrt{\Delta-1}}$

$\beta = 0.396608... + 0.917988...i$.



Conjecture and bottleneck

Corollary:

$Z_{\text{Ising}}(H;\beta) = 0$ for H with maximum degree $\Delta - 1$ $\implies$ IsingNorm$(\beta, \Delta, 1.01)$ and IsingArg$(\beta, \Delta, \pi/3)$ are #P-hard.

Proof idea:

Choose H with minimum number of edges and Implement -1. ■

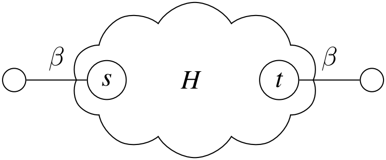
Conjecture:

$Z_{\text{Ising}}(H;\beta) = 0$ for H with maximum degree Δ $\implies$ IsingNorm$(\beta, \Delta, 1.01)$ and IsingArg$(\beta, \Delta, \pi/3)$ are #P-hard.

Bottleneck:

Our approach needs

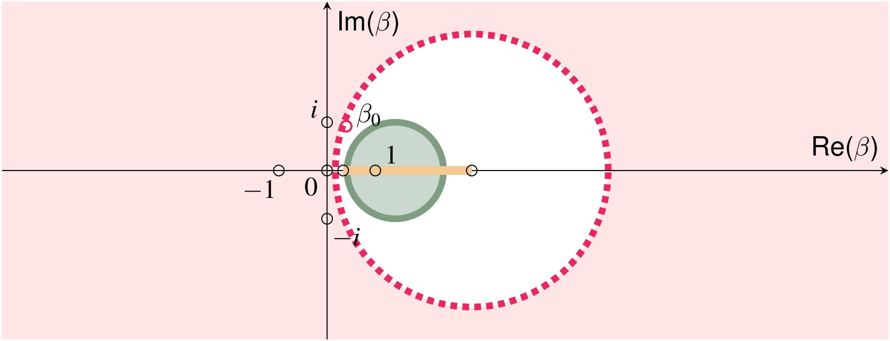
◦ $\max\{\deg(s), \deg(t)\} \leq \Delta - 1$



Independent set polynomial: we can use trees without pinnings!

Open problems

1. Maximal zero-free region containing $(1/\beta_c, \beta_c)$.
2. If a tree with pinnings has ratio r, can we (Δ, β)-implement r (without pinnings)?
3. Hardness when $|\frac{\beta-1}{\beta+1}| > \frac{1}{\Delta-1}$? (now $|\frac{\beta-1}{\beta+1}| > \frac{1}{\sqrt{\Delta-1}}$)
4. Zero on graph with maximum degree $\Delta \implies$ hardness?



Results for $\Delta = 3$.