How to calculate partition functions using convex programming hierarchies: provable bounds for variational methods

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July 13, 2016

Abstract

We consider the problem of approximating partition functions for Ising models. We make use of recent tools in combinatorial optimization: the Sherali-Adams and Lasserre convex programming hierarchies, in combination with variational methods to get algorithms for calculating partition functions in these families. These techniques give new, non-trivial approximation guarantees for the partition function beyond the regime of correlation decay. They also generalize some classical results from statistical physics about the Curie-Weiss ferromagnetic Ising model, as well as provide a partition function counterpart of classical results about max-cut on dense graphs (Arora et al., 1995). With this, we connect techniques from two apparently disparate research areas – optimization and counting/partition function approximations. (i.e. #P type of problems).

Furthermore, we design to the best of our knowledge the first provable, convex variational methods. Though in the literature there are a host of convex versions of variational methods (Wainwright et al.; 2005; Heskes, 2006; Meshi et al., 2009), they come with no guarantees (apart from some extremely special cases, like e.g. the graph has a single cycle (Weiss, 2000)). We consider dense and low threshold rank graphs, and interestingly, the reason our approach works on these types of graphs is because local correlations propagate to global correlations – completely the opposite of algorithms based on correlation decay. In the process we design novel entropy approximations based on the low-order moments of a distribution.

Our proof techniques are very simple and generic, and likely to be applicable to many other settings other than Ising models. 1

1 Introduction

Calculating partition functions is a common task in machine learning: for a distribution \( p \) over a domain \( D \), specified up to normalization i.e. \( p(x) \propto f(x), x \in D \) for some explicit function \( f(x) \), we want to calculate the partition function (i.e. the normalization constant) \( \sum_{x \in D} f(x) \). 2 This task arises naturally in almost any problem involving learning, performing inference (i.e. calculating marginals) over graphical models, or estimating posterior distributions in latent variable models.

Broadly, two approaches are used for calculating partition functions: one is based on using Markov Chains to sample from the distribution \( p \); the other is variational methods, which involve characterizing the partition function as the solution of a certain (intractable) optimization problem over the polytope of valid distributions over \( D \). In theory, the former are much better studied, the crowning achievements of which are probably (Jerrum et al., 2004) and (Jerrum and Sinclair, 1993), who proved certain Markov Chains mix rapidly in the case of permanent with non-negative entries and the ferromagnetic Ising model.

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1This paper was accepted for presentation at Conference on Learning Theory (COLT) 2016

2\( D \) can also be continuous of course, in which case the sum becomes an integral, though in this paper we only will be concerned with discrete domains.
In practice however, variational methods are quite popular (Wainwright and Jordan, 2008; Blei et al., 2003; 2016). There are various reasons for this, the main being that they can be quite a bit faster than Markov Chain methods and they tend to be easier to parallelize. With the exception of belief propagation (which can be viewed as a particular way to solve a certain non-convex relaxation of the optimization problem for calculating the partition function (Yedidia et al., 2003)) there is essentially no theoretical understanding. Additionally, the guarantees for belief propagation usually apply only in the regime of decay of correlations and locally tree-like graphs.

The contributions of our paper are two-fold.

First, we bring to bear recent tools in combinatorial optimization: the Sherali-Adams and Lasserre convex programming hierarchies, in combination with variational methods to get algorithms for calculating partition functions of Ising models. These techniques give new, non-trivial approximation guarantees for the partition function beyond the regime of correlation decay. They also generalize some classical results from statistical physics about the Curie-Weiss ferromagnetic Ising model, as well as provide a partition function counterpart of classical results about max-cut on dense graphs (Arora et al., 1995). With this, we connect techniques from two apparently disparate research areas – optimization and counting/partition function approximations. (i.e. #P type of problems).

Second, we design to the best of our knowledge the first provable, convex variational methods. Though in the literature there are a myriad of convex versions of variational methods (Wainwright et al.; 2005; Heskes, 2006; Meshi et al., 2009), they come with no guarantees at all (except in some extremely special cases, like e.g. the graph has a single cycle (Weiss, 2000)). Our methods tackle dense and low threshold rank graphs, and interestingly, the reason our approach works on these types of graphs is because local correlations propagate to global correlations – which is completely the opposite of algorithms based on correlation decay. In the process we design novel entropy approximations based on the low-order moments of a distribution.

Our proof methods are extremely simple and generic and we believe they can be applied to many other families of partition functions.

Finally, one more important reason to study variational methods (albeit more theoretical in nature) is derandomization, since variational methods are usually deterministic. The gap between the state of the art in partition function calculation with and without randomization is huge. For instance, for the case of calculating permanents of non-negative matrices the algorithm due to (Jerrum et al., 2004) gets a factor 1 + \( \epsilon \) approximation in time \( \text{poly}(n, 1/\epsilon) \) with high probability (i.e. it’s an FPRAS). In contrast, the best deterministic algorithm due to (Gurvits and Samorodnitsky, 2014) achieves only a factor \( 2^n \) approximation in time \( \text{poly}(n) \). (To make the situation even more drastic, the approach in (Gurvits and Samorodnitsky, 2014) can at best lead to a factor \( \sqrt{2^n} \) approximation (Wigderson).)

## 2 Overview of results

We focus on densely Ising models first: an Ising model \( p(x) \propto \exp \left( \sum_{i,j} J_{i,j} x_i x_j \right) \), \( x \in \{-1, 1\}^n \) is \( \Delta \)-dense if it satisfies \( \Delta |J_{i,j}| \leq \frac{1}{\Delta}, \forall i, j \in [n]\), where \( J_T = \sum_{i,j} |J_{i,j}| \).

This is a natural generalization of the typical way to define density for combinatorial optimization problems (see e.g. (Yoshida and Zhou, 2014)). To see this consider a graph \( G = (V, E) \) with \( |E| = cn^2 \). For optimization problems like max-cut or more generally CSPs, we care about objectives that look like

\[
E_{e \in E} f(e) = \sum_{e \in E} \frac{1}{|E|} f(e)
\]

for some function \( f \). Hence, the “weight” in front of each pair \((i, j)\) in the objective is 0 if there is no edge or \( \frac{1}{|E|} \).

This corresponds to \( \Delta = \frac{1}{c} \) in our definition. For partition function problems, however, scale matters (i.e. we cannot assume \( \sum_{i,j} J_{i,j} = 1 \)), so the above generalization appears very organic.

### Theorem 1

For \( \Delta \)-dense Ising models, there is an algorithm based on Sherali-Adams hierarchies which achieves an additive approximation of \( \epsilon J_T \) to \( \log Z \), where \( Z = \sum_{x \in \{-1, 1\}^n} \exp \left( \sum_{i,j} J_{i,j} x_i x_j \right) \) and runs in time \( n^O\left( \frac{1}{\Delta \epsilon^2} \right) \).

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3Markov Chain methods always produce the right answer in the end, but might take longer to converge; variational methods are based on solving an optimization problem, for which it is potentially possible to get stuck in a local optimum, but generally convergence is faster.
Our second contribution are analogous claims for Ising models whose potentials look like low rank matrices. (More precisely, adjacency matrices of low threshold rank graphs, a concept introduced by (Arora et al., 2010) in the context of their algorithm for Unique Games.)

Concretely, an Ising model \( p(x) \propto \exp \left( \sum_{i,j} J_{i,j} x_i x_j \right) \), \( x \in \{-1,1\}^n \) is regular if \( \sum_j |J_{i,j}| = J', \forall i \). The adjacency matrix of a regular Ising model is the matrix \( A_{i,j} = |J_{i,j}| / J' \). Then, we show:

**Theorem 2.** There is an algorithm based on Lasserre hierarchies which achieves an additive approximation of \( en.J' \) to \( \log Z \), where \( Z = \sum_{x \in \{-1,1\}^n} \exp \left( \sum_{i,j} J_{i,j} x_i x_j \right) \), and runs in time \( n^{\text{rank}(\Omega(\epsilon^3) / \Omega(\epsilon^2))} \), where \( \text{rank}(\tau) \) is the number of eigenvalues of the adjacency matrix \( A \) greater than or equal to \( \tau \).

It’s interesting that this property of the graph, previously introduced for purposes of combinatorial optimization problems like small-set expansion, Unique Games (Steurer, 2010; Arora et al., 2010), also helps with counting type problems.

Note that since we prove additive factor guarantees to \( \log Z \), using the fact the \( e^x \leq 1 + 2e \) for small enough \( e \), we can easily turn them to multiplicative factor guarantees on \( Z \). While these guarantees are not as strong as one usually gets in the correlation decay regime (i.e. \( 1 + \epsilon \) multiplicative factor approximations to \( Z \) in time \( \text{poly}(n, 1/\epsilon) \)), to the best of our knowledge, these are the first approximations guarantees for \( Z \) when correlation decay does not hold. We discuss interesting regimes of the potentials \( J_{i,j} \) in Section 5.

### 2.1 Outline of the techniques

Our approach can be summarized as follows. We first express the value of the log-partition function as the solution of a certain (intractable) optimization problem, by using a variational characterization of the log-partition function dating all the way back to Gibbs. (See Lemma 3.) To be more precise, we express it as \( \log Z = \max_{\mu \in M} \{ E(\mu) + H(\mu) \} \), where \( M \) is the polytope of distributions over \( \{-1,1\}^n \), \( E(\mu) \) is an average energy term, which depends on pairwise marginals of \( \mu \) only, and \( H(\mu) \) is the Shannon entropy of \( \mu \).

The source of intractability comes from the fact that we cannot optimize over the polytope \( M \): we will instead optimize over a larger polytope \( M' \), which will come by considering pseudo-distributions, derived from either Sherali-Adams or Lasserre hierarchies. Additionally, we need to design a relaxation of \( H(\mu) \), since in general we cannot hope to express the entropy of a distribution as a function its low-order marginals only.

The entropy relaxation \( \tilde{H}(\mu) \) needs to satisfy \( \tilde{H}(\mu) \geq H(\mu) \) for \( \mu \in M \) and needs to be concave in the variables used in the Sherali-Adams and Lasserre relaxations. The relaxation we use (See Section 4) will be based upon the chain rule for entropy, so it will be easy to prove that it upper bounds \( H(\mu) \) (Proposition 7).

The analysis of the quality of the relaxation proceeds by rounding the pseudo-distributions to an actual distribution. This is slightly different from the roundings in combinatorial optimization, as there we only care about producing a single good \( \{-1,1\}^n \) solution. Here, because of the entropy term, we must crucially produce a distribution over \( \{-1,1\}^n \). The observation then is that we can view correlation rounding, a rounding previously used in works on combinatorial optimization (Barak et al., 2011; Yoshida and Zhou, 2014) as producing a distribution over \( \{-1,1\}^n \) which has the same entropy as the \( \tilde{H}(\mu) \) we defined. (Theorems 11, 13).

### 3 Preliminaries

We proceed with designing approximation algorithms for partition functions of Ising models first. Recall, an Ising model is a distribution \( p : \{-1,1\}^n \to [0,1] \) that has the form \( p(x) \propto \exp \left( \sum_{i,j=1}^n J_{i,j} x_i x_j \right) \) and its partition function is \( Z = \sum_{x \in \{-1,1\}^n} \left( \sum_{i,j=1}^n J_{i,j} x_i x_j \right) \).

They are very commonly used in practical applications in machine learning because of their flexibility (and other appealing properties like being max-entropy distributions subject to moment constraints), and are extensively studied in theoretical computer science, statistical physics and probability theory.

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4There are many generalizations of this, allowing linear or higher order terms, as well as different domains than \( \{-1,1\}^n \). Most results we prove can be generalized appropriately to these settings completely mechanically, so for clarity sake we focus on this case.
A full survey is out of the scope of this paper, but we just mention that it can be shown that approximating $Z$ within any polynomial factor is NP-hard for general potentials $J_{i,j}$ (Jerrum and Sinclair, 1993). When the potentials $J_{i,j}$ are all non-negative (also known as the ferromagnetic Ising model), (Jerrum and Sinclair, 1993) exhibit an FPRAS for computing $Z$.

Let us set up the basic tools we will be using.

### 3.1 Variational methods

One of the main ideas all the algorithms will use is the following simple lemma, which characterizes $Z$ as the solution of an optimization problem. It essentially dates back to Gibbs (Ellis, 2012), who used it in the context of statistical mechanics, though it has been rediscovered by machine learning researchers (Wainwright and Jordan, 2008; Yedidia et al., 2003). For completeness, we reprove it here:

**Lemma 3** (Variational characterization of $\log Z$). For any distribution $\mu : \{-1, 1\}^n \to [0, 1]$,

$$
\sum_{i,j} J_{i,j} \mathbb{E}_\mu [x_i x_j] + H(\mu) \leq \log Z
$$

with equality at $\mu = p$.

**Proof.** For any distribution $\mu : \{-1, 1\}^n \to [0, 1]$, we can write the KL divergence between $\mu$ and $p$ as

$$
KL(\mu||p) = \mathbb{E}_\mu [\log \mu(x)] - \mathbb{E}_\mu [\log p(x)] = -H(\mu) - \sum_{i,j} J_{i,j} \mathbb{E}_\mu [x_i x_j] + \log Z
$$

Since the KL divergence is always non-negative, $-H(\mu) - \sum_{i,j} J_{i,j} \mathbb{E}_\mu [x_i x_j] + \log Z \geq 0$. Hence, $\log Z \geq H(\mu) + \sum_{i,j} J_{i,j} \mathbb{E}_\mu [x_i x_j]$ which proves the first claim of the lemma. However, equality is achieved whenever the KL divergence is 0, which happens when $\mu = p$. This finishes the second part of the lemma.

An immediate consequence of the above is the following:

**Corollary 4.** $\log Z = \max_{\mu \in \mathcal{M}} \left\{ \sum_{i,j} J_{i,j} \mathbb{E}_\mu [x_i x_j] + H(\mu) \right\}$, where $\mathcal{M}$ is the polytope of distributions over $\{-1, 1\}^n$.

We will use the above corollary as follows: instead of considering $\mu \in \mathcal{M}$, which is a polytope we cannot optimize over in polynomial time, we will consider $\mu \in \mathcal{M}'$, for a polytope $\mathcal{M}'$ satisfying $\mathcal{M} \subseteq \mathcal{M}'$, and feasible to optimize over. In fact, $\mathcal{M}'$ will be a polytope of pseudo-distributions, associated with either Sherali-Adams or Lasserre hierarchies. This idea is not new – it has appeared implicitly or explicitly in works on various types of belief propagation. (Wainwright and Jordan, 2008)

The novel thing is how we handle the entropy portion of the objective. Since $\mu \in \mathcal{M}'$ is no longer necessarily a distribution, we need to design surrogates for the entropy of $\mu$. A popular choice in the literature is the so-called Bethe entropy, which roughly arises by taking the expression for the entropy of $\mu$ in terms of the pairwise marginals when the graph is a tree. (Of course, this expression is exact only if the graph is a tree. (Yedidia et al., 2003)) However, this approximation is not a relaxation of $\log Z$ in the standard sense – the Bethe entropy is not an upper bound of the entropy, and the constructed approximation to $\log Z$ is not concave in general, so the analysis proceeds by analyzing the belief propagation messages directly.\(^5\)

We take a completely different approach. To get a proper relaxation for $\log Z$, we design functionals $\bar{H}(\mu)$ defined on $\mu \in \mathcal{M}'$, s.t. $\bar{H}(\mu) \geq H(\mu)$ whenever $\mu \in \mathcal{M}$. In brief, we will use the following Corollary to 4:

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\(^5\)This approach usually works for graphs that are locally-tree-like (i.e. don’t have short cycles), and for which some form of correlation decay holds.
Corollary 5. If $\mathcal{M} \subseteq \mathcal{M}'$ and $H(\mu) \leq \hat{H}(\mu)$ for $\mu \in \mathcal{M}$, then

$$\log Z \leq \max_{\mu \in \mathcal{M}'} \left\{ \sum_{i<j} J_{i,j} E_{\mu} [x_i x_j] + \hat{H}(\mu) \right\}$$

Subsequently, we will round the pseudo-distributions to actual distributions, in a manner that doesn’t lose too much in terms of the value of the objective function.

3.2 Sherali-Adams and Lasserre hierarchies

We will be strongly using hierarchies of convex relaxations, capturing constraints on low-order moments and marginals of distributions. These are where our polytope $\mathcal{M}'$ will come from. While convex hierarchies have recently become relatively well-known in theoretical computer science, we still provide a (very) brief overview for completeness sake. For more details, the reader can consult (Barak et al., 2011; 2014; Laurent, 2009).

Recall, we are considering relaxations of the polytope of distributions over $\{-1, 1\}^n$. The $k$-level Sherali-Adams hierarchy (henceforth SA($k$)) has variables $\mu_S(x_S), x_S \in \{-1, 1\}^{\left| S \right|}$ specifying local distributions over all subsets $S \subseteq [n], |S| \leq k$. The distributions $\mu_S : \{-1, 1\}^{\left| S \right|} \rightarrow \{0, 1\}$ and $\mu_T : \{-1, 1\}^{\left| T \right|} \rightarrow \{0, 1\}$, for any $S, T$ s.t. $|S \cup T| \leq k$ must be “consistent” on $S \cap T$. More precisely, it’s the case that

$$\Pr_{x_S \sim \mu_S} [x_{S \cap T} = \alpha] = \Pr_{x_T \sim \mu_T} [x_{S \cap T} = \alpha], \forall S, T \subseteq [n], |S \cup T| \leq k$$

The fact that these constraints can be written as a linear program is well-known. (See e.g. (Barak et al., 2011))

We can also define a conditioning operation thanks to the existence of these local distributions. More precisely, for a vertex $v$, conditioning on $v$ involves sampling $v$ according to the local distribution $\mu_{\{v\}}$. This operation specifies a solution to the $k-1$st level SA hierarchies: just define $\mu_S(x_S) = \mu_{S \cup \{v\}}(x_S \cup v)$.

The additional power we get from the $k$-th level of the Lassere hierarchy (henceforth LAS($k$)) is that the semidefinite program provides vectors $v_{S, \alpha}$ for each subset $S$ and possible assignment of values $\alpha$ to it, s.t. $\langle v_{S, \alpha} , v_{T, \beta} \rangle = \Pr_{\mu_{S \cup T}} (x_S = \alpha, x_T = \beta)$, if $|S \cup T| \leq k$.

4 Entropy respecting roundings

In this section we consider the functionals acting as surrogates for entropy. Recall, these need to be upper bounds on the entropy of a distribution $\mu$ on which we have essentially no handle other than having the first few moments. A clear candidate to do this is the chain rule.

Notice that for any set $S$ of size at most $k$, where $k$ is the number of levels of the Sherali-Adams or Lasserre hierarchy, $H(\mu_S)$ is a well-defined quantity: it’s exactly

$$H(\mu_S) = \sum_{x_S \in \{-1, 1\}^{|S|}} \mu_S(x_S) \log(\mu_S(x_S))$$

Since these local quantities are essentially all the information about the joint distribution $\mu$ we have, our functional must involve such quantities only.

The simplest functional one can design surely is the following:

Definition. The mean-field pseudo-entropy functional $H_{MF}(\mu)$ is defined as $H_{MF}(\mu) = \sum_{i=1}^{n} H(\mu_i)$.

Remark. Note, this is not the same as the usual mean-field approximation in statistical physics. The mathematical program analogue of that approximation would be to enforce that $E_{\mu}[x_i x_j] = E_{\mu}[x_i]E_{\mu}[x_j]$ — which would result in a non-convex relaxation generally. We think the name is appropriate though, since the bound on the entropy is mean-field, i.e. results by treating $\mu$ as if it were a product distribution.
Almost trivially for any $\mu \in \mathcal{M}$, the following proposition holds:

**Proposition 6.** For any distribution $\mu : \{-1,1\}^n \rightarrow [0,1]$, $H(\mu) \leq H_{MF}(\mu)$

**Proof.** By the chain rule, $H(\mu) = \sum_{i=1}^n H(\mu_i|\mu_{[i-1]})$, where $[i-1]$ denotes the set $\{1, 2, \ldots, i-1\}$ and $H(X|Y)$ is the conditional entropy of $X$ given $Y$. However, since $H(\mu_i|\mu_{[i-1]}) \leq H(\mu_i)$ the claim trivially holds. \hfill $\Box$

We will also consider generalizations of the above – where before applying the above "mean-field" bound on the entropy, one can condition on a small subset first. Namely,

**Definition.** The augmented mean-field pseudo-entropy functional for subsets of size $k$, $H_{aMF,k}(\mu)$ is defined as $H_{aMF,k}(\mu) = \min_{|S|\leq k} \{H(\mu_S) + \sum_{i \notin S} H(\mu_i|\mu_S)\}$.

The same proof as in Proposition 6 implies:

**Proposition 7.** $H(\mu) \leq H_{aMF,k}(\mu)$

Furthermore, it’s quite easy to show that $H_{aMF,k}(\mu)$, like $H_{MF}(\mu)$, is a concave function.

**Lemma 8.** The pseudo-entropy functional $H_{aMF,k}(\mu) = \min_{|S|\leq k} \{H(\mu_S) + \sum_{i \notin S} H(\mu_i|\mu_S)\}$ is concave in the variables $\{\mu_{S \cup \{i\}}(x_{S \cup \{i\}}) || S| \leq k, i \in [n]\}$.

**Proof.** Since $H_{aMF,k}(\mu) = \min_{|S|\leq k} \{H(\mu_S) + \sum_{i \notin S} H(\mu_i|\mu_S)\}$, and the minimum of concave functions is concave, all we need to show is that $H(\mu_S) + \sum_{i \notin S} H(\mu_i|\mu_S)$ is concave for all $S$. It’s well known that entropy is a concave function, and $H(\mu_S)$ is concave. What remains to be shown is that $\sum_{i \notin S} H(\mu_i|\mu_S)$ is concave. But, since the sum of concave functions is concave, it suffices to prove $H(\mu_i|\mu_S)$ is concave.

The proof of this is essentially the same as the proof of concavity of entropy. Abusing notation a bit, we will denote as $\mu_A|x_B$ the conditional distribution on the variables in $A$, conditioned on the variables in $B$ having the value $x_B$. We recall that

\[
H(\mu_i|\mu_S) = \sum_{x_S \in \{-1,1\}^{|S|}} \mu_s(x_S)H(\mu_i|x_s)
\]

\[
= -\sum_{x_S \in \{-1,1\}^{|S|}} \sum_{x \in \{-1,1\}} \mu_s(x_S)\mu_i|x_s(x_i) \log(\mu_i|x_s(x_i))
\]

\[
= -\sum_{x_S \in \{-1,1\}^{|S|}} \sum_{x \in \{-1,1\}} \mu_{S\cup\{i\}}(x_{S\cup\{i\}}) \log(\mu_i|x_s(x_i))
\]

\[
= -\sum_{x_S \in \{-1,1\}^{|S|}} \sum_{x_i \in \{-1,1\}} \mu_{S\cup\{i\}}(x_{S\cup\{i\}}) \log \left( \frac{\mu_{S\cup\{i\}}(x_{S\cup\{i\}})}{\mu_s(x_S)} \right)
\]

We rewrite the last expression as a KL divergence as follows:

\[
-\sum_{x_S \in \{-1,1\}^{|S|}} \sum_{x_i \in \{-1,1\}} \mu_{S\cup\{i\}}(x_{S\cup\{i\}}) \log \left( \frac{\mu_{S\cup\{i\}}(x_{S\cup\{i\}})}{\mu_s(x_S)} \right) + 1 = -KL(\mu_{S\cup\{i\}}||(\mu_s \times r)) + 1 \quad (4.1)
\]

where $r$ is a uniform distribution over $\{-1,1\}$.

Then, if $\mu^1_{S\cup\{i\}} = \lambda \mu^1_S + (1-\lambda)\mu^2_{S\cup\{i\}}$, we want to show

\[
H(\mu^1_i|\mu^1_S) \geq \lambda H(\mu^1_i|\mu^1_S) + (1-\lambda)H(\mu^2_i|\mu^2_S)
\]

By (4.1) and the convexity of KL divergence,

\[
H(\mu^1_i|\mu^1_S) = -KL(\mu^1_{S\cup\{i\}}||(\mu^1_S \times r)) + 1 \\
\geq -\lambda KL(\mu^1_{S\cup\{i\}}||(\mu^1_S \times r)) - (1-\lambda)KL(\mu^2_{S\cup\{i\}}||(\mu^2_S \times r)) + 1 \\
= \lambda H(\mu^1_i|\mu^1_S) + (1-\lambda)H(\mu^2_i|\mu^2_S)
\]

which is what we want. \hfill $\Box$
4.1 Dense Ising models

We finally turn to designing an algorithm for “dense” Ising models.

There are multiple reasons to study this particular subclass: from the theoretical computer science point of view, we have various PTAS for constraint satisfaction problem when the constraint graph is dense (Yoshida and Zhou, 2014; Arora et al., 1995) so we might hope to get results better than the worst-case ones for partition function calculation as well.

Another motivation comes from mean-field ferromagnetic Ising model (also known as the Curie-Weiss model (Ellis and Newman, 1978)), which is frequently studied as a very simplified model of ferromagnetism because one can get relatively easily results about global properties of the model like the partition function, magnetization, etc. In the mean-field model, each spin interacts (equally strongly) with every other spin.

We will, in this section, generalize the classical results about the ferromagnetic Curie-Weiss model, as well as provide the natural counterpart of the results in (Yoshida and Zhou, 2014; Arora et al., 1995) for partition functions.

Let us first review the standard results about Curie-Weiss. Recall, this model follows the distribution $p(x) \propto \exp(\sum_{i,j=1}^{n} \frac{J_{i,j}}{n} x_i x_j)$, $J > 0$. It is easy to analyze because $p(x)$ factorizes and can be “reparametrized” in terms of the magnetization. Namely, since $\sum_{i,j=1}^{n} \frac{1}{n} x_i x_j = \frac{1}{n} (\sum_{i} x_i)^2$, and $(\sum_{i} x_i)^2 \in [-n, n]$, one can show (Ellis and Newman, 1978):

**Theorem 9** (Ellis and Newman, 1978). For the Curie-Weiss model,

$$\log \mathcal{Z} = (1 \pm o(1)) \left( n \max_{m \in [-1, 1]} \left( J m^2 + \frac{1 - m}{2} \log \frac{1 - m}{2} + \frac{1 + m}{2} \log \frac{1 + m}{2} \right) \right)$$

The proof of this theorem involves rewriting the expression for $\mathcal{Z}$ as follows:

$$\mathcal{Z} = \sum_{x \in \{-1, 1\}^n} \exp \left( \sum_{i,j} J_{i,j} \frac{1}{n} x_i x_j \right) = \sum_{l} \exp \left( \frac{J_l^2}{n} \right) \cdot n_l$$

where $n_l$ is the number of terms where $\sum_{i=1}^{n} x_i = l$. Then, using Stirling’s formula and some more algebraic manipulation, one can estimate the dominating term in the summation. The claim of the theorem then follows.

We significantly generalize the above claim using notions from theoretical computer science. The goal is to prove Theorem 1.

Let $J_{l} = \sum_{i,j} |J_{i,j}|$. As discussed in Section 2, we define the following notion of density inspired by the definition of a dense graph in combinatorial optimization (Yoshida and Zhou, 2014):

**Definition.** An Ising model is $\Delta$-dense if $\forall i \neq j, \Delta |J_{i,j}| \leq \frac{J_{l}}{n}$, $\Delta \in (0, 1]$.

We will consider the relaxation for $\log \mathcal{Z}$ given by the augmented pseudo-entropy functional and the level $k = O(1/(\Delta \epsilon^2))$ Sherali-Adams relaxation, namely:

$$\max_{\mu \in \text{SA}(k), k = O(1/(\Delta \epsilon^2))} \left\{ \sum_{i,j} J_{i,j} \mathbb{E}_{\mu} [x_i x_j] + H_{\text{SMF}, k}(\mu) \right\}$$

(4.2)

We also recall correlation rounding as defined in (Barak et al., 2011). In correlation rounding, we pick a “seed set” of a certain size, condition on it, and round the rest of the variables independently. The usual thing to prove is that there is a good “seed set” of a small size to condition on. In particular, for the dense case, the following lemma was proven in (Yoshida and Zhou, 2014):

**Lemma 10** (Yoshida and Zhou, 2014). There exists a set $S$ of size $k = O(1/(\Delta \epsilon^2))$, s.t.

$$\left| \sum_{i,j} J_{i,j} \mathbb{E}_{\mu} [x_i x_j | x_S] - \sum_{i,j} J_{i,j} \mathbb{E}_{\mu} [x_i | x_S] \mathbb{E}_{\mu} [x_j | x_S] \right| \leq \frac{100}{\Delta k} J_{T}$$

7
With this in hand, we proceed to the main theorem of this section:

**Theorem 11** (Restatement of Theorem 1). The output of 4.2 is an \( \epsilon J_T \) additive approximation to \( \log Z \).

**Proof.** The function 4.2 is optimizing a sum of two terms: \( \sum_{i\neq j} J_{i,j} \mathbb{E}_\mu [x_i x_j] \) and an entropy term. Following standard terminology in statistical physics, we will call the former term average energy.

We will analyze the quality of the convex relaxation by exhibiting a rounding of the pseudo-distribution to an actual distribution. There is a difference in what this means compared to the roundings we use in combinatorial optimization: we produce a distribution. There we only care about producing a single \( \{+1, -1\} \) solution. Here, because of the entropy term, it’s essential that we produce a distribution over \( \{+1, -1\} \) solutions.

We use the fact that correlation rounding can be viewed as producing distributions with a fairly explicit expression for their entropy. Let \( \tau \) be the threshold rank from \((\text{Restatement of Theorem 4.2})\). We want to prove Theorem 11.

Consider the average energy first. By Lemma 10,

\[
| \sum_{i,j} J_{i,j} \mathbb{E}_\mu [x_i x_j | x_S] - \sum_{i,j} J_{i,j} \mathbb{E}_{\tilde{\mu}} [x_i x_j | x_S] | \leq J_T \epsilon
\]

Now consider the entropy term. The entropy of the distribution \( \tilde{\mu} \) is \( H(\tilde{\mu}) = H(\mu_S) + \sum_{i \notin S} H(\mu_i | \mu_S) \). But, since \( H_{\text{MF},k}(\mu) = \min_{|S| \leq k} \{ H(\mu_S) + \sum_{i \notin S} H(\mu_i | \mu_S) \} \), \( H_{\text{MF},k}(\mu) \leq H(\tilde{\mu}) \) follows. This immediately implies that

\[
\left( \sum_{i,j} J_{i,j} \mathbb{E}_\mu [x_i x_j] + H_{\text{MF},k}(\mu) \right) - \left( \sum_{i,j} J_{i,j} \mathbb{E}_{\tilde{\mu}} [x_i x_j] + H(\tilde{\mu}) \right) =
\]

\[
\left( \sum_{i,j} J_{i,j} \mathbb{E}_\mu [x_i x_j] - \sum_{i,j} J_{i,j} \mathbb{E}_{\tilde{\mu}} [x_i x_j] \right) + (H_{\text{MF},k}(\mu) - H(\tilde{\mu})) \leq J_T \epsilon
\]

This exactly proves the claim we want.

Notice, in the case of the Curie-Weiss model, since \( J > 0 \), the value of the relaxation 4.2 is at least \( J_T \). Theorem 11 gives a \( 1 + \epsilon \) multiplicative factor approximation to \( \log Z \) for any constant \( \epsilon \), so generalizes the statement of Theorem 9 to cases where the potentials \( J_{i,j} \) might vary in magnitude and sign.

### 4.2 Low threshold rank Ising models

If we use the added power of the Lasserre hierarchy, we can also handle Ising models whose weights look like low rank matrices. We want to prove Theorem 2.

We will consider for simplicity in this section regular Ising models in the weighted sense, meaning \( \sum_j |J_{i,j}| = J_i \), \( \forall i \). The adjacency matrix of an Ising model will be the doubly-stochastic matrix with entries \( |J_{i,j}| / J \).

Let’s recall the definition of threshold rank from (Arora et al., 2010):

**Definition.** The \( \tau \)-threshold rank of a regular graph is the number of eigenvalues of the normalized adjacency matrix greater than or equal to \( \tau \).

We will, in analogy, define the threshold rank of an Ising model.

---

6Notice this is an actual, well-defined distribution, and not only a pseudo-distribution anymore.

7Though we remind again, all of the claims can be appropriately generalized at the expense of more bothersome notation.
**Definition.** The \( \tau \)-threshold rank of a regular Ising model is the number of eigenvalues of its adjacency matrix greater than or equal to \( \tau \).

We will consider the following convex program:

\[
\max_{\mu \in \mathcal{LAS}(k)} \left\{ \sum_{i,j} J_{i,j} \mathbb{E}_\mu [x_i x_j] + H_{aMF,k}(\mu) \right\}
\]  

(4.3)

Consider the vectors \( v_i, i \in [n], \) s.t. \( (v_j, v_j) = \mathbb{E}_\mu [x_i x_j] \). Then, (Barak et al., 2011) prove that when the graph has low threshold rank, “local” correlations propagate to “global” correlations, and as a consequence of this, there is a set of size at most rank \( (\Omega(\epsilon^2))/\Omega(\epsilon^2) \), such that conditioning on it causes the \( \sum_{i,j} J_{i,j} \mathbb{E}_\mu [x_i x_j | x_S] - \sum_{i,j} J_{i,j} \mathbb{E}_\mu [x_i | x_S] \mathbb{E}_\mu [x_j | x_S] \) to drop below \( \epsilon J_T \). More precisely:

**Lemma 12** (Barak et al., 2011). There exists a set \( S \) of size \( t \leq \text{rank}(\Omega(\epsilon^2))/\Omega(\epsilon^2) \), where \( \text{rank}(\tau) \) is the \( \tau \)-threshold rank of the Ising model, s.t.  

\[
\left| \sum_{i,j} J_{i,j} \mathbb{E}_\mu [x_i x_j | x_S] - \sum_{i,j} J_{i,j} \mathbb{E}_\mu [x_i | x_S] \mathbb{E}_\mu [x_j | x_S] \right| \leq \epsilon J_T
\]

Hence, analogously as in Theorem 11, we get:

**Theorem 13** (Restatement of Theorem 2). The output of 4.3 is a \( \epsilon J_T \)-additive approximation to \( \log Z \).

## 5 Discussion on interpreting the results

Since the above results are stated in terms of the additive approximation they provide for \( \log Z \), we discuss how one should interpret them in different “temperature regimes” i.e. different scales of the potentials \( J_{i,j} \). Note that partition function approximation problems are not scale-invariant, and their hardness is sensitive to the size of the coefficients \( J_{i,j} \).

For simplicity of the discussion, let’s focus on the case where there is an underlying graph \( G = (V, E) \), such that \( J_{i,j} = \pm J \), for \( (i, j) \in E(G) \), and 0 otherwise. Furthermore, let’s assume the graph \( G \) is \( d \)-regular.

There are generically three regimes for the problem:

- “High temperature regime”, i.e. when \( |J| = O \left( \frac{1}{\epsilon} \right) \) for a sufficiently small constant in the \( O (\cdot) \) notation. In this case, standard techniques like Dobrushin’s uniqueness criterion show that there is correlation decay. This is the regime where generically Markov Chain methods work. Note that using such methods, generally one can get a \( (1 + \epsilon) \)-factor approximation for \( Z \) in time \( n \) \( \cdot \Theta(\frac{1}{\epsilon^2}) \), which is unfortunately much stronger than what our method gets in that regime. It would be extremely interesting to see if the methods in our paper can be modified to subsume this regime as well.

- “Around the transition threshold”, i.e. when \( |J| = \Theta(\frac{1}{\epsilon^d}) \) for a sufficiently large constant in the \( \Theta \) notation, such that there is no correlation decay. Generally, unless there is some special structure, Markov Chain methods will provide no non-trivial guarantee in this regime – however, we get an order \( \epsilon n \) additive factor approximation to \( \log Z \), which translates to a \( (1 + \epsilon)^n \) factor approximation of \( Z \). We do not, to the best of our knowledge, know how to get such results using any other methods.

- “Low temperature regime”, i.e. when \( |J| = \omega(1/d) \). In this case, in light of the variational characterization of \( \log Z \) and the fact that the entropy is upper bounded by \( n \), the dominating term will typically be the energy term \( \sum_{(i,j) \in E(G)} J_{i,j} \mathbb{E}_\mu [x_i x_j] \), so essentially the quality of approximation will be dictated by the hardness of the optimization problem corresponding to the energy term. (e.g., for the anti-ferromagnetic case, where all the potentials \( J_{i,j} \) are negative, the optimization problem corresponding to the energy term is just max-cut, and we cannot hope for more than a constant factor approximation to \( \log Z \) for general (negative) potentials.)

\( ^8 \)Note, \( J_T = n J' \) in this case.
6 Conclusion

We presented simple new algorithms for calculating partition functions in Ising models based on variational methods and convex programming hierarchies. To the best of our knowledge, these techniques give new, non-trivial approximation guarantees for the partition function when correlation decay does not hold, and are the first provable, convex variational methods. Our guarantees are for dense or low threshold rank graphs, and in the process we design novel entropy approximations based on the low-order moments of a distribution.

We barely scratched the surface, and we leave many interesting directions open. Our methods are very generic, and are probably applicable to many other classes of partition functions apart from Ising models. One natural candidate is weighted matchings due to the connections to calculating non-negative permanents.

Another intriguing question is to determine if there is a similar approach that can subsume prior results on partition function calculation in the regime of correlation decay, as our guarantees are much weaker there. This would give a convex relaxation interpretation of these types of results.

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