Zeros of polynomials, phase transitions, and algorithms

ಪೀಯೂಷ ಶ್ರೀವಾಸ್ತವ (Piyush Srivastava)

SPML, ICTS

January 9, 2020

Tata Institute, Mumbai
Joint work with Jingcheng Liu and Alistair Sinclair

Naṭanāmāni

Phase transitions

Complex zeros of polynomials

Decay of correlations

Computational complexity

Naṭanāmāni

Phase transitions

Complex zeros of polynomials

Yang–Lee theory

Decay of correlations

Uniqueness of Gibbs Measures

Computational complexity

"Sampling and counting"

Naṭanāmāni

Phase transitions

Complex zeros of polynomials

Yang-Lee theory

Decay of correlations

Uniqueness of Gibbs Measures

Computational complexity

"Sampling and counting"

Markov chain Monte Carlo

Phase transitions

Complex zeros of polynomials
Yang-Lee theory

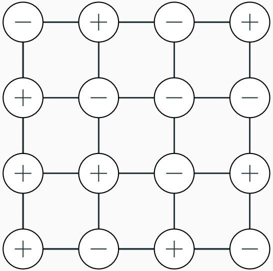
Decay of correlations
Uniqueness of Gibbs Measures

Computational complexity
"Sampling and counting"

Markov chain Monte Carlo

Apology: Survey of results; few/no proofs (questions welcome!)

Ising model

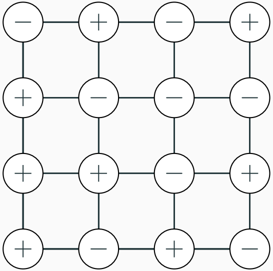


Gibbs distribution

$$\mu(\sigma) \propto \exp\left(J \sum_{u \sim v} \sigma_u \sigma_v\right)$$

The state of each node is independent of other nodes conditioned on its neighbors

Ising model



Gibbs distribution

$$\mu(\sigma) \propto \exp\left(J \sum_{u \sim v} \sigma_u \sigma_v \right)$$

The state of each node is independent of other nodes conditioned on its neighbors

The Ising model is "spatially" Markovian

Probabilistic graphical models/Markov Random fields

Probability distributions with such independence constraints

Graphical models: Beyond magnets

Even the Ising model makes an appearance in a rather wide variety of areas:

Graphical models: Beyond magnets

Even the Ising model makes an appearance in a rather wide variety of areas:

- Individual choice theory, as the logit response

  e.g. [McKelvey & Palfrey, *Games and Econ. Behaviour*, 1995]

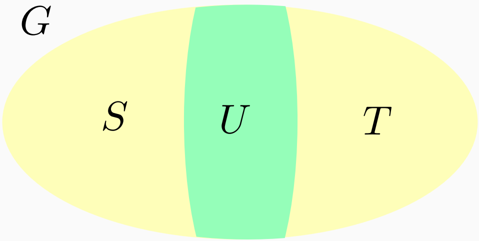
- Spread of opinions in social networks

  e.g. [Montanari & Saberi, *PNAS*, 2010]

- Computer vision

  e.g. [Geman & Graffigne, *Proc. of the ICM*, 1986]

Counting in Markov Random Fields/Spin systems

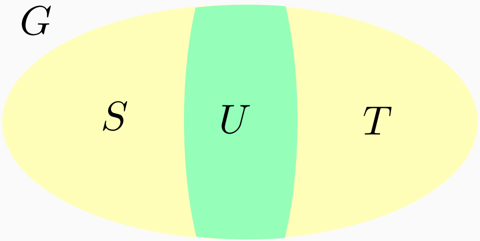


Gibbs Distribution μ s.t.

$$\sigma_S \perp\!\!\!\perp \sigma_T | \sigma_U$$

if U disconnects S from T in G

Counting in Markov Random Fields/Spin systems



Gibbs Distribution μ s.t.

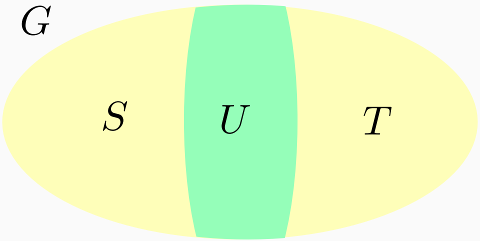
$$\sigma_S \perp\!\!\!\perp \sigma_T | \sigma_U$$

if U disconnects S from T in G

Questions

- (Approximately) **sample** from the Gibbs distribution μ
- (Approximately) compute **marginals** of μ

Counting in Markov Random Fields/Spin systems



Gibbs Distribution μ s.t.

$$\sigma_S \perp\!\!\!\perp \sigma_T | \sigma_U$$

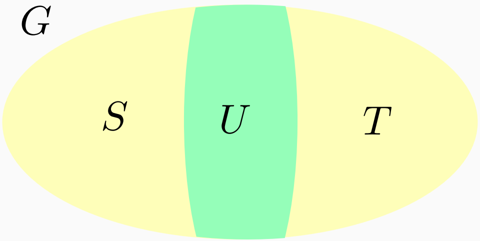
if U disconnects S from T in G

Questions

- (Approximately) **sample** from the Gibbs distribution μ
- (Approximately) compute **marginals** of μ
- Approximate the partition function …next slide!

These are often equivalent problems…

Counting in Markov Random Fields/Spin systems



Gibbs Distribution μ s.t.

$$\sigma_S \perp\!\!\!\perp \sigma_T | \sigma_U$$

if U disconnects S from T in G

Questions

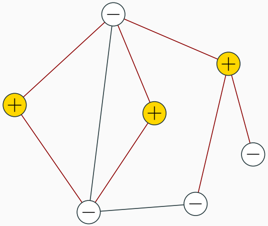
- (Approximately) **sample** from the Gibbs distribution μ
- (Approximately) compute **marginals** of μ
- Approximate the partition function ...next slide!

These are often equivalent problems...

- Learn the model from **samples** of μ ...not in this talk!

Ising model

[Ising, 1925]



Vertex activity

$$\mu(\sigma) \propto w(\sigma) = \lambda^{\#(+)} \beta^{|\mathrm{cut}(\sigma)|}$$

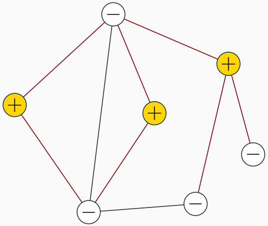
Edge activity

Partition function $Z(\beta, \lambda) := \sum_{\sigma : V \to \{+,-\}} w(\sigma)$

Approximate Z on input G and fixed β and λ?

Ising model

[Ising, 1925]



$$\mu(\sigma) \propto w(\sigma) = \lambda^{\#(+)} \beta^{|\mathrm{cut}(\sigma)|}$$

Vertex activity: λ

Edge activity: β

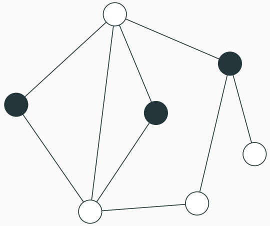
Partition function $Z(\beta, \lambda) := \sum_{\sigma : V \to \{+,-\}} w(\sigma)$

Approximate Z on input G and fixed β and λ?

Ferromagnetic vs. Antiferromagnetic Ising

$\beta < 1$ and $\beta > 1$ are qualitatively very different

Hard core lattice gas/Independent sets



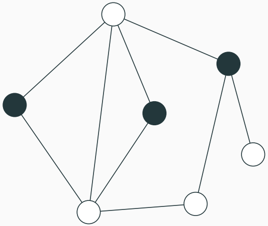
Partition function

$$Z_G(\lambda) = \sum_{I\,:\,\text{ind. set in } G} \lambda^{|I|}$$

Approximate the number of independent sets

$$\mu_\lambda(I) = \frac{1}{Z(\lambda)}\lambda^{|I|}$$

Hard core lattice gas/Independent sets



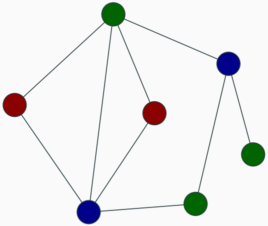
Partition function

$$Z_G(\lambda) = \sum_{I\ :\ \text{ind. set in } G} \lambda^{|I|}$$

Approximate $Z_G(\lambda)$
for input G and fixed λ

$$\mu_\lambda(I) = \frac{1}{Z(\lambda)} \lambda^{|I|}$$

Zero temperature anti-ferromagnetic Potts/Proper colourings



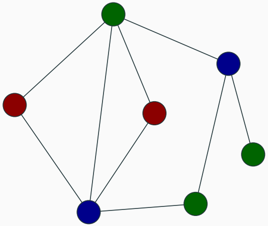
Partition function

$$Z_{G,q}(w) = \sum_{\sigma : V \to [q]} w^{|\{\{u,v\} \in E : \sigma(u) = \sigma(v)\}|}$$

Approximate the number of proper colourings with q colours

$$\mu_{G,q}(\sigma) = \frac{1}{Z_{G,q}(0)} \cdot [\sigma \text{ is a proper colouring}]$$

Zero temperature anti-ferromagnetic Potts/Proper colourings



Partition function

$$Z_{G,q}(w) = \sum_{\sigma : V \to [q]} w^{|\{\{u,v\} \in E : \sigma(u) = \sigma(v)\}|}$$

Approximate $Z_{G,q}(0)$
for input G

$$\mu_{G,q}(\sigma) = \frac{1}{Z_{G,q}(0)} \cdot [\sigma \text{ is a proper colouring}]$$

Spin systems with higher order interactions

More general Ising models:

- A **hypergraph** $G = (V, H)$. Let $n = |V|, m = |E|$
- **Configuration:** $\sigma \in \Sigma := \{+, -\}^V$
- **Hyperedge potentials:** $\varphi_e : \Sigma^{|e|} \to \mathbb{C}$. W.l.o.g. $\varphi_e(-, \ldots, -) = 1$
- **Vertex potentials:** $\psi_v : \Sigma \to \mathbb{C}$. W.l.o.g. $\psi_v(+) = \lambda_v, \psi_v(-) = 1$

Partition function

$$Z_G^{\boldsymbol{\varphi}}(\lambda) = \sum_{\boldsymbol{\sigma}: V \to \{+,-\}} \underbrace{\prod_{e \in H} \varphi_e\left(\boldsymbol{\sigma}\big|_e\right) \prod_{v \in V} \psi(\boldsymbol{\sigma}(v))}_{\text{weight of configuration } \boldsymbol{\sigma}}$$

$$= \sum_{\boldsymbol{\sigma}: V \to \{+,-\}} \prod_{e \in H} \varphi_e\left(\boldsymbol{\sigma}\big|_e\right) \prod_{v : \boldsymbol{\sigma}_v = +} \lambda_v$$

Fully polynomial time approximation

Fully polynomial approximation scheme (FPTAS)

Input: G, ϵ. Output: $\hat{Z}$. Run time: $\mathrm{poly}(|G|, 1/\epsilon)$

$$\left|\hat{Z} - Z\right| \leq \epsilon \, |Z|$$

Fully polynomial time approximation

Fully polynomial randomized approximation scheme (FPRAS)

Input: G, ϵ, δ. Output: $\hat{Z}$. Run time: $\text{poly}(|G|, 1/\epsilon, \log(1/\delta))$

$$\left|\hat{Z} - Z\right| \leq \epsilon |Z|, \text{ with probability } \geq 1 - \delta$$

We are interested in deterministic algorithms:

The P vs. BPP question

"When is randomization essential for efficient algorithms"?

Fully polynomial time approximation

Fully polynomial approximation scheme (FPTAS)

Input: G, ϵ. Output: $\hat{Z}$. Run time: $\mathrm{poly}(|G|, 1/\epsilon)$

$$\left|\hat{Z} - Z\right| \leq \epsilon \, |Z|$$

We are interested in deterministic algorithms:

The P vs. BPP question

"When is randomization essential for efficient algorithms"?

Sampling vs counting

Partition functions	$\equiv$	Gibbs measures
$Z_G(\lambda) = \sum_{I:\text{ind. in } G} \lambda^{\lvert I \rvert}$	$\equiv$	$\mu_G(I) \sim \lambda^I$
Approximate Z	$\equiv$	Approximately sample from μ [Jerrum et al., 1986; Randall and Wilson, 1999]

Sampling vs counting

Partition functions	$\equiv$	Gibbs measures
$Z_G(\lambda) = \sum_{I:\text{ind. in } G} \lambda^{\|I\|}$	$\equiv$	$\mu_G(I) \sim \lambda^I$
Approximate Z	$\equiv$	Approximately sample from μ

[Jerrum et al., 1986; Randall and Wilson, 1999]

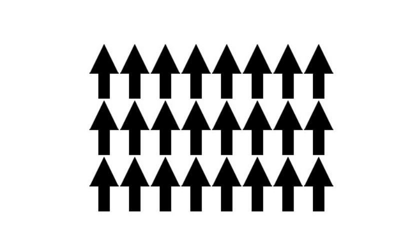
Classical approximate counting methods

- Markov chain Monte Carlo (via approximate samples from μ)
- Exploiting "correlation decay" in μ

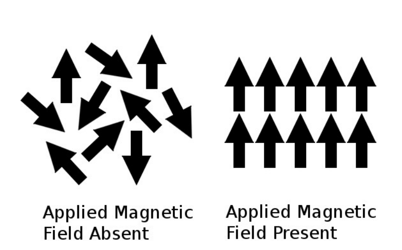
Phase transitions: Statistical Physics and Algorithms

Phase transitions: magnets

Some magnetic materials lose their magnetism just above a critical temperature (Curie temperature)



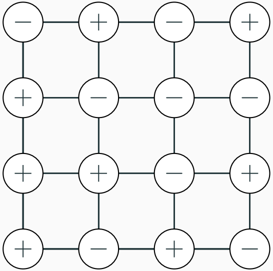
$T < T_c$



$T > T_c$

Perhaps the first phase transition to be abstracted: Ising model (1925)

Ising model



Gibbs distribution

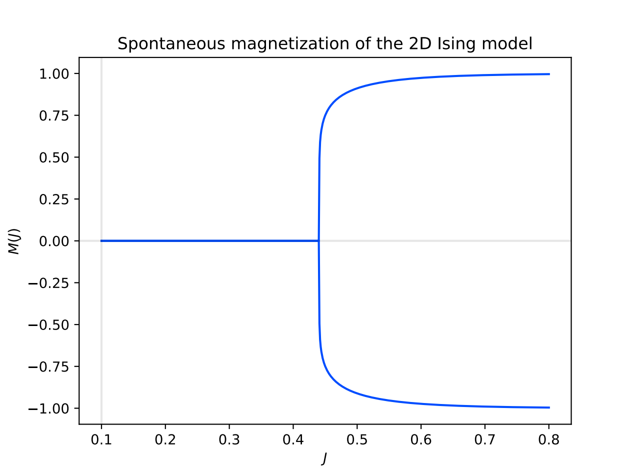
$$\mu(\sigma) \propto \exp\left(J \sum_{u \sim v} \sigma_u \sigma_v\right)$$

- Nodes "represent" magnetic domains, J represents inverse temperature $1/T$
- Mean magentization: Average of $\sum_v \sigma_v$ according to μ

$$M(J) = \mathop{E}_{\sigma \sim \mu}[\sum_v \sigma_v]$$

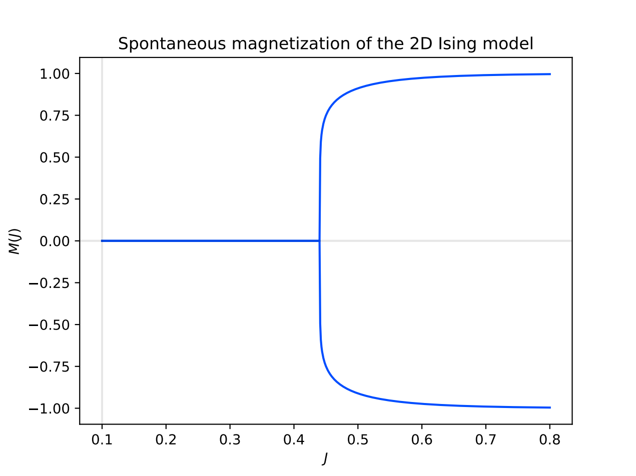
Phase transition in the Ising model

[Onsager, 1944]



Phase transition in the Ising model

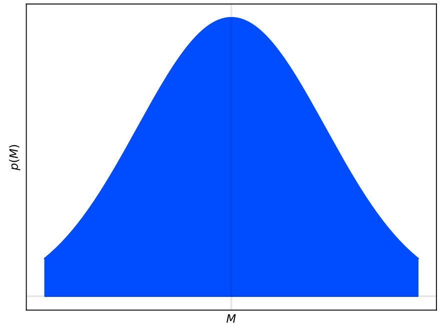
[Onsager, 1944]



- Need to take an infinite volume limit to actually see this

Phase transition in the Ising model: finite volume

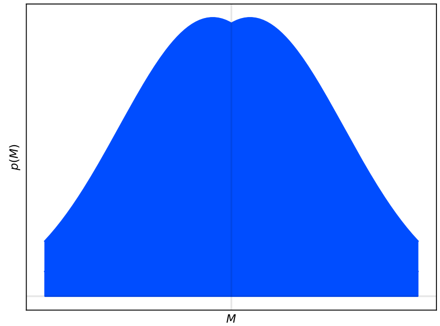
- But one can see a “phase transition” in some finite settings as well
- As the size of the “lattice” increases, the bimodal nature of μ becomes more pronounced



!Cartoon not to scale!

Phase transition in the Ising model: finite volume

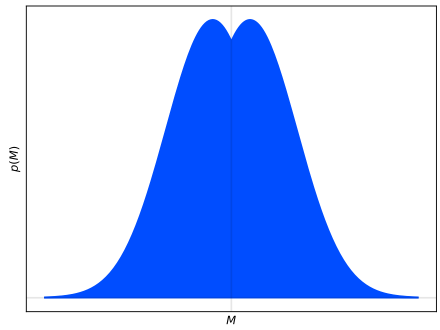
- But one can see a "phase transition" in some finite settings as well
- As the size of the "lattice" increases, the bimodal nature of μ becomes more pronounced



!Cartoon not to scale!

Phase transition in the Ising model: finite volume

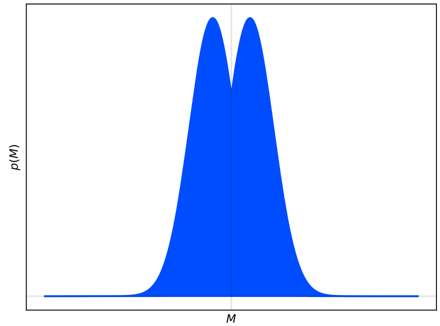
- But one can see a "phase transition" in some finite settings as well
- As the size of the "lattice" increases, the bimodal nature of μ becomes more pronounced



!Cartoon not to scale!

Phase transition in the Ising model: finite volume

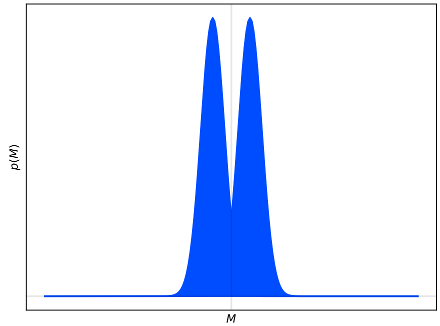
- But one can see a “phase transition” in some finite settings as well
- As the size of the “lattice” increases, the bimodal nature of μ becomes more pronounced



!Cartoon not to scale!

Phase transition in the Ising model: finite volume

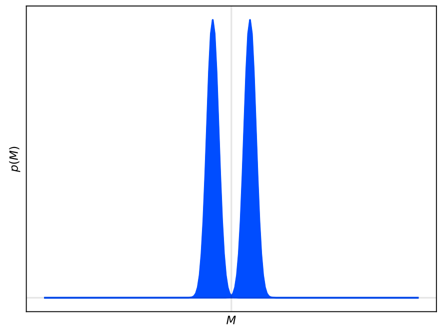
- But one can see a "phase transition" in some finite settings as well
- As the size of the "lattice" increases, the bimodal nature of μ becomes more pronounced



!Cartoon not to scale!

Phase transition in the Ising model: finite volume

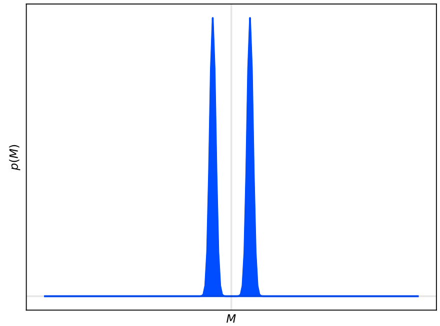
- But one can see a "phase transition" in some finite settings as well
- As the size of the "lattice" increases, the bimodal nature of μ becomes more pronounced



!Cartoon not to scale!

Phase transition in the Ising model: finite volume

- But one can see a “phase transition” in some finite settings as well
- As the size of the “lattice” increases, the bimodal nature of μ becomes more pronounced

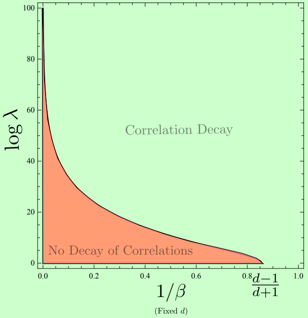


!Cartoon not to scale!

Examples: Antiferromagnetic Ising model

Approximation on graphs of degree at most d

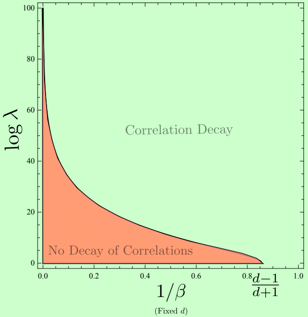
[Sinclair, S., Thurley; 2014]



Deterministic FPTAS in the Non-red region

Examples: Antiferromagnetic Ising model

Approximation on graphs of degree at most d [Sinclair, S., Thurley; 2014]



Deterministic FPTAS in the Non-red region

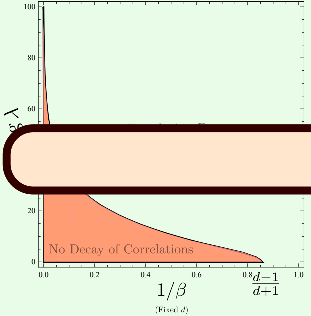
This is tight!

Theorem [Sly and Sun, 2014]

No FPRAS in red region for $Z_G(\lambda)$ for d-regular graphs, unless NP=RP

Examples: Antiferromagnetic Ising model

Approximation on graphs of degree at most d [Sinclair, S., Thurley; 2014]



Where does this boundary come from?

This is tight!

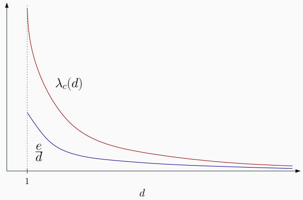
Theorem [Sly and Sun, 2014]

No FPRAS in red region for $Z_G(\lambda)$ for d-regular graphs, unless NP=RP

Examples: Hard code model

Approximation on graphs of degree at most d [Weitz, 2006]

$$\lambda < \lambda_c(d) := \frac{(d-1)^{d-1}}{(d-2)^d} \downarrow \frac{e}{d-1} \text{ as } d \uparrow \infty$$

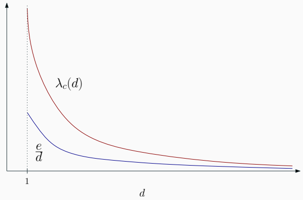


Critical activity

Examples: Hard code model

Approximation on graphs of degree at most d [Weitz, 2006]

$$\lambda < \lambda_c(d) := \frac{(d-1)^{d-1}}{(d-2)^d} \downarrow \frac{e}{d-1} \text{ as } d \uparrow \infty$$



Critical activity

This is also tight!

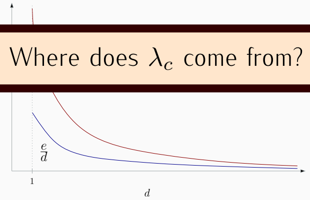
Theorem [Sly, 2010; Galanis et al., 2014; Sly and Sun, 2014]

$\lambda > \lambda_c(d) \implies$ no FPRAS for $Z_G(\lambda)$ for d-regular graphs, unless NP=RP

Examples: Hard code model

Approximation on graphs of degree at most d [Weitz, 2006]

$$\lambda < \lambda_c(d) := \frac{(d-1)^{d-1}}{(d-2)^d} \downarrow \frac{e}{d-1} \text{ as } d \uparrow \infty$$



Where does λ_c come from?

Critical activity

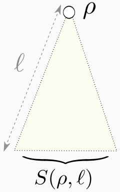
This is also tight!

Theorem [Sly, 2010; Galanis et al., 2014; Sly and Sun, 2014]

$\lambda > \lambda_c(d) \implies$ no FPRAS for $Z_G(\lambda)$ for d-regular graphs, unless NP=RP

Correlation decay on the d-ary tree

Gibbs measure on the d-ary tree: $\mu(I) \propto \lambda^{|I|}$



$$p_\ell(\rho|+) \triangleq \mathop{\mathbb{P}}_{I \sim \mu}[\rho \in I \,|\, \text{level } \ell \text{ fully occupied}]$$

$$p_\ell(\rho|-) \triangleq \mathop{\mathbb{P}}_{I \sim \mu}[\rho \in I \,|\, \text{level } \ell \text{ fully unoccupied}]$$

Phase transition on the d-ary tree

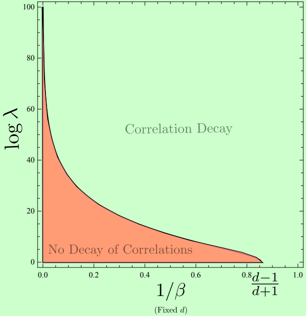
There is a critical activity $\lambda_c(d) > 0$ such that

$$|p_\ell(\rho|+) - p_\ell(\rho|-)| = \begin{cases} \exp\left(-\Theta(\ell)\right), & \lambda < \lambda_c(d) \text{ ("correlation decay")} \\ \Theta(1), & \lambda > \lambda_c(d) \end{cases}$$

- Correlation decay corresponds to the uniqueness of Gibbs distribution

Antiferromagnetic Ising model: fully understood

Approximation on graphs of degree at most d [Sinclair, S., Thurley; 2014]



Deterministic FPTAS in the Non-red region

This is *also* tight!

Theorem [Sly and Sun, 2014]

No FPRAS in red region for $Z_G(\lambda)$ for d-regular graphs, unless NP=RP

Ferromagnetic Ising model

- There is also a uniqueness phase transition in the ferromagnetic regime

Ferromagnetic Ising model

- There is also a uniqueness phase transition in the ferromagnetic regime
- …but there is **no corresponding approximability transition:**

Theorem [Jerrum & Sinclair, 1993]

For $0 < \beta < 1$ and $\lambda > 0$, there exists a randomized MCMC algorithm (FPRAS) for approximating the partition function of the ferromagnetic Ising model on all graphs

Results: Beyond correlation decay and Monte Carlo

Ferromagnetic Ising model: Deterministic approximation

Deterministic approximation: was known only up to the uniqueness threshold

Theorem [Zhang, Liang and Bai, 2011]

For $\frac{\Delta-1}{\Delta+1} < \beta < 1$ and $\lambda > 0$, there exists an FPTAS for approximating the partition function of the ferromagnetic Ising model on graphs of maximum degree Δ

- The presence of the uniqueness phase transition is an obstacle to *decay of correlations*,
- …but not an obstacle to approximability

Ferromagnetic Ising model: Deterministic approximation

Deterministic approximation: was known only up to the uniqueness threshold

Theorem [Zhang, Liang and Bai, 2011]

For $\frac{\Delta-1}{\Delta+1} < \beta < 1$ and $\lambda > 0$, there exists an FPTAS for approximating the partition function of the ferromagnetic Ising model on graphs of maximum degree Δ

- The presence of the uniqueness phase transition is an obstacle to *decay of correlations*,
- ...but not an obstacle to approximability

Question

Is there a deterministic algorithm that matches MCMC methods?

Ferromagnetic Ising model: Deterministic approximation

Deterministic approximation: was known only up to the uniqueness threshold

Theorem [Zhang, Liang and Bai, 2011]

For $\frac{\Delta-1}{\Delta+1} < \beta < 1$ and $\lambda > 0$, there exists an FPTAS for approximating the partition function of the ferromagnetic Ising model on graphs of maximum degree Δ

- The presence of the uniqueness phase transition is an obstacle to *decay of correlations*,
- ...but not an obstacle to approximability

Question

Is there a deterministic algorithm that matches MCMC methods...

...at least on bounded degree graphs?

Zeros of polynomials and algorithms

Theorem [Liu, Sinclair, S., *Proc. IEEE FOCS*, 2017]

Deterministic approximation of Z for ferromagnetic Ising on bounded degree graphs when λ bounded away from 1

- A randomized MCMC approximation was first discovered in 1990s
- But unlike the anti-ferromagnetic case, correlation decay is provably incapable of matching this [Sinclair, S., Thurley, *J. Stat. Phys. (155)*, 2014]

Beyond pairwise interactions

New algorithms for the case of Ising model on hypergraphs: in cases where even MCMC algorithms are not yet known

Zeros of polynomials and algorithms

Theorem [Liu, Sinclair, S., *Proc. IEEE FOCS*, 2017

Deterministic approximation of Z for ferromagnetic Ising on bounded degree graphs when λ bounded away from 1

- A randomized MCMC approximation was first discovered in 1990s
- But unlike the anti-ferromagnetic case, correlation decay is provably incapable of matching this [Sinclair, S., Thurley, *J. Stat. Phys. (155)*, 2014]

Beyond pairwise interactions

New algorithms for the case of Ising model on hypergraphs: in cases where even MCMC algorithms are not yet known

Zeros of Z

- Based on results on the location of complex roots of the partition function

Zeros of polynomials and algorithms

Theorem [Liu, Sinclair, S., *Proc. IEEE FOCS*, 2017

Deterministic approximation of Z for ferromagnetic Ising on bounded degree graphs when λ bounded away from 1

- A randomized MCMC approximation was first discovered in 1990s
- But unlike the anti-ferromagnetic case, correlation decay is provably incapable of matching this [Sinclair, S., Thurley, *J. Stat. Phys. (155)*, 2014]

Beyond pairwise interactions

New algorithms for the case of Ising model on hypergraphs: in cases where even MCMC algorithms are not yet known

Zeros of Z

- Based on results on the location of complex roots of the partition function
- **Aside:** Slightly sharper versions of similar results imply hardness of exactly computing marginals [Sinclair, S., *Comm. Math. Phys. 329 (3)*, 2014]

Zeros of polynomials and approximation of Z

$(1 \pm \epsilon)$-factor approximation for $Z(\lambda)$ $\equiv$ $\pm\epsilon$-additive approximation for $\log Z(\lambda)$

Zeros of polynomials and approximation of Z

$(1 \pm \epsilon)$-factor approximation for $Z(\lambda)$ $\equiv$ $\pm\epsilon$-additive approximation for $\log Z(\lambda)$

- Taylor expand $\log Z$ around 0! [Yang and Lee, 1952; Barvinok, 2015a,b]

$$\log Z(x) = \sum_{i=0}^{k} c_i x^i + \mathrm{err},$$

where

$$\mathrm{err} = O\left(\left(\frac{|x|}{R}\right)^{k+1} \mathrm{poly}\,(n)\right)$$

if

$Z(x) \neq 0$ when x in $D(0, R)$

Zeros of polynomials and approximation of Z

$(1 \pm \epsilon)$-factor approximation for $Z(\lambda)$ $\equiv$ $\pm\epsilon$-additive approximation for $\log Z(\lambda)$

- Taylor expand $\log Z$ around 0! [Yang and Lee, 1952; Barvinok, 2015a,b]

$$\log Z(x) = \sum_{i=0}^{k} c_i x^i + \mathrm{err},$$

where

$$\mathrm{err} = O\left(\left(\frac{|x|}{R}\right)^{k+1} \mathrm{poly}\,(n)\right)$$

if

$Z(x) \neq 0$ when x in $D(0, R)$

"$Z(x)$ is stable with respect to $D(0, R)$"

"$\log Z(x)$ is analytic in $D(0, R)$"

Zeros of polynomials and approximation of Z

$$\log Z(x) = \sum_{i=0}^{k} c_i x^i + \mathrm{err},$$

- c_i's are closely related to the lowest k coefficients of Z
- These correspond to k-point correlations

Zeros of polynomials and approximation of Z

$$\log Z(x) = \sum_{i=0}^{k} c_i x^i + \text{err},$$

- c_i's are closely related to the lowest k coefficients of Z
- These correspond to k-point correlations

Results on zero's of Z and $k = \Theta(\log n)$ give $n^{O(\log n)}$ algorithms: [Barvinok, 2015a]

- **Independent sets:** $Z(\lambda) \neq 0$ for $|\lambda| < \frac{1}{ed_{\max}}$

  [Shearer, 1985; Scott and Sokal, 2005]

- **Ising model:** $Z(\beta, \lambda) \neq 0$ for $|\lambda| \neq 1$ when $\beta < 1$

  [Lee and Yang, 1952]

Zeros of polynomials and approximation of Z

$$\log Z(x) = \sum_{i=0}^{k} c_i x^i + \text{err},$$

- c_i's are closely related to the lowest k coefficients of Z
- These correspond to k-point correlations

Results on zero's of Z and $k = \Theta(\log n)$ give $n^{O(\log n)}$ algorithms: [Barvinok, 2015a]

- **Independent sets:** $Z(\lambda) \neq 0$ for $|\lambda| < \frac{1}{ed_{\max}}$

  [Shearer, 1985; Scott and Sokal, 2005]

- **Ising model:** $Z(\beta, \lambda) \neq 0$ for $|\lambda| \neq 1$ when $\beta < 1$

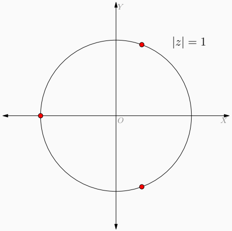
  [Lee and Yang, 1952]

Patel and Regts [2016] give techniques to make some of these polynomial on bounded degree graphs

Zeros of partition functions: The Lee-Yang theorem

Theorem [Lee & Yang, 1952]

For $0 < \beta \leq 1$, the zeros of $Z_G^{\beta}(\lambda)$ (viewed as a polynomial in λ) satisfy $|\lambda| = 1$



$Z^{\beta}(\lambda)$ is *zero-free* except on the unit circle in complex plane

Results

Definition (Ising Model on Hypergraphs)

$$Z_H^{\beta}(\lambda) = \sum_{S \subseteq V} \beta^{|E(S,V \setminus S)|} \lambda^{|S|}$$

A hyperedge $e \in E(S, V \setminus S)$ if and only if e intersects **both** S and $V \setminus S$

Theorem

Fix any $\Delta > 0$ and $k \geq 2$. There is an FPTAS for the Ising partition function $Z_H^{\beta}(\lambda)$ in all hypergraphs H of maximum degree Δ and maximum edge size k, for all edge activities β such that

$$-\frac{1}{2^{k-1}-1} \leq \beta \leq \frac{1}{2^{k-1}\cos^{k-1}\left(\frac{\pi}{k-1}\right)+1}$$

and all vertex activities $|\lambda| \neq 1$

Results

Based on a new Lee-Yang theorem for hypergraphs:

Theorem (Lee-Yang Theorem for Hypergraphs)

Let $H = (V, E)$ be a hypergraph with maximum hyperedge size $k \geq 2$. Then

$$Z_H^{\beta}(\lambda) = 0 \qquad \equiv \qquad |\lambda| = 1$$

if the edge activity β satisfies

$$-\frac{1}{2^{k-1} - 1} \leq \beta \leq \frac{1}{2^{k-1}\cos^{k-1}\left(\frac{\pi}{k-1}\right) + 1}.$$

This range of β is tight

Results

Based on a new Lee-Yang theorem for hypergraphs:

Theorem (Lee-Yang Theorem for Hypergraphs)

Let $H = (V, E)$ be a hypergraph with maximum hyperedge size $k \geq 2$. Then

$$Z_H^\beta(\lambda) = 0 \qquad \equiv \qquad |\lambda| = 1$$

if the edge activity β satisfies

$$-\frac{1}{2^{k-1}-1} \leq \beta \leq \frac{1}{2^{k-1}\cos^{k-1}\left(\frac{\pi}{k-1}\right)+1}.$$

This range of β is tight

- ...and a generalization of the method of **Patel and Regts** [2016] to general hypergraph models

Summary

Root location as a primitive for approximate counting

- Ising model on graphs
  - Lee–Yang theorem + **Patel and Regts** [2016]/generalizations
  - Deterministic approximation beyond correlation decay
- Ising model on hypergraphs ("higher order interactions")
  - New Lee–Yang theorem for hypergraphs
    + generalizations of **Patel and Regts** [2016]
  - Deterministic approximation where MCMC algorithms also not currently known

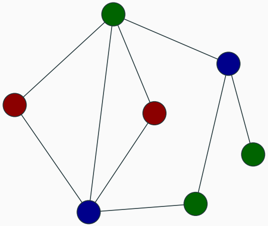
Summary

Root location as a primitive for approximate counting

- Ising model on graphs
  - Lee-Yang theorem + **Patel and Regts** [2016]/generalizations
  - Deterministic approximation beyond correlation decay
- Ising model on hypergraphs/general two-spin systems ("higher order interactions")
  - New Lee-Yang theorem for hypergraphs/Suzuki-Fisher theorem + generalizations of **Patel and Regts** [2016]
  - Deterministic approximation where MCMC algorithms also not currently known

Results: Potts model/random colourings

Zero temperature anti-ferromagnetic Potts/Proper colourings



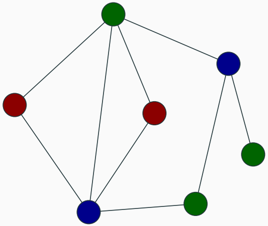
Partition function

$$Z_{G,q}(w) = \sum_{\sigma : V \to [q]} w^{|\{\{u,v\} \in E : \sigma(u)=\sigma(v)\}|}$$

Approximate the number of proper colourings with q colours

$$\mu_{G,q}(\sigma) = \frac{1}{Z_{G,q}(0)} \cdot [\sigma \text{ is a proper colouring}]$$

Zero temperature anti-ferromagnetic Potts/Proper colourings



Partition function

$$Z_{G,q}(w) = \sum_{\sigma : V \to [q]} w^{|\{\{u,v\}\in E:\sigma(u)=\sigma(v)\}|}$$

Approximate $Z_{G,q}(0)$
for input G

$$\mu_{G,q}(\sigma) = \frac{1}{Z_{G,q}(0)} \cdot [\sigma \text{ is a proper colouring}]$$

Random colourings

Question

INPUT: Graph of bounded degree Δ; q colours
OUTPUT: $(1 \pm \epsilon)$-approximation of $Z_{G,q}(0)$

Random colourings

Question

INPUT: Graph of bounded degree Δ; q colours

OUTPUT: $(1 \pm \epsilon)$-approximation of $Z_{G,q}(0)$

Known results

- NP-hard: $q < \Delta$ (q even)

  [Galanis, Štefankovič & Vigoda, 2014]

Random colourings

Question

INPUT: Graph of bounded degree Δ; q colours

OUTPUT: $(1 \pm \epsilon)$-approximation of $Z_{G,q}(0)$

Known results

- NP-hard: $q < \Delta$ (q even)

  [Galanis, Štefankovič & Vigoda, 2014]

- Randomized algorithms, "complicated" MCMC analyses: $q > (11/6 - \epsilon)\Delta$

  [Chen, Delcourt, et al., 2019; Vigoda 2000]

- Randomized algorithms, "simple" MCMC analysis: $q \geq 2\Delta$

  [Jerrum, 1995; Bubley & Dyer, 1997, based on their elegant *path coupling* technique]

Random colourings

Question

INPUT: Graph of bounded degree Δ; q colours

OUTPUT: $(1 \pm \epsilon)$-approximation of $Z_{G,q}(0)$

Known results

- NP-hard: $q < \Delta$ (q even)

  [Galanis, Štefankovič & Vigoda, 2014]

- Randomized algorithms, "complicated" MCMC analyses: $q > (11/6 - \epsilon)\Delta$

  [Chen, Delcourt, et al., 2019; Vigoda 2000]

- Randomized algorithms, "simple" MCMC analysis: $q \geq 2\Delta$

  [Jerrum, 1995; Bubley & Dyer, 1997, based on their elegant *path coupling* technique]

- Deterministic algorithms, "correlation decay": $q \geq 2.581\Delta + 1$

  [Lu and Yin, 2013; see also Gamarnik & Katz, 2007]

Random colourings

Question

INPUT: Graph of bounded degree Δ; q colours

OUTPUT: $(1 \pm \epsilon)$-approximation of $Z_{G,q}(0)$

Known results

- NP-hard: $q < \Delta$ (q even)
  [Galanis, Štefankovič & Vigoda, 2014]
- Randomized algorithms, "complicated" MCMC analyses: $q > (11/6 - \epsilon)\Delta$
  [Chen, Delcourt, et al., 2019; Vigoda 2000]
- Randomized algorithms, "simple" MCMC analysis: $q \geq 2\Delta$
  [Jerrum, 1995; Bubley & Dyer, 1997, based on their elegant *path coupling* technique]
- Deterministic algorithms, "correlation decay": $q \geq 2.581\Delta + 1$
  [Lu and Yin, 2013; see also Gamarnik & Katz, 2007]

Not even "simple" MCMC analyses are matched by deterministic algorithms!

Approaching path coupling

Main result [Liu, Sinclair, S., *IEEE FOCS*, 2019]

Fix constants $\Delta \geq 3$ and $q \geq 2\Delta$.

There is an FPTAS that on input a graph G of maximum degree at most Δ, outputs a $(1 \pm \epsilon)$-approximation to the number of colourings of G in time $O((n/\epsilon)^{c(\Delta,q)})$

Approaching path coupling

Main result [Liu, Sinclair, S., *IEEE FOCS*, 2019]

Fix constants $\Delta \geq 3$ and $q \geq 2\Delta$.
There is an FPTAS that on input a graph G of maximum degree at most Δ, outputs a $(1 \pm \epsilon)$-approximation to the number of colourings of G in time $O((n/\epsilon)^{c(\Delta,q)})$

Previous work

Deterministic $(1 \pm \epsilon)$-approximation in time $((n/\epsilon)^{c(\Delta,q)})$ when $q \geq 2.58\Delta + 1$

[Lu and Yin, 2013; see also Gamarnik & Katz, 2007]

Zeros of the Potts partition function

Main technical result

$$Z_{G,q}(w) = \sum_{\sigma \,:\, V \to [q]} w^{|\{\{u,v\} \in E : \sigma(u) = \sigma(v)\}|}$$

Fix $\Delta \geq 3$ and $q \geq 2\Delta$. Then there exists $\delta = \delta(\Delta, q) > 0$ such that for any graph G of maximum degree at most Δ

$$d(\omega, [0,1]) \leq \delta \implies Z_{G,q}(\omega) \neq 0$$

Zeros of the Potts partition function

Main technical result

$$Z_{G,q}(w) = \sum_{\sigma : V \to [q]} w^{|\{\{u,v\}\in E : \sigma(u)=\sigma(v)\}|}$$

Fix $\Delta \geq 3$ and $q \geq 2\Delta$. Then there exists $\delta = \delta(\Delta, q) > 0$ such that for any graph G of maximum degree at most Δ

$$d(\omega, [0,1]) \leq \delta \implies Z_{G,q}(\omega) \neq 0$$

Comments

- Improves upon [Bencs, Davis, Patel & Regts, 2018] who established this under $q > e\Delta$

Zeros of the Potts partition function

Main technical result

$$Z_{G,q}(w) = \sum_{\sigma : V \to [q]} w^{|\{\{u,v\} \in E : \sigma(u) = \sigma(v)\}|}$$

Fix $\Delta \geq 3$ and $q \geq 2\Delta$. Then there exists $\delta = \delta(\Delta, q) > 0$ such that for any graph G of maximum degree at most Δ

$$d(\omega, [0,1]) \leq \delta \implies Z_{G,q}(\omega) \neq 0$$

Comments

- Improves upon [**Bencs, Davis, Patel & Regts, 2018**] who established this under $q > e\Delta$
- The main new ingredient: “lifting” the MCMC path coupling argument to the complex plane

Aside: Independent sets

Other applications: Independent sets and the Lovász Local lemma

Non-positive activities

$Z(\lambda)$ for negative and complex λ

Other applications: Independent sets and the Lovász Local lemma

Non-positive activities

$Z(\lambda)$ for negative and complex λ

Shearer's version of the Lovász Local Lemma

$$Z_G(\lambda) \neq 0 \text{ for } \lambda \in \overline{D(0,p)}$$
$$\equiv$$
$$\text{LLL on } G \text{ holds with probability } p$$

- Approximation of Z in this setting using "correlation decay" and zeros

  [Harvey, S., Vondrák, *ACM-SIAM SODA* 2018; Patel & Regts, *SIAM J. Comp.* 2017]

  - ...with a curious speed advantage for correlation decay
  - ...leading to a new "rounding based" sub-exponential time algorithmic LLL

Aside

Zeros of polynomials and Phase transitions

or

Why was the Lee–Yang theorem proven?

> *"It has been written that the shortest and best way between two truths of the real domain often passes through the imaginary one."*
>
> – Jacques Hadamard, paraphrasing Paul Painlevé

Skip

Ising model: The free energy

Free energy per unit volume: $F(\beta, \lambda) \triangleq -\frac{1}{|V|} \log Z(\beta, \lambda)$

- Physically interesting quantities can be expressed in terms of the free energy, e.g., the average fraction of '+' spins:

$$\frac{\mu(\beta,\lambda)}{|V|} = \frac{1}{|V|} \cdot \frac{\sum_\sigma \#(+) w(\sigma)}{Z(\beta,\lambda)} = \frac{1}{|V|} \cdot \frac{\lambda Z'}{Z} = -\lambda F(\beta,\lambda)'$$

Ising model: The free energy

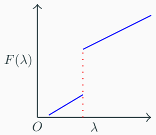
Free energy per unit volume: $F(\beta,\lambda) \triangleq -\frac{1}{|V|}\log Z(\beta,\lambda)$

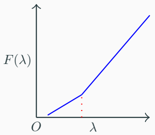
- Physically interesting quantities can be expressed in terms of the free energy, e.g., the average fraction of '+' spins:

$$\frac{\mu(\beta,\lambda)}{|V|} = \frac{1}{|V|}\cdot\frac{\sum_\sigma \#(+)w(\sigma)}{Z(\beta,\lambda)} = \frac{1}{|V|}\cdot\frac{\lambda Z'}{Z} = -\lambda F(\beta,\lambda)'$$

Phase transitions

Singularities/discontinuities in F or its derivatives.





The Ising model: Phase transitions

- Of course, F is always analytic for a finite graph
  - …no phase transitions?

The Ising model: Phase transitions

- Of course, F is always analytic for a finite graph
  - …no phase transitions?

- For an infinite graph G (often the integer lattice $\mathbb{Z}^2$), take a sequence of finite graphs G_n "tending to" G and define

$$F_G(J, \lambda) = \lim_{n \to \infty} F_{G_n}(J, \lambda)$$

- **Onsager, 1944**: the second derivative of $F_{\mathbb{Z}^2}(J, \lambda)$ (with respect to J) has a singularity!
  - Captures the physical phenomenon of magnets showing a phase transition with respect to temperature ("Curie temperature")

The Ising model: Phase transitions with respect to field

Question

Does the Ising model have any phase transitions in the λ parameter?

…i.e., with respect to the magnetic field?

Equivalently, when is $F_G(\beta, z) = -\lim_{n\to\infty} \frac{1}{|V_n|} \log Z_{G_n}(\beta, z)$ analytic?

The Ising model: Phase transitions with respect to field

Question

Does the Ising model have any phase transitions in the λ parameter?

…i.e., with respect to the magnetic field?

Equivalently, when is $F_G(\beta, z) = -\lim_{n\to\infty} \frac{1}{|V_n|} \log Z_{G_n}(\beta, z)$ analytic?

Theorem [Yang and Lee, 1952]

If $Z_{G_n}(\beta, z)$ is non-vanishing in an open region $S \subset \mathbb{C}$ containing some portion of $\mathbb{R}^+$, then

$$F_G(\beta, z) \triangleq -\lim_{n\to\infty} \frac{1}{|V|} \log Z_{G_n}(\beta, z)$$

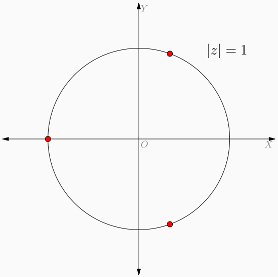
is analytic in S

- In particular, there are no phase transitions for any positive real $\lambda \in S$
- The first application appeared in a companion paper in the same journal issue…

Zeros of the partition function: The Lee-Yang theorem

Theorem [Lee and Yang, 1952]

When $0 < \beta \leq 1$, the zeros of $Z(\beta, z)$ satisfy $|z| = 1$.



Thus, there are no phase transitions with respect to λ, except possibly in the "zero-field" case $\lambda = 1$

- Since then, the Lee-Yang approach has been explored for several other systems: Asano [1970]; Suzuki and Fisher [1971]; Heilmann and Lieb [1972]; Newman [1974]; Biskup et al. [2004]; …

Correlation decay and zero-freeness

- More examples for

$$\text{Correlation decay algorithms} \longrightarrow \text{Zero-freeness results}$$

[Peters & Regts, 2017, 2018, Liu, Sinclair, S., 2019]

Correlation decay implies absence of "Fisher zeros" [Liu, Sinclair, S., *J. Math. Phys. (60)*, 2019]

Fix a degree Δ. Recall the correlation decay regime for the Ising model: $I_\Delta = \left(\frac{\Delta-2}{\Delta}, \frac{\Delta}{\Delta-2}\right)$. Then,

$$\beta \in I_\Delta$$

$$\downarrow$$

There is a complex neighborhood N of β s.t.

$\forall$ graphs G of degree at most Δ and $\forall\ \gamma \in N$

$$Z_G(\gamma, 1) \neq 0$$

- Fisher initiated the study of zeros in the β parameter in the 1960s
  - . . . but unlike the Lee-Yang case, very little is known in general

Discussion

- A primitive for estimation based on understanding complex roots of the partition function
- Like correlation decay and MCMC, inspired by phase transition formalisms
- But applicable in many situations where the other two methods are not yet known to be

[Barvinok, 2017]

However...

- When MCMC can be proved to work, the run time guarantees are of the form

$$O(f(\Theta)\,\mathrm{poly}\,(n))$$

- For the two deterministic methods, the run time guarantees are typically of the form

$$O(n^{g(\Theta)})$$

Θ: represents model parameters (temperature, activity, degree etc.)

Discussion

- A primitive for estimation based on understanding complex roots of the partition function
- Like correlation decay and MCMC, inspired by phase transition formalisms
- But applicable in many situations where the other two methods are not yet known to be

[Barvinok, 2017]

Question

Just a matter of inadequacy of techniques?

…or is there a more fundamental randomized/deterministic separation at work?

- For the two deterministic methods, the run time guarantees are typically of the form

$$O(n^{g(\Theta)})$$

Θ: represents model parameters (temperature, activity, degree etc.)

Conclusion

More connections between locations of zeros, MCMC and the correlation decay approaches?

Conclusion

More connections between locations of zeros, MCMC and the correlation decay approaches?

Aside

- J. Liu, A. Sinclair, and P. Srivastava. *A deterministic algorithm for counting colorings with* 2Δ *colors*. Extended abstract in *Proc. IEEE Annual Symposium on Foundations of Computer Science (FOCS), 2019.*
- J. Liu, A. Sinclair, and P. Srivastava. *Fisher zeros and correlation decay in the Ising model. J. Math. Phys. (60)*, 2019. Extended abstract in *Proc. Innovations in Theoretical Computer Science (ITCS) conference, 2019.*
- N. J. A. Harvey, P. Srivastava, J. Vondrák. *Computing the independence polynomial: From the tree threshold down to the roots.* Extended abstract in *Proc. ACM-SIAM Annual Symposium on Discrete Algorithms (SODA), 2018.*
- J. Liu, A. Sinclair, and P. Srivastava. *The Ising Partition Function: Zeros and Deterministic Approximation. J. Stat. Phys. (174)*, 2019. Extended abstract in *Proc. IEEE Annual Symposium on Foundations of Computer Science (FOCS), 2017.*
- P. Srivastava. *The Lee-Yang theory of phase transitions.* Companion note for a tutorial at IEEE FOCS, 2013. Available from `https://www.tifr.res.in/~piyush.srivastava/research.html#Notes`

Hanabusa Itchō (1652–1724 CE)

Wikimedia Commons, public domain

ಧನ್ಯವಾದಗಳು!

https://www.tifr.res.in/~piyush.srivastava

References

Taro Asano. Lee-Yang theorem and the Griffiths inequality for the anisotropic Heisenberg ferromagnet. *Phys. Rev. Lett.*, 24(25):1409–1411, June 1970. doi: 10.1103/PhysRevLett.24.1409. URL `http://link.aps.org/doi/10.1103/PhysRevLett.24.1409`.

Alexander Barvinok. Computing the partition function for cliques in a graph. *Theory of Computing*, 11(13):339–355, 2015a.

Alexander Barvinok. Computing the permanent of (some) complex matrices. *Found. Comput. Math.*, 16(2):329–342, January 2015b. ISSN 1615-3375, 1615-3383. doi: 10.1007/s10208-014-9243-7. URL `http://link.springer.com/article/10.1007/s10208-014-9243-7`. https://arxiv.org/abs/1405:1303.

M. Biskup, C. Borgs, J. Chayes, L. Kleinwaks, and R. Kotecký. Partition function zeros at first-order phase transitions: A general analysis. *Communications in Mathematical Physics*, 251(1):79–131, October 2004. doi: http://dx.doi.org/10.1007/s00220-004-1169-5. URL `http://dx.doi.org/10.1007/s00220-004-1169-5`.

Andreas Galanis, Qi Ge, Daniel Štefankovič, Eric Vigoda, and Linji Yang. Improved inapproximability results for counting independent sets in the hard-core model. *Random Struct. Algorithms*, 45(1):78–110, 2014. ISSN 1098-2418. URL `https://dx.doi.org/10.1002/rsa.20479`.

Ole J. Heilmann and Elliott H. Lieb. Theory of monomer-dimer systems. *Comm. Math. Phys.*, 25 (3):190–232, 1972. ISSN 0010-3616. doi: 10.1007/BF01877590. URL `https://dx.doi.org/10.1007/BF01877590`.

Mark Jerrum, Leslie G. Valiant, and Vijay V. Vazirani. Random generation of combinatorial structures from a uniform distribution. *Theor. Comput. Sci.*, 43:169–188, 1986.

T. D. Lee and C. N. Yang. Statistical theory of equations of state and phase transitions. II. Lattice gas and Ising model. *Phys. Rev.*, 87(3):410–419, August 1952. doi: 10.1103/PhysRev.87.410.

Charles M. Newman. Zeros of the partition function for generalized Ising systems. *Commun. Pure Appl. Math.*, 27(2):143–159, March 1974. ISSN 1097-0312. doi: 10.1002/cpa.3160270203. URL `http://onlinelibrary.wiley.com/doi/10.1002/cpa.3160270203/abstract`.

Lars Onsager. Crystal statistics. I. A two-dimensional model with an order-disorder transition. *Phys. Rev. (2)*, 65:117–149, 1944.

Viresh Patel and Guus Regts. Deterministic polynomial-time approximation algorithms for partition functions and graph polynomials, July 2016. https://arxiv.org/abs/1607.01167.

Dana Randall and David Wilson. Sampling spin configurations of an Ising system. In *Proc. 10th ACM-SIAM Symp. Discret. Algorithms (SODA)*, SODA '99, pages 959–960, Philadelphia, PA, USA, 1999. SIAM. ISBN 0-89871-434-6. URL `http://dl.acm.org/citation.cfm?id=314500.314945`.

Alexander D. Scott and Alan D. Sokal. The repulsive lattice gas, the independent-set polynomial, and the Lovász local lemma. *J. Stat. Phys.*, 118(5-6):1151–1261, March 2005. ISSN 0022-4715, 1572-9613. doi: 10.1007/s10955-004-2055-4. URL `http://link.springer.com/article/10.1007/s10955-004-2055-4`.

James B. Shearer. On a problem of Spencer. *Combinatorica*, 5(3), 1985.

Allan Sly. Computational transition at the uniqueness threshold. In *Proc. 51st IEEE Symp. Found. Comput. Sci. (FOCS)*, pages 287–296. IEEE Computer Society, 2010.

Allan Sly and Nike Sun. Counting in two-spin models on d-regular graphs. *Ann. Probab.*, 42(6): 2383–2416, November 2014. ISSN 0091-1798, 2168-894X. doi: 10.1214/13-AOP888. URL `http://projecteuclid.org/euclid.aop/1412083628`.

Masuo Suzuki and Michael E Fisher. Zeros of the partition function for the Heisenberg, ferroelectric, and general Ising models. *J. Math. Phys.*, 12(2):235–246, February 1971. ISSN 00222488. doi: doi:10.1063/1.1665583. URL `http://jmp.aip.org/resource/1/jmapaq/v12/i2/p235_s1`.

Dror Weitz. Counting independent sets up to the tree threshold. In *Proc. 38th ACM Symp. Theory Comput. (STOC)*, pages 140–149. ACM, 2006. ISBN 1-59593-134-1. doi: http://doi.acm.org/10.1145/1132516.1132538.

C. N. Yang and T. D. Lee. Statistical theory of equations of state and phase transitions. I. Theory of condensation. *Phys. Rev.*, 87(3):404–409, August 1952. doi: 10.1103/PhysRev.87.404.