On the zeros and approximation of the Ising partition function

ALEXANDER BARVINOK

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Partition function

Let $f: \{-1,1\}^n \longrightarrow \mathbb{R}, \mathbb{C}$ be a function.

• We want to efficiently compute (approximate)

$$\sum_{x \in \{-1,1\}^n} e^{f(x)}.$$

A closely related question:

When

$$\sum_{x \in \{-1,1\}^n} e^{f(x)} \neq 0?$$



Partition function

We are interested in the cases when f is

quadratic:
$$f(x) = \sum_{1 \le i < j \le n} a_{ij} \xi_i \xi_j + \sum_{i=1}^n b_i \xi_i$$

or cubic:
$$f(x) = \sum_{1 \le i < j < k \le n} c_{ijk} \xi_i \xi_j \xi_k + \sum_{1 \le i < j \le n} a_{ij} \xi_i \xi_j + \sum_{i=1}^n b_i \xi_i.$$

for $x = (\xi_1, ..., \xi_n)$.

Remark: If

$$f(x) = \alpha + \sum_{i=1}^{n} b_i \xi_i$$

is affine, then

$$\sum_{\mathsf{x} \in \{-1,1\}^n} e^{f(\mathsf{x})} = e^{lpha} \prod_{i=1}^n \left(e^{b_i} + e^{-b_i}
ight)$$

and everything is easy (need e^{b_i} as an input),



Quadratic f

Theorem (Theorem 1)

Suppose that f is quadratic and that for some $0 < \delta < 1$, we have

$$\sum_{j:\;j\neq i}|\Re\,a_{ij}|\;\leq\;1-\delta,\quad \sum_{j:\;j\neq i}|\Im\,a_{ij}|\;\leq\;\frac{\delta^2}{10}\quad\text{and}\quad |\Im\,b_i|\;\leq\;\frac{\delta^2}{10}$$

for $i = 1, \ldots, n$. Then

$$\sum_{x\in\{-1,1\}^n}e^{f(x)}\neq 0.$$

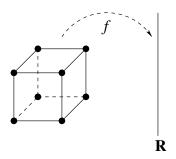
Corollary: By interpolation, $\sum_{x \in \{-1,1\}^n} e^{f(x)}$ can be approximated within relative error $0 < \epsilon < 1$ in quasi-polynomial $n^{O(\ln n - \ln \epsilon)}$ time, provided $a_{ii}, b_i \in \mathbb{R}$ and

$$\sum_{i:\ i\neq i}|a_{ij}|\ \le\ 1-\delta\quad\text{for}\quad i=1,\ldots,n.$$



Quadratic f

Again, we need e^{b_i} as an input. Geometrically, everything is easy if the Lipschitz constant of the non-linear part of f is strictly less than 1, with respect to the ℓ^1 metric on $\{-1,1\}^n$.



Cubic f

Theorem (Theorem 2)

Suppose that f is cubic and that for some $0 < \delta < 1/2$, we have

$$\begin{split} \sum_{j,k:\ j,k\neq i} |\Re\ c_{ijk}| + \sum_{j:\ j\neq i} |\Re\ a_{ij}| &\leq 1-\delta \\ \sum_{j,k:\ j,k\neq i} |\Im\ c_{ijk}| + \sum_{j:\ j\neq i} |\Im\ a_{ij}| &\leq \frac{\delta^2}{10} \quad \textit{and} \\ |\Im\ b_i| &\leq \frac{\delta^2}{10} \quad \textit{for} \quad i = 1,\ldots,n. \end{split}$$

Then

$$\sum_{x \in \{-1,1\}^n} e^{f(x)} \neq 0.$$



Cubic f

Corollary: By interpolation, $\sum_{x \in \{-1,1\}^n} e^{f(x)}$ can be approximated within relative error $0 < \epsilon < 1$ in quasi-polynomial $n^{O(\ln n - \ln \epsilon)}$ time, provided $c_{ijk}, a_{ij}, b_i \in \mathbb{R}$ and

$$\sum_{j,k:\;j,k
eq i} |c_{ijk}| + \sum_{j:\;j
eq i} |a_{ij}| \;\leq\; 1-\delta \quad ext{for} \quad i=1,\ldots,n.$$

Again, we need e^{b_i} as an input.

General f

Generally, if $f: \{-1,1\}^n \longrightarrow \mathbb{R}, \mathbb{C}$ is a polynomial of degree d,

$$f(x) = \sum_{\substack{I \subset \{1,\dots,n\} \ |I| \leq d}} a_I \prod_{i \in I} \xi_i \quad \text{where} \quad x = (\xi_1,\dots,\xi_n),$$

then similar results can be obtained assuming that

$$\sum_{I:\ i\in I}|a_I|\ \le\ \frac{\gamma}{\sqrt{d}},$$

where $\gamma > 0$ is an absolute constant.

In the cases of d=2 and d=3 we get asymptotically optimal bounds.

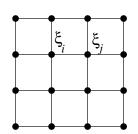


Ising model on graphs

Let G = (V, E) be a graph with vertices $V = \{1, ..., n\}$ and edges E. For a real a, let us choose

$$a_{ij} = \begin{cases} a & \text{if } \{i,j\} \in E \\ 0 & \text{otherwise} \end{cases}$$

and suppose that $b_i = b$ for some $b \in \mathbb{C}$ and i = 1, ..., n.



Ising model on graphs: zeros

Let $\Delta \geq 3$ be the largest degree of a vertex of G and suppose that either

$$a = \frac{1}{2} \ln \frac{\Delta}{\Delta - 2} \quad \text{(ferromagnetic interactions)} \quad \text{or}$$

$$a = \frac{1}{2} \ln \frac{\Delta - 2}{\Delta} \quad \text{(antiferromagnetic interactions)}.$$

As G ranges over the graphs with largest degree Δ , the zeros of the functions

$$b \longmapsto \sum_{x \in \{-1,1\}^n} e^{f(x)}$$

can get arbitrarily close to 0: [Barata and Goldbaum, 1991], [Barata and Marchetti, 1997], [Bencs, Buys, Guerini and Peters 2019], [Peters and Regts, 2020].

Now, in this case

$$\sum_{i:\ i\neq i} |\Re \ a_{ij}| \ \le \ \frac{\Delta}{2} \ln \frac{\Delta}{\Delta-2} \longrightarrow 1 \quad \text{as} \quad \Delta \longrightarrow \infty,$$

Ising model on graphs: complexity

and hence "1" in Theorems 1 and 2 is optimal. Let us choose any

$$a < \frac{1}{2} \ln \frac{\Delta - 2}{\Delta}$$
 (antiferromagnetic interactions).

The problem of approximation of

$$\sum_{x \in \{-1,1\}^n} e^{f(x)}$$

is NP-hard on graphs of the largest degree $\Delta \geq 3$ under randomized reductions [Sly and Sun, 2014], [Galanis, Štefankovič and Vigoda, 2016]. Hence "1" is optimal in the corollaries.

The interpolation lemma

Lemma

Let $U \subset \mathbb{C}$ be a connected open set containing 0 and 1. Then there is a constant $\gamma = \gamma(U) > 0$ such that the following holds: If

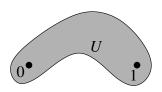
$$g(z) = \sum_{k=0}^{n} c_k z^k, \quad n \geq 2$$

is a polynomial such that $g(z) \neq 0$ for all $z \in U$ then, for any $0 < \epsilon < 1$, the value of g(1), up to relative error ϵ , is determined by the coefficients c_k with $k \leq \gamma (\ln n - \ln \epsilon)$ and can be computed in $n^{O(1)}$ time from those coefficients.

Remark: We say that $w_1 \neq 0$ approximates $w_2 \neq 0$ within relative error ϵ if we can write $w_1 = e^{z_1}$ and $w_2 = e^{z_2}$ with $|z_1 - z_2| \leq \epsilon$.



The interpolation lemma



lf

$$g(z) = \sum_{k=0}^{n} c_k z^k$$

and $g(z) \neq 0$ in an open connected set containing 0 and 1, then, up to relative error $0 < \epsilon < 1$, the value of g(1) is determined by only $O(\ln n - \ln \epsilon)$ lowest coefficients of g. Roughly,

$$\gamma(U) \sim \frac{1}{\beta-1}$$

where $\beta > 1$ is the largest radius of the disc $\mathbb{D} = \{z : |z| < \beta\}$ with a holomorphic map $\phi: \mathbb{D} \longrightarrow U$ satisfying $\phi(0) = 0$ and $\phi(1) = 1$

Zero freeness \Longrightarrow approximation

Given

$$f(x) = \sum_{1 \le i < j \le n} a_{ij} \xi_i \xi_j + \sum_{i=1}^n b_i \xi_i \text{ for } x = (\xi_1, \dots, \xi_n),$$

we write

$$\begin{split} e^{f(x)} &= \exp\left\{-\sum_{1 \leq i < j \leq n} a_{ij}\right\} \left(\prod_{1 \leq i < j \leq n} e^{a_{ij}(\xi_1 \xi_j + 1)}\right) \left(\prod_{i=1}^n e^{b_i \xi_i}\right) \\ &= \exp\left\{-\sum_{1 \leq i < j \leq n} a_{ij}\right\} \left(\prod_{1 \leq i < j \leq n} (1 + c_{ij})^{N(\xi_i \xi_j + 1)}\right) \left(\prod_{i=1}^n e^{b_i \xi_i}\right) \end{split}$$

where $c_{ij}=e^{a_{ij}/N}-1$ and $N=n^2$ and apply the Interpolation Lemma to the polynomial

$$g(z) = \sum_{x \in \{-1,1\}^n} \prod_{1 \le i < j \le n} (1 + zc_{ij})^{N(\xi_i \xi_j + 1)} \left(\prod_{i=1}^n e^{b_i \xi_i} \right).$$

The idea of the proofs of Theorems 1 and 2

A face F of the cube $\{-1,1\}^n$ consists of the points $x=(\xi_1,\ldots,\xi_n)$, where

$$\xi_i = 1$$
 for $i \in I_+$ and $\xi_i = -1$ for $i \in I_-$

while the remaining coordinates ξ_i : $i \notin I_+ \cup I_-$ are free to take either value.

We prove by induction on the dim F that if $F_+ \subset F$ and $F_- \subset F$ are the faces of F obtained by fixing a free coordinate to 1 and -1 respectively, then

$$s_{+} = \sum_{x \in F_{+}} e^{f(x)} \neq 0, \quad s_{-} = \sum_{x \in F_{-}} e^{f(x)} \neq 0$$

and the angle between s_+ and s_- (as vectors in $\mathbb{R}^2 = \mathbb{C}$) does not exceed some $\theta = \theta(\delta) > 0$.



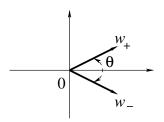
A bit of geometry, d = 2

For d = 2, the proof uses the following geometric lemma.

Lemma (Lemma 1)

Let $w_+, w_- \in \mathbb{C} \setminus \{0\}$ be numbers such that the angle between w_+ and w_- does not exceed some $0 \le \theta < \pi$. Then

$$\left|\Im\,\frac{w_+-w_-}{w_++w_-}\right| \,\,\leq\,\, \tan\frac{\theta}{2}.$$



A bit of geometry, d = 3

For d = 3, the proof uses the following geometric lemma.

Lemma (Lemma 2)

Let $w_{++}, w_{+-}, w_{-+}, w_{--} \in \mathbb{C} \setminus \{0\}$ be numbers such that the angles

between w_{++} and w_{+-}

between w_{++} and w_{-+}

between w_{--} and w_{+-}

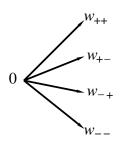
between w_{--} and w_{-+}

do not exceed θ for some $0 \le \theta < \pi/2$. Then

$$\left|\Im\,\frac{w_{++}-w_{-+}-w_{+-}+w_{--}}{w_{++}+w_{-+}+w_{+-}+w_{--}}\right| \,\,\leq\,\, \tan\frac{\theta}{2}.$$



A bit of geometry, d = 3



Reduces to Lemma 1 if we let

$$w_{+} = w_{++} + w_{--}$$
 and $w_{-} = w_{-+} + w_{+-}$.

The obvious extension to eight vectors

$$W_{+++}, W_{++-}, W_{+-+}, W_{-++}, W_{+--}, W_{-+-}, W_{---}, W_{---}$$

fails (it would have taken care of d = 4).

