The Ising Partition Function: Zeros and Deterministic Approximation

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Spin systems (aka MRFs or graphical models)

We focus on two-state systems only:

- An undirected graph (or hypergraph) $G = (V, E)$. Let $n = |V|$, $m = |E|$.
- Configuration: $\sigma \in \Sigma$, where $\Sigma := \{+, -\}^V$.
- Edge potentials: $\varphi_e : \Sigma \times \Sigma \times \cdots \times \Sigma \to \mathbb{C}$. W.l.o.g. $\varphi_e(-, \ldots, -) = 1$.
- Vertex potentials: $\psi_v : \Sigma \to \mathbb{C}$. W.l.o.g. $\psi_v(+) = \lambda, \psi_v(-) = 1$.

Definition (Partition function)

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

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

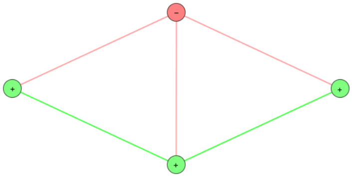
Example: Ising model on graphs

For $\beta, \lambda \in \mathbb{R}_+$,

- Configuration: $\sigma \in \{+, -\}^V$
- Edge potentials: $f_e = \begin{pmatrix} 1 & \beta \\ \beta & 1 \end{pmatrix}$ – related to the “temperature”
- Vertex potentials: $f_v = \begin{pmatrix} \lambda \\ 1 \end{pmatrix}$ – “external field”

Ising model

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



A spin configuration with weight $\beta^3 \lambda^3$

- $\beta < 1$: Ferromagnetic; the model favors small cuts
- $\beta > 1$: Anti-ferromagnetic; the model favors large cuts

Approximating the partition fucntion

We will be interested in multiplicative approximation of Z

Definition (Fully polynomial-time approximation scheme)

An FPTAS for a function $f(\cdot)$ is an algorithm with:

- *Input:* $\varepsilon > 0, \boldsymbol{x}$
- *Output:* $\widetilde{f(\boldsymbol{x})}$ *such that* $\left|f(\boldsymbol{x}) - \widetilde{f(\boldsymbol{x})}\right| \leq \varepsilon \left|f(\boldsymbol{x})\right|$
- *Running time:* $\mathrm{poly}(|\boldsymbol{x}|, 1/\varepsilon)$

☺ For *self-reducible* problems, this notion of approximability is robust.

Antiferromagnetic Ising model: fully understood

Theorem (Weitz, Sinclair-Srivastava-Thurley, Li-Lu-Yin, Sly-Sun, Galanis-Stefankovic-Vigoda)

For any $\beta > 1, \lambda > 0$, there is a threshold $\beta_c(\lambda, d)$ s.t.

- *If $\beta < \beta_c(\lambda, d)$, then there is an FPTAS to approximate Z on graphs of maximum degree d; (Weitz's algorithm)*
- *If $\beta > \beta_c(\lambda, d)$, then it is NP-hard to approximate Z on d-regular graphs.*

Remark

This threshold $\beta_c(\lambda, d)$ coincides with the threshold for uniqueness of the Gibbs measure on the infinite d-regular tree.

Ferromagnetic Ising model

There is also a uniqueness phase transition in the ferromagnetic regime, but there is no 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 graphs.*

Deterministic approximation is currently 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

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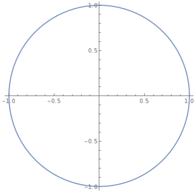
Zeros of partition functions

Instead of making use of the uniqueness property, we appeal to the classical notion of phase transition, as zeros of the partition function:

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

Our results

Theorem

Fix any $\Delta > 0$. There is a FPTAS for the Ising partition function $Z_G^{\beta}(\lambda)$ in all graphs G of maximum degree Δ for all edge activities $-1 \leq \beta \leq 1$ and all (possibly complex) vertex activities λ with $|\lambda| \neq 1$.

Remark

This is the first deterministic FPTAS for (almost) the whole range of β, λ. We can also allow edge-dependent activities β_e provided all of them lie in $[-1, 1]$.

Our results (cont'd)

Definition (Ising Model on Hypergraphs)

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

Theorem (Lee-Yang Theorem for Hypergraphs)

Let $H = (V, E)$ be a hypergraph with maximum hyperedge size $k \geq 3$. Then all the zeros of the Ising model partition function $Z_H^\beta(\lambda)$ lie on the unit circle if and only if the edge activity β lies in the range

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

Our results (cont'd)

In combination with our Lee-Yang theorem for hypergraphs:

Theorem

Fix any $\Delta > 0$ and $k \geq 3$. 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 $|\lambda| \neq 1$.

Recall

$$Z_G^{\varphi}(\lambda) = \sum_{\sigma: V \to \{+,-\}} \prod_{e \in E} \varphi_e\left(\sigma\big|_e\right) \lambda^{|\{v:\sigma(v)=+\}|}$$

Together with Suzuki-Fisher 1971 (Lee-Yang theorem for general ferromagnetic 2-spin models):

Theorem

Fix any $\Delta > 0$ and $k \geq 2$ and a family of edge activities $\boldsymbol{\varphi} = \{\varphi_e\}$ satisfying

- *symmetry:* $\varphi_e(\sigma) = \overline{\varphi_e(-\sigma)}$;
- *"ferromagnetism":* $|\varphi_e(+, \cdots, +)| \geq \frac{1}{4} \sum_{\boldsymbol{\sigma} \in \{+,-\}^V} |\varphi_e(\boldsymbol{\sigma})|$.

Then there exists an FPTAS for the partition function $Z_H^{\varphi}(\lambda)$ in all hypergraphs H of maximum degree Δ and maximum edge size k for all vertex activities $\lambda \in \mathbb{C}$ such that $|\lambda| \neq 1$.

Overview

Approximation via the log-partition function

Theorem (Barvinok, Barvinok and Soberon)

For a zero free region, $\log Z$ *can be approximated to within* $\pm\varepsilon$ *by its k-th order Taylor series, for* $k = O(\log(n/\varepsilon))$.

To make use of the analyticity of $\log Z$

- Taylor expansion of $\log Z$ around $\lambda = 0$
- By Lee-Yang theorem, $|\lambda| < 1$ is zero free
- The first k terms of the Taylor series require the first $k+1$ coefficients of Z

$$Z_G^{\beta}(\lambda) = \sum_{i=0}^{n} \left(\sum_{\substack{S \subseteq V \\ |S| = i}} \beta^{|E(S,\bar{S})|} \right) \lambda^i,$$

$$\log Z = \sum_{i=0}^{k-1} \frac{\lambda^i}{i!} \left(\frac{\mathrm{d}^i}{\mathrm{d}\lambda^i} \log Z \Big|_{\lambda=0} \right) + \cdots$$

Naively, computing the first k coefficients of Z takes time $O(n^k) \implies$ quasi-polynomial time algorithm

Computing coefficients of Z

Theorem (Patel and Regts)

If the first k coefficients can be represented as a sum over induced subgraphs, one can compute them in time $\Delta^{O(k)} = \text{poly}(n/\varepsilon)$ for graphs of bounded degree Δ. In particular, for the Ising model, if $\lambda = 1$ and $|\beta - 1| < 0.34/\Delta$, there is an FPTAS.

For graphs of maximum degree Δ:

- the number of labeled *induced subgraphs* of size k is $O(n^k)$
- the number of labeled *connected* induced subgraphs of size k is at most $n(e\Delta)^k$

Main idea: reduce a sum over all induced subgraphs to sum over connected induced subgraphs.

☹ The Ising model, when viewed as a polynomial in λ, is **not** a sum over induced subgraphs.

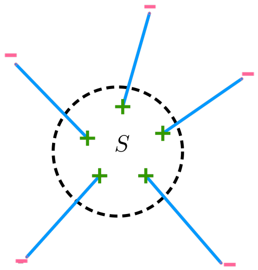
Insects in graphs

Main idea: Generalize the notion of *induced subgraphs* to *induced sub-insects.*

Recall the Ising partition function:

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

Given a configuration $\boldsymbol{\sigma}$, let S be the set of vertices assigned $+$-spins:

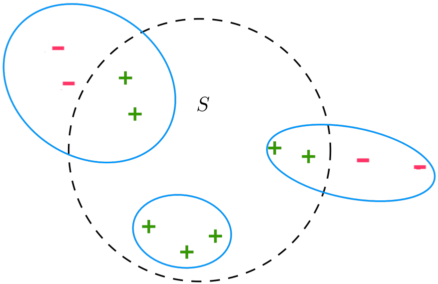


The coefficient $\beta^{|E(S,V\setminus S)|}$ of a configuration depends only on the *induced sub-insect* $G^{+}[S]$

Insects in hypergraphs

Recall that w.l.o.g $\varphi_e(-,\cdots,-)=1$.

$$Z_H^{\varphi}(\lambda)=\sum_{\boldsymbol{\sigma}:V\to\{+,-\}}\prod_{e\in E}\varphi_e\left(\boldsymbol{\sigma}\big|_e\right)\lambda^{|\{v:\boldsymbol{\sigma}(v)=+\}|}=\sum_{S\subseteq V}\prod_{e:e\cap S\neq\emptyset}\varphi_e(S)\lambda^{|S|}.$$



The coefficient $\prod_{e:e\cap S\neq\emptyset}\varphi_e\left(\boldsymbol{\sigma}\big|_e\right)$ of a configuration depends only on the induced sub-insect $H^+[S]$

Note: the number of labeled *connected* sub-insects of size t is at most $n(e\Delta k)^t$.

Reducing to a connected sub-insect count

Let $r_1, \cdots, r_n$ be the complex zeros of $Z_G^{\varphi}(\lambda)$:

$$Z_G^{\varphi}(\lambda) = \prod_{i=1}^{n}(1 - \lambda/r_i) = \sum_{i=0}^{n}(-1)^i e_i(G)\lambda^i,$$

Review of our goal:

- To compute the Taylor series of $\log Z$, we need the coefficients $e_i(G)$
- $e_i(G)$ is the elementary symmetric polynomial evaluated at $(\frac{1}{r_1}, \cdots, \frac{1}{r_n})$
- From the definition of Z,

$$e_i(G) = (-1)^i \sum_{\substack{S \subseteq V \\ |S|=i}} \prod_{e: e \cap S \neq \emptyset} \varphi_e(S)$$

- Notice that $e_i(G)$ is a *weighted sub-insect count*, but not necessarily connected

Instead, we consider a related quantity: the t-th power sum given by $p_t = \sum_{i=1}^{n} 1/r_i^t$

Reducing to a connected sub-insect count (cont'd)

Let $p_t = \sum_{i=1}^{n} 1/r_i^t$ be the t-th power sum. By Newton's identities:

$$p_t = \sum_{i=1}^{t-1} (-1)^{i-1} p_{t-i} e_i + (-1)^{t-1} t e_t.$$

Proof sketch

- Recall that e_i is a *weighted sub-insect count*
- **Lemma**: product of *weighted sub-insect counts* is also a *weighted sub-insect count*
- Thus p_t is also a *weighted sub-insect count*
- Notice that p_t is additive in the sense that $p_t(G_1 \cup G_2) = p_t(G_1) + p_t(G_2)$
- **Lemma**: a weighted sub-insect count is additive **iff** it is a *connected* sub-insect count
- Thus p_t is supported only on *connected* sub-insects up to size t.

Summary of FPTAS for $Z_G^{\boldsymbol{\beta}}(\lambda)$

Taylor approximation:

- Since $Z_G^{\boldsymbol{\beta}}(\lambda) = \lambda^n \cdot Z_G^{\boldsymbol{\beta}}(1/\lambda)$, w.l.o.g. $|\lambda| < 1$
- To get a $(1 \pm \varepsilon)$ multiplicative approximation of Z, it suffices to get a $\pm\frac{\varepsilon}{4}$ additive approximation of $\log Z$ (by standard complex analysis)
- By Barvinok et. al., the t-th order Taylor series of $\log Z$ around $\lambda = 0$ is a $\pm\varepsilon$ approximation for $t = O\left(\log(n/\varepsilon)\right)$ at any point λ such that $B(0, |\lambda|)$ is a zero-free region
- By the Lee-Yang theorem, there are no zeros of Z in $|\lambda| < 1$

Summary of FPTAS for $Z_G^{\boldsymbol{\beta}}(\lambda)$

Computing coefficients by reducing to a connected sum:

- The t-th order Taylor series of $\log Z$ depends only on the first $t+1$ coefficients
- Recall that $Z_G^{\boldsymbol{\beta}}(\lambda) = \sum_{i=0}^{n} (-1)^i e_i(G)\lambda^i$, e_i is the i-th coefficient
- e_t can be computed using Newton's identities given p_t
- p_t can be computed efficiently by enumerating over *connected* sub-insects for $t = O(\log(n/\varepsilon))$

Overview

Lee-Yang theorem

Definition (Lee-Yang property)

A multilinear polynomial P is said to have the *Lee-Yang property*, denoted by $P \in \mathrm{LY}$, if $P(\lambda_1, \cdots, \lambda_n) \neq 0$ for any $\lambda_1, \cdots, \lambda_n$ such that $|\lambda_i| \geq 1$ for all i, and $|\lambda_i| > 1$ for some i.

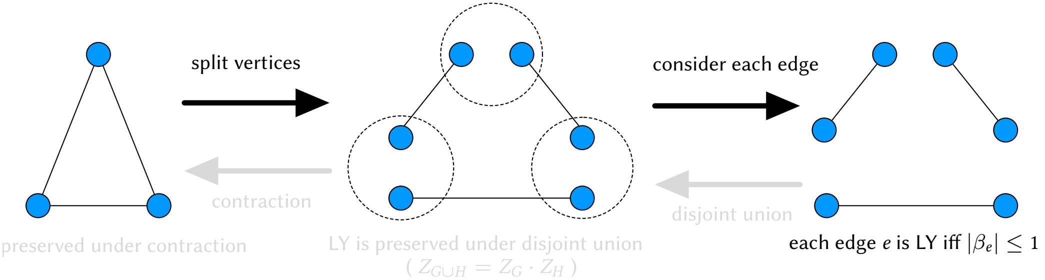
Definition (Multivariate Ising model)

$$Z_G^{\vec{\beta}}(\lambda_1, \cdots, \lambda_n) = \sum_{S \subseteq V} \prod_{e \in E(S, \overline{S})} \beta_e \prod_{i \in S} \lambda_i$$

Theorem (Lee-Yang Theorem 1952)

If $0 < \beta_e < 1$, *then* $Z_G^{\vec{\beta}}(\lambda_1, \cdots, \lambda_n)$ *has the Lee-Yang property.*

Asano's proof of the Lee-Yang theorem



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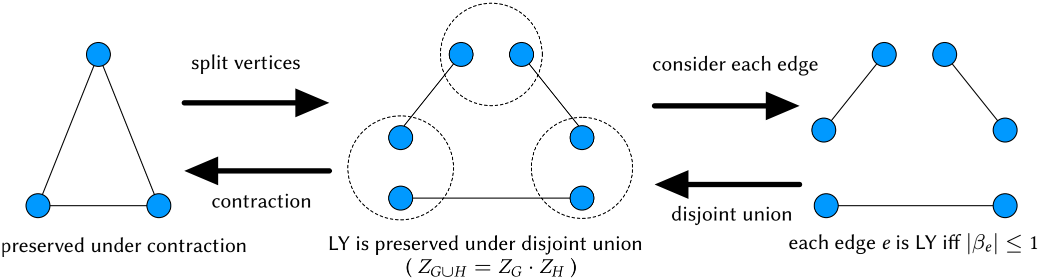

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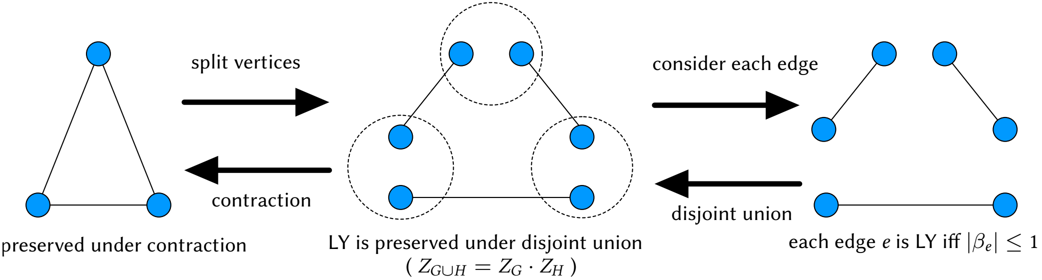


What about hypergraphs? The above scheme is very general except:

- LY holds for each hyperedge
- LY is preserved under contraction

Characterizing Lee-Yang theorems for symmetric polynomials

Lemma (Criterion for Lee-Yang property)

Given a multilinear polynomial $P(z_1, z_2, \ldots, z_n)$, define multilinear polynomials A_j and B_j in the variables $z_1, \ldots, z_{j-1}, z_{j+1}, \ldots, z_n$ such that

$$P = A_j z_j + B_j$$

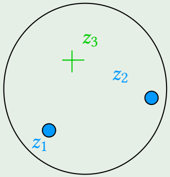
If P is symmetric, i.e., $P(\boldsymbol{z}) = \prod_{i=1}^{n} z_i \cdot \overline{P(1/\boldsymbol{z})}$, then $P \in \mathrm{LY}$ if and only if $A_j \in \mathrm{LY}$ for all j.

- For a single hyperedge: LY for one of the leading coefficients A_j implies LY for a hyperedge.
- For contraction: LY for the disjoint union implies that LY for all the leading coefficients.

Lee-Yang theorem on a single hyperedge

The leading coefficients A_j

Recall that $Z = A_j z_j + B_j$,



$A_3 = z_1 z_2 + \beta z_1 + \beta z_2 + \beta$ in a hyperedge of size 3.

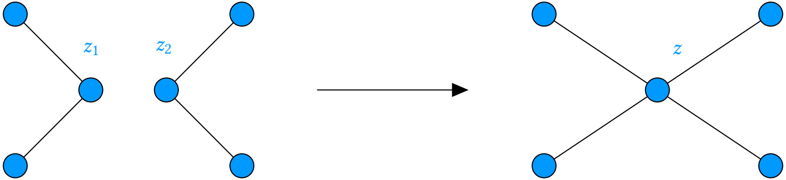
More generally, $A_j \in \mathrm{LY}$ (that is, $A_j = 0$ for $|z_i| \geq 1$) is equivalent to

$$\frac{1}{\beta} = 1 - \prod_{\substack{i=1 \\ i \neq j}}^{k} \left(1 + \frac{1}{z_i}\right).$$

This characterizes the range in our theorem:

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

Asano contraction



Asano contraction: suppose that $Az_1z_2 + Bz_1 + Cz_2 + D \in \mathrm{LY}$, need to show $Az + D \in \mathrm{LY}$.

- $Az_1z_2 + Bz_1 + Cz_2 + D \neq 0$ for $|z_1|, |z_2| > 1$
- $Az^2 + (B + C)z + D = 0$ only if $|z| \leq 1$
- $\left|\frac{D}{A}\right| \leq 1$, using Vieta's formula for product of zeros
- By our lemma, $A \in \mathrm{LY}$, so $A \neq 0$. Thus $Az + D = 0$ only if $|z| = \left|\frac{D}{A}\right| \leq 1$
- $Az + D \in \mathrm{LY}$

Discussions and Open problems

Open problem

What about $\lambda = 1$?

- There are zeros arbitrarily close to $\lambda = 1$ at low temperature
- Our algorithm works for all $|\beta| \leq 1$. FPTAS for $\lambda = 1$ and $-1 < \beta < 0$ would give FPTAS for counting perfect matchings in general (non-bipartite) graphs

Open problem

Connections of locations of zeros, and algorithms such as MCMC and the correlation decay approach?

- Jerrum-Sinclair's MCMC works in subgraphs world instead of the spins world, which by Lee-Yang theorem is real-rooted
- Analog of Griffiths inequality for the self-avoiding walk tree