Improved Estimation of High-dimensional Ising Models

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Abstract

We consider the problem of jointly estimating the parameters as well as the structure of binary valued Markov Random Fields, in contrast to earlier work that focus on one of the two problems. We formulate the problem as a maximization of $\ell_1$-regularized surrogate likelihood that allows us to find a sparse solution. Our optimization technique efficiently incorporates the cutting-plane algorithm in order to obtain a tighter outer bound on the marginal polytope, which results in improvement of both parameter estimates and approximation to marginals. On synthetic data, we compare our algorithm on the two estimation tasks to the other existing methods. We analyze the method in the high-dimensional setting, where the number of dimensions $p$ is allowed to grow with the number of observations $n$. The rate of convergence of the estimate is demonstrated to depend explicitly on the sparsity of the underlying graph.

1 Introduction

Undirected graphical models, also known as Markov random fields (MRFs), have been successfully applied in a variety of domains, including natural language processing, computer vision, image analysis, spatial data analysis and statistical physics. In most of these domains, the structure of the graphical models is constructed by hand. However, in certain complex domains we have little expertise about interactions between features in data and we need a method that automatically selects a model that represents data well. We propose an algorithm that is able to learn a sparse model that fits data well and has an easily interpretable structure.

Let $X = (X_1, \ldots, X_p)^T$ be a random vector with distribution $P$ that can be represented by an undirected graph $G = (V, E)$. Each vertex from the set $V$ is associated with one component of the random vector $X$. The edge set $E$ of the graph $G$ encodes certain conditional independence assumptions among subsets of the $p$-dimensional random vector $X_i$; $X_i$ is conditionally independent of $X_j$ given the other variables if $(i, j) \notin E$. Let $D = \{x^{(i)} = (x_1^{(i)}, \ldots, x_p^{(i)})\}_{i=1}^n$ be an i.i.d. sample. Our task is to estimate the edge set $E$ as well as the parameters of the distribution that generated the sample. The main contribution of our paper is twofold: the development of an efficient algorithm that estimates the undirected graphical model from data, and the high-dimensional asymptotic analysis of its estimates. We find that the rate of convergence of the estimate explicitly depends on the sparsity of the underlying graph.
variables and iteratively enlarge the set until optimality is achieved. However, the resulting graph structure is not necessarily sparse. [1] used the log-determinant relaxation of the log-partition function [19] to obtain a surrogate likelihood that can be easily optimized.

In this paper we are interested in learning both the parameters and the structure of a binary valued Markov Random Field with pairwise interactions from observed data. An important insight into the problem of structure estimation is that even if a sparse graph is estimated, that does not necessarily mean that the inference in the model is tractable (e.g. inference in a grid, in which each node has only 4 neighbors, is not tractable). Since we are interested in using the estimated model for inference, we use the insight obtained from [16]: i.e. we use the same approximate procedure for estimating the parameters and for inference, as the bias introduced in estimation phase can compensate for the error in the inference phase. Our method is mostly related to [1], as we propose to optimize the $\ell_1$ penalized surrogate likelihood based on the log-determinant relaxation. However, in order to obtain a better estimate, we efficiently incorporate the cutting-plane algorithm [13] for obtaining a tighter outer bound on the marginal polytope into our optimization procedure. Using a better approximation to the log-partition function is crucial in reducing the approximation error of the estimate. In many applications, the ambient dimensionality of the model $p$ is larger than the sample size $n$ and the classical asymptotic analysis, where the model is fixed and the sample size increases, does not give a good insight into the model behavior. We analyze our estimate in the high-dimensional setting, i.e. we allow the dimension $p$ to increase with the sample size $n$. Doing so, we are allowing a procedure to select a more complex model that can represent a larger class of distributions.

2 Preliminaries

In this section we briefly introduce MRFs. We present why the exact inference in discrete MRFs, in general, is intractable, and how to formulate approximate inference as a convex optimization problem. In Section 3, we derive our learning algorithm using methods presented here.

Markov Random Fields. Consider an undirected graph $G$ with vertex set $V = \{1, 2, \ldots, p\}$ and edge set $E \subseteq V \times V$. A Markov random field consists of a random vector $X = (X_1, \ldots, X_p)^T \in \mathbb{R}^p$, where the random variable $X_s$ is associated with vertex $s \in V$. In this paper we will consider binary pairwise MRFs, the Ising model, in which the probability distribution factorizes as $P(x) = \exp(\langle \theta, \varphi(x) \rangle - A(\theta))$ and $X \in \{-1, 1\}^p$. Here $\langle \theta, \varphi(x) \rangle$ denotes the dot product between the parameter vector $\theta \in \mathbb{R}^d$ and potentials $\varphi(x) \in \mathbb{R}^d$, and $A(\theta) = \log \sum_{x \in X} \exp(\langle \theta, \varphi(x) \rangle)$ is the log-partition function. Since we are considering binary pairwise MRFs, potentials are functions over nodes and edges of the form $\varphi(x_v) = x_v$ and $\varphi(x_u, x_v) = x_u x_v$. For future use, we introduce a shorthand notation for the mean parameters $\eta_v = E_{\theta}[\varphi(x_v)]$ and $\eta_{uv} = E_{\theta}[\varphi(x_u, x_v)]$.

Log-partition function. Evaluating the log-partition function involves summing over exponentially many terms and, in general, is intractable. The log-partition function can be expressed as an optimization problem, as a variational formulation, using its Fenchel-Legendre conjugate dual $A^*(\eta)$:

$$A(\theta) = \sup_{\eta \in \mathcal{M}} \{ \langle \theta, \eta \rangle - A^*(\eta) \},$$

where $\mathcal{M} := \{ \eta \in \mathbb{R}^d \mid \exists p(X) \text{ s.t. } \eta = E_{\theta}[\varphi(x)] \}$ is the set of realizable mean parameters $\eta$ and the dual function $A^*(\eta) = -H(p(x; \eta(\theta)))$ is equal to the negative entropy of the distribution parametrized by the mean parameters $\eta$. For each parameter $\theta$ there is a corresponding mean parameter $\eta \in \mathcal{M}$ that maximizes (1). The relation is given as:

$$\eta = \nabla A(\theta) = E_{\theta}[\varphi(x)].$$

[18, 19] list other properties of log-partition function.

Log-partition relaxations. The log-partition function written in equation (1) defines an optimization problem restricted to the set $\mathcal{M}$. Since the set $\mathcal{M}$ is a polytope, it can be represented as an intersection of a finite number of hyperplanes; however, the number of hyperplanes needed to describe the set $\mathcal{M}$ grows exponentially with the number of nodes $p$. It is important to find an outer bound on $\mathcal{M}$ that can be easily characterized and as tight as possible. One outer bound can be obtained using the set of points that satisfy local consistency conditions $\text{LOCAL}(G) := \{ \eta \in [-1, 1]^d \mid \forall (u, v) \in E : \eta_{uv} - \eta_u + \eta_v \leq 1 \}$.

By construction, we have $\mathcal{M} \subseteq \text{LOCAL}(G)$, but points in $\text{LOCAL}(G)$ do not necessarily represent mean parameters of any probability distribution. Another outer bound can be obtained observing that the second moment matrix $M_1(\eta) = E_{\theta}[1 x]^T (1 x)$ is positive semi-definite. Therefore we have $\mathcal{M} \subseteq \text{SDEF}_1(G) := \{ \eta \in \mathbb{R}^d \mid M_1(\eta) \succeq 0 \}$.

The outer bound on the polytope $\mathcal{M}$ can be further tightened by relating it to the cut polytope $\text{CUT}(G)$ (e.g. [3]) and using known relaxations to the cut polytope. Mapping between $\mathcal{M}$ and the cut polytope can
be done using the suspension graph $G' = (V', E')$ of the graph $G$, where $V' = V \cup \{p + 1\}$ and $E' = E \cup \{(v, p + 1) \mid v \in V\}$. The suspension graph is created by adding an additional node $p + 1$ to the graph $G$ and connecting each node $v \in V$ to the newly created node $p + 1$.

**Definition 1.** Let $w_{uv}$ denote the weight of an edge in $G'$. The linear bijection $\xi_{cut}$ that maps points $\eta \in \mathcal{M}$ to points $w \in \text{CUT}(G')$ is given by $w_{v, n + 1} = \frac{1}{2}(\eta_v + 1)$ for $v \in V$ and $w_{uv} = \frac{1}{2}(1 - \eta_{uv})$ for $(u, v) \in E$.

Using a separation algorithm, it is possible to separate a class of inequalities that define the cut polytope and add them to the inequalities defining $\text{LOCAL}(G)$ to tighten the outer bound. Efficient separation algorithms are known for several classes of inequalities [3], but in this paper we will use the simplest one, cycle-inequalities. Cycle-inequalities can be written as:

\[
\sum_{uv \in C \setminus F} w_{uv} + \sum_{uv \in F} (1 - w_{uv}) \geq 1
\]

where $C$ is a cycle in $G'$ and $F \subseteq C$ and $|F|$ is odd. The class of cycle-inequalities can be efficiently separated using Dijkstra’s shortest path algorithm in $O(n^2 \log n + n|E|)$.

To further relax the problem (1), we approximate the negative entropy $A^*(\eta)$ by a function $B^*(\eta)$ to obtain the approximation $B(\theta)$ to $A(\theta)$:

\[
B(\theta) = \sup_{\eta \in \text{OUT}(G)} \langle \theta, \eta \rangle - B^*(\eta),
\]

where $\text{OUT}(G)$ is a convex and compact set acting as an outer bound to $\mathcal{M}$. Even though it is not required, many of the existing entropy approximations are strictly convex (e.g. the convexified Bethe entropy [17], the Gaussian-based log-determinant relaxation [19] or the reweighted Kikuchi approximations [20]), which guarantees uniqueness of the solution to (4).

**Inference in MRFs.** The inference task in MRFs refers to finding or approximating the marginal probabilities (or the mean vector). It can be seen from equation (2) that the log-partition plays an important role in inference and a good approximation to it is essential in obtaining good estimates of the marginals. Many known approximate inference algorithms can be explained using the framework explained above; they create an outer bound $\text{OUT}(G)$ and use an entropy approximation to estimate the marginals (e.g. the log-determinant relaxation [19], Belief Propagation [21] and tree-reweighted sum-product (TRW) [17] to name few). Recent work proposed a cutting-plane algorithm [13] that iteratively tightens the outer bound on the polytope $\mathcal{M}$ using cycle-inequalities and empirically obtains improved estimates of marginals.

### 3 Structure learning and parameter estimation

In this section we address the problem of structure learning and parameter estimation. Given a sample $D$, we obtain our estimate of the edge set $E$ and parameters $\theta$ associated with edges as a maximizer of the $l_1$ penalized surrogate log-likelihood:

\[
\hat{\theta}^n = \arg\max_{\theta \in \mathbb{R}^d} (\ell(\theta; D) - \lambda^n \sum_{uv \in E} |\theta_{uv}|)
\]

\[
= \arg\max_{\theta \in \mathbb{R}^d} (\theta, \tilde{\eta}^n) - B(\theta) - \lambda^n \sum_{uv \in E} |\theta_{uv}|,
\]

where $\tilde{\eta}^n$ denotes the mean parameter estimated from the sample. $\lambda^n$ is a tuning parameter that sets the strength of the penalty. Note that a solution to the problem (5) simultaneously gives the estimate of the edge set $E$ and the parameter vector $\theta$, since if $\theta_{uv} = 0$ then the estimated graph does not contain the edge between nodes $u$ and $v$. Since the $l_1$ penalty shrinks the edge parameters towards 0, the estimation is biased towards sparse models.

In the remainder of this section we will explain our algorithm that efficiently solves (5). Since the problem (5) is convex one could use, for example, the subgradient method for non-differentiable functions [2]. However, computing the gradient of the log-likelihood $\frac{\partial \ell(\theta; D)}{\partial \theta}$ requires inference over the model with current values of the parameters. Since the inference is only approximate, the accuracy of the computed gradient heavily depends on the approximation used. Note again that the sparsity of the graph does not necessarily imply that the inference is tractable. Applying the cutting-plane algorithm [13] for approximate inference could achieve good accuracy, however it would be computationally prohibitive, since at each iteration of the subgradient algorithm, the cutting plane algorithm have to be run anew to obtain the mean parameters. Hence, computational inefficiency stems from the fact that for each parameter $\theta$, we have to compute the corresponding mean parameter $\eta$. We present a way to exploit the structure of the log-determinant relaxation to obtain both $\theta$ and $\eta$ and obtain computationally efficient algorithm. We will use the convenient way of representing parameters in a matrix:

\[
R(\theta) = \begin{pmatrix}
0 & \theta_1 & \theta_2 & \ldots & \theta_p \\
\theta_1 & 0 & \theta_{12} & \ldots & \theta_{1p} \\
\vdots & \vdots & \ddots & \ldots & \vdots \\
\theta_p & \theta_{1p} & \theta_{2p} & \ldots & 0
\end{pmatrix}
\]

Algorithm 1 describes our proposed method for structure learning. To obtain the solution of (5) efficiently,
we use variational representation of $B(\theta)$ using the log-determinant relaxation and jointly optimize over $\theta$ and $\eta$. Starting with $\text{LOCAL}(G)$ as an outer bound to $\mathcal{M}$, the algorithm alternates between finding the best parameters and tightening the outer bound $\text{OUT}(G)$ by incorporating the cycle inequalities that are violated by the current mean parameters $\eta$. The algorithm is similar, in spirit, to the cutting-plane algorithm [13] for inference. However, optimization in line 3 of Algorithm 1 is done over all parameters jointly, which produces some technical challenges. We proceed with a procedure for solving the optimization problem (5).

The formulation in line 3 arose from using the variational form (4) of $B(\theta)$ in the surrogate likelihood (5). The idea behind the log-determinant relaxation [19] is to upper bound the log-partition function by using the Gaussian-based entropy approximation: 

$$A(\theta) \leq \sup_{\eta \in \text{OUT}(G)} \frac{1}{2} \log \det (R(\eta) + \text{diag}(m)) + \langle \theta, \eta \rangle,$$

where $m \in \mathbb{R}^{p+1} = \{1, \frac{4}{3}, \ldots, \frac{4}{3} \}$. To make use of this upper bound, we have to rewrite it so that both parameters $\theta$ and $\eta$ can be extracted from it. Before we rewrite the upper bound, notice that after $k$ iterations of repeat-until loop in Algorithm 1, we have added $k$ cycle-inequalities. It will be useful to rewrite equation (3) in a matrix form as $\text{Tr}(A_k R(\eta)) \geq b_k$, where $A_k$ is a symmetric matrix for the $k$-th inequality.

**Lemma 2.** After $k$ iterations of algorithm, we write the log-partition relaxation as

$$B(\theta) = \frac{p}{2} \log \left( \frac{\text{det}(\mathbb{I})}{2} \right) - \frac{1}{2} (p + 1) - \frac{1}{2} \max_{\nu, \alpha \geq 0} \{ \nu^T m - \alpha^T b + \log \det (-R(\theta) - \text{diag}(\nu) + \sum_{i=1}^{k} \alpha_i A_i) \}. \quad (6)$$

To obtain the mean vector $\eta^*$ corresponding to $\theta$ we take off diagonal elements of the matrix 

$$Z = (-R(\theta) - \text{diag}(\nu) + \sum_{i=1}^{k} \alpha_i A_i)^{-1}$$

defined for optimal $\nu, \alpha$, i.e. $R(\eta^*) = Z - \text{diag}(Z)$. 

**Proof.** Due to the lack of space, we leave out technical details of the proof and just give a sketch of the main idea. The proof is similar to the proof of Lemma 5 in [1]. We start from equation (4), where the Gaussian-based entropy is used as $B^*(\eta)$, and rewrite it in the Lagrangian form with $\alpha_i$ as a Lagrangian multiplier for $i$-th cycle-inequality. The lemma follows from rewriting the Lagrangian in the dual form. \hfill \square

Using Lemma 2, we can rewrite the problem in line 3 of Algorithm 1 so that both $\theta$ and $\eta$ can be extracted. Defining $Y := -R(\theta) - \text{diag}(\nu)$ and dropping constant terms the optimization problem is written as:

$$\max_{\alpha \geq 0} \left\{ \log \det (Y + \sum_i \alpha_i A_i) - \text{Tr}(Y \sum_i \alpha_i A_i) + \text{diag}(m)) \right\}.$$  

(7)

With $\alpha = 0$, the problem (7) is identical to the problem analysed in [1, 7], where $Y$ can be found using a block coordinate descent. However, due to the terms that arise from the added cycle-inequalities, the Lagrangian multipliers $\alpha \neq 0$ are different from zero and we need a different method to obtain the optimal $Y$ and $\alpha$.

We propose Algorithm 2 for solving the problem (7). The algorithm iterate between solving $Y$ and $\alpha$. For fixed $\alpha$, the dual of (7) is given as

$$\max_{W \in \mathcal{W}} \left\{ \log \det (W + R(\eta^*)) + \text{diag}(m)) - \text{Tr}(W \sum_i \alpha_i A_i) \right\}, \quad (8)$$

where

$$\mathcal{W} = \left\{ \begin{array}{ll} W_{uv} = 0 & \text{for } u = 1, v = 1, u = v \\ |W_{uv}| \leq \lambda^u & \text{otherwise} \end{array} \right\}. \quad (9)$$

To solve for $Y$ we apply the subgradient method, in which we optimize the dual variable $W$ with the projection step onto the box constraint defined in (9). The gradient direction is given as $\nabla W = (R(\eta^*)) + \text{diag}(m) + W^{-1} - \sum_i \alpha_i A_i$ and the step size can be defined as $\gamma_i = \gamma_i / \sqrt{\delta_i}$. For fixed $Y$, the problem (7) reduces to one in line 5 of Algorithm 2. Since the dimension of $\alpha$, corresponding to the number of cycle-inequalities, is not large, we can apply any optimization method to find an optimal $\alpha$. 

**Algorithm 1** Structure learning with cutting-plane algorithm

1: $\text{OUT}(G) \leftarrow \text{LOCAL}(G)$
2: repeat
3: $\hat{\theta}^*, \hat{\eta} \leftarrow \max_{\theta, \eta} \{ \langle \theta, \eta \rangle - \lambda^u \sum_{\nu, \alpha \geq 0} \{ \nu^T m - \alpha^T b \} \}$
4: $w \leftarrow \text{Create_Separate_Cycle_Inequalities}(w)$
5: $C \leftarrow \text{Separate_Cycle_Inequalities}(w)$
6: $\text{OUT}(G) \leftarrow \text{OUT}(G) \cap C$
7: until $C = \emptyset$

**Algorithm 2** Finding best parameters

1: $W, \alpha \leftarrow \text{Initialize}()$
2: repeat
3: $W \leftarrow \max_{W \in \mathcal{W}} \left\{ \log \det (W + R(\eta^*)) + \text{diag}(m)) - \text{Tr}(W \sum_i \alpha_i A_i) \right\}$
4: $Y \leftarrow (W + R(\eta^*)) + \text{diag}(m))^{-1} - \sum_i \alpha_i A_i$
5: $\alpha \leftarrow \max_{\alpha_{\geq 0}} \{ \log \det (Y + \sum_i \alpha_i A_i) - \alpha^T b \}$
6: until stop criterion
Algorithm 2 is guaranteed to converge, which can be shown from the standard results for block coordinate optimization (e.g. [14]). Using the same results, we could perform the analysis of the convergence rate, but that is beyond the scope of this paper. The computational complexity of Algorithm 2 is roughly $O(p^3)$, so the overall complexity of the structure learning is $O(p^3)$. The method has lower complexity than the method [1] and same as graphical lasso [7]. A useful trick for boosting the performance of the structure learning algorithm is to use a warm-start strategy for Algorithm 2, i.e. initialize $Y$ and $\alpha$ to the optimal solution of the previous iteration.

An important advantage of our algorithm, over other block-coordinate descent algorithms [1, 7], is that we can readily modify it to the case when the regularization is given as a constraint on $\ell_1$ ball in which parameters lie, e.g. $\sum_{uv \in E} |\theta_{uv}| \leq C$. In that case, we can solve directly the primal problem, to obtain $Y$, using an efficient algorithm for projection onto the $\ell_1$ ball [6]. The algorithm for efficient projection onto the $\ell_1$ ball was also exploited for learning sparse inverse covariance matrices under the Gaussian assumption on data [5]. Finally, the structure learning algorithm could be extended to the non-binary MRFs using a generalization to the log-determinant relaxation [19] and projecting the marginal polytope to different binary marginal polytopes [13].

4 Asymptotic analysis

In this section, we state our main theoretical result on the convergence rate of the $\ell_1$ penalized log-likelihood estimate. As opposed to the algorithm described in the last section, where we used the log-determinant approximation, our theoretical result is applicable to any strongly convex surrogate for the log-partition function. The asymptotic analysis presented here is high-dimensional in nature, i.e. we analyse the estimate in the case when both the model dimension $p$ and the sample size $n$ tend to infinity. Traditionally, asymptotic analysis is performed for a fixed model letting the sample size $n$ to increase, however, that type of analysis does not reflect the situation that occurs in many real data sets where the dimensionality $p$ is larger than the sample size $n$ (e.g. gene arrays, fMRIs). To get insight into the behaviour of the estimate, it is therefore important to perform the high-dimensional analysis.

The first question to ask is whether the estimate $\hat{\theta}^n$ converges to $\theta^*$, the true parameter associated with the distribution? Unfortunately, in general, the answer to this question is no, since we are using an approximation to the log-partition function. Note that we could obtain such consistency result if we are willing to assume that the true graph can be found in a restricted class of models, e.g. trees for which the approximation will give the exact solution.

The next best thing we can hope for is that our procedure produces an estimate that is close to the best parameter $\hat{\theta}$ in the class using the surrogate $B(\theta)$. In general, we cannot tell how far is the best parameter in the class $\hat{\theta}$ from the true $\theta^*$, however, letting the dimension of the model $p$ to increase with the size of the sample and using a good approximation $B(\theta)$ we are able to represent an increasing number of distributions and, hence, reduce the size of the approximation error.

Naturally, the next question is whether the estimate $\hat{\theta}^n$ at least converges to $\hat{\theta}$? This convergence would be obviously true if the model had been fixed, however, we are dealing with models of increasing dimensionality. In order to guarantee the closeness of the estimate $\hat{\theta}^n$ to the best parameter $\hat{\theta}$ we will have to assume that the model is sparse and we will show how the rate of convergence explicitly depends on the sparsity. We proceed with the main result.

Let $\eta^*$ be the true mean vector corresponding to $\theta^*$. Since we use strictly convex conjugate dual pair $B$ and $B^*$, the gradient mapping $\nabla B$ is one-to-one and onto the relative interior of the constrain set $\text{OUT}(G)$ [11]. In the limit of infinite amount of data, the asymptotic value of the parameter estimate is given by $\overline{\theta} = \nabla^{-1}B(\eta^*)$. Let $S = \{\beta \mid \beta \neq 0\}$ be the index set of non zero elements of $\theta$ and let $\overline{S}$ be its complement. Note that the set $S$ indexes nodes and edges in the graph and that the size of the set is related to the sparsity of the estimated graph. Denote $s = |S|$ the number of the non-zero elements. The following theorem gives us the asymptotic behaviour of the parameter estimate $\hat{\theta}^n$. To prove the theorem we follow a method of Rothman et al. [12].

Theorem 3. Let $\hat{\theta}^n$ be the minimizer of (5). If $B(\theta)$ is strongly convex and $\lambda_n \propto \sqrt{\frac{\log p}{n}}$ then,

$$\left\|\hat{\theta}^n - \theta^*\right\|_2 = O_P\left(\sqrt{\frac{(p+s)\log p}{n}}\right).$$

Proof. Let $G : \mathbb{R}^d \mapsto \mathbb{R}$ be a map defined as $G(\delta) := \ell(\hat{\theta} + \delta; D) - \lambda^s \sum_{uv} |\delta_{uv}| + \ell(\theta; D) + \lambda^s \sum_{uv} |\theta_{uv}|$. Using the Taylor expansion and the fact that $\nabla B(\theta) = \eta^*$, we have $B(\theta + \delta) - B(\theta) = (\eta^*, \delta) + \frac{1}{2}\delta^T \nabla^2 \left[B(\hat{\theta} + \alpha\delta)\right]\delta$, for $\alpha \in [0, 1]$. Now, we may write $G$ as:

$$G(\delta) = (\delta, \hat{\theta}^n - \eta^*) - \frac{1}{2}\delta^T \nabla^2 \left[B(\hat{\theta} + \alpha\delta)\right]\delta - \lambda^s \sum_{uv} (|\hat{\theta}_{uv}^n + \delta_{uv}| - |\hat{\theta}_{uv}|).$$

(10)
By construction, our estimate $\hat{\delta}^n = \hat{\theta}^n - \hat{\theta}$ maximizes $G$ and we have $G(\delta^n) \geq G(0) = 0$. The proof continues by showing that for some $L > 0$ and $||\delta||_2 = L$ we have $G(\delta) < 0$, which implies that $||\delta^n||_2 \leq L$ because of concavity of $G$. Appropriately choosing $L$, we show that $\delta$ converges to 0.

We proceed by bounding each term in (10). The first term can be written as:

$$|\langle \hat{\theta}^n - \hat{\theta} \rangle| \leq \sum_{uv \in E} |\delta_{uv}| + \sum_{v \in V} |\delta_v| \leq (*) + (**) .$$

Using the union sum inequality and Hoeffding's inequality, with probability tending to 1, we have

$$\max_{uv} |\hat{\theta}^n_{uv} - \hat{\theta}_{uv}| \leq C_1 \sqrt{\frac{\log p}{n}} ,$$

and a bound $(*) \leq C_1 \sqrt{\frac{\log p}{n}} \sum_u |\delta_u|$. Using the Cauchy-Schwartz inequality and Hoeffding’s inequality the second term is bounded as

$$(**) \leq \left( \sum_u (|\hat{\theta}^n_v - \hat{\theta}_v|^2)^{1/2} \right) \left( \sum_u |\delta_u|^2 \right)^{1/2} \leq C_2 \sqrt{\frac{\log p}{n}} \left( \sum_u |\delta_u|^2 \right)^{1/2} .$$

The Hessian of a strongly convex function is positive definite, so the second term in (10) can be bound as follows

$$\text{Tr}(\delta^T \nabla^2 B(\theta + \alpha \delta) \delta) \geq C_3 ||\delta||_2^2 ,$$

where $C_3$ is a constant that depends on the minimum eigenvalue of the Hessian. Using the triangular inequality on the third term, we have

$$\sum_{uv' \in S} (|\hat{\theta}_{uv'} + \delta_{uv'}| - |\hat{\theta}_{uv'}|) \geq \left( \sum_{uv' \in S} |\delta_{uv'}| \right) - \left( \sum_{uv' \in S} |\delta_{uv'}| \right) .$$

Now we can define the constant $L$ as

$$L = M \left( \sqrt{\frac{s \log p}{n}} + \sqrt{\frac{\log p}{n}} \right) \to 0 .$$

Taking $\lambda^n = C_2 \sqrt{\frac{\log p}{n}}$, we have an upper bound on $G$:

$$G(\delta) \leq C_1 \sqrt{\frac{\log p}{n}} (1 - \frac{1}{\epsilon}) \sum_{uv \in S} |\delta_{uv}| + C_1 \sqrt{\frac{\log p}{n}} (1 + \frac{1}{\epsilon}) \sum_{uv \in S} |\delta_{uv}| + C_2 \frac{\log p}{n} \left( \sum_u |\delta_u|^2 \right)^{1/2} - C_3 ||\delta||_2^2 .$$

First term is negative for small $\epsilon$ so we can remove it from the upper bound. Using the fact that

$$\sum_{uv \in S} |\delta_{uv}| \leq \sqrt{s} (\sum_{uv \in S} \delta_{uv}^2)^{1/2} ,$$

the upper bound becomes

$$G(\delta) \leq \frac{(C_1(1+\epsilon) - C_3) (\sum_{uv \in S} \delta_{uv}^2)^{1/2}}{\epsilon} + (C_2(1 - \epsilon) - C_3) ||\delta||_2^2 < 0$$

for sufficiently large $M$ and the theorem follows.

5 Experimental Results

In this section we compare the performance of our estimation method for sparse graphs as well as Banerjee et al. [1] and Wainwright et al. [15] on simulated data. In order to assess the performance we compare speed, accuracy of the structure selection and accuracy of the estimated parameters. Method of Wainwright et al. [15] produces two estimates $\hat{\theta}_{uv}$ and $\hat{\theta}_{vu}$ for each edge parameter. There are two ways how we can symmetrize the solution:

$$\hat{\theta}_{uv} = \begin{cases} \hat{\theta}_{uv} & \text{if } |\hat{\theta}_{uv}| < |\hat{\theta}_{vu}| \text{ “Wainwright min”,} \\
\hat{\theta}_{vu} & \text{if } |\hat{\theta}_{uv}| \geq |\hat{\theta}_{vu}| \text{ “Wainwright max”.} \end{cases}$$

We have implemented the method of Wainwright et al. [15] using a coordinate descent algorithm for logistic regression [8]. To compare the method of Banerjee et al. [1] we used “COVSEL” package available from the authors website.

We use three types of graphs for experiments: (a) 4-nearest-neighbor grid models, (b) sparse random graphs, and (c) sparse random graphs with dense subgraphs. The grid model represents a simple sparse graph, which does not allow for exact inference due to the large tree width. To create a random sparse graph, we choose a total number of edges and add them between random pairs of nodes, taking into account the maximum node degree. Random graphs with dense subgraphs are globally sparse, i.e. they have few edges, however there are local subgraphs that are very dense, with strong interactions between nodes. To generate them, we first create dense components and then randomly add edges between different components. For a given graph, we assign each node a parameter $\theta_v \sim \mathcal{U}[-1,1]$ and each edge a parameter $\theta_{uv} \sim \mathcal{U}[-\xi,\xi]$, where $\xi$ is the coupling strength. For a given distribution $P_{\theta^*}$ of the model we generate random data sets $\{x^{(i)}, x^{(2)}, \ldots, x^{(n)}\}$ of i.i.d. points using Gibbs sampling. Every experimental result is averaged over 50 runs.

We first comment on the speed of convergence of the methods. We have decided not to plot graphs with speed comparisons due to the use of different programming languages, however, from our limited experience
we observe that the method of Wainwright et al. [15] is the fastest and the running time does not depend much on the underlying sparsity of the graph. Our method compared favorably to the method of Banerjee et al. [1], however, increasing the density of the graph or increasing the coupling strength \( \xi \) resulted in an increase of the number of added cycle-inequalities needed for the approximation and in a slower convergence. From the comments on the speed of the methods, we can suspect that there is a trade-off between speed and accuracy.

Next, we compare the accuracy of the edge selection. For this experiment we create a random sparse graphs with \( p = 50 \) nodes and 100 edges, such that the coupling strength is \( \xi = 0.5 \). Then we vary the sample size \( n \) from 100 to 1000. Figure 1 shows precision and recall of edges included into the graph for a regularization parameter set as \( \lambda_n = 2 \sqrt{\log p/n} \). We have excluded the method of Banerjee et al. [1] in the figure, since for this experiment the estimated structure was identical. From plots we can see that our method and “Wainwright min” produce similar results and perform better than “Wainwright max”. Similar conclusions can be drawn for the grid model (results not shown). To shed some more light on these results, it is instructive to discuss the speed at which the edges get included into the model as the function of parameter \( \lambda_n \). “Wainwright max” produces estimates that include edges the fastest and the resulting graph is the densest which can explain low precision due to many spurious edges that get included into the model. “Wainwright min” includes edges most conservatively, while our solution produces graphs that according to their denseness fall in between “Wainwright min” and “Wainwright max” estimates. Next, we move onto a harder problem of estimating the structure of graphs that have strong couplings between nodes. For this experiment, we construct a random graph with two dense subgraphs, which are fully connected graphs of size 8. Graphs have total of \( p = 50 \) nodes and 100 edges. We vary the coupling strength \( \xi \) in interval [1, 10]. The structure is estimated from a sample size of \( n = 500 \) and the results are presented in Figure 2. In this experiment we start to notice a difference between the estimated models using our method and the method [1]. As the coupling strength increases, the mean parameter is not captured within the constraints defined by the cycle-inequalities and our method has to add the violated cycle-inequalities to the constraint set \( \text{OUT}(G) \) which produces a different estimate.

Final set of experiments measures how well the estimated model fits the observed data and for that purpose we use surrogate log-likelihood. While the true measure of the fit should be the log-likelihood, it is not possible to use it due to the problem of evaluating the log-partition function. Furthermore, in practise we always use the surrogate log-likelihood when choosing a model from data, so our experiments can be justified. Figure 3 shows the fit for data generated from the grid model. As in estimation of the structure, for this sparse model, there is no difference between our method and the method of Banerjee et al. [1]. One explanation of this result is that the outer bound on the polytope \( \mathcal{M} \), implicitly defined through log-determinant that act as a log-barrier, captures the estimated mean parameter and all the cycle-inequalities are satisfied. Next, similarly to the structure estimation, we generate a graph with dense subgraphs and present results in Figure 3. Again, we can see that our method start to perform better as we increase the strength of couplings. On Figure 3 we also plot the fit for parameters estimated from the method of Wainwright et al. [15], however, since the method uses a different pseudo-likelihood, it performs worse than the other two methods.

To summarize, we have shown that on the task of estimating the structure our method performs similarly to the method of Banerjee et al. [1] and that both methods estimate structure that falls between “Wainwright min” and “Wainwright max” estimates. When measuring how well do learned models fit the data, we observe that our method outperforms the method of Banerjee et al. [1] when the model has dense subgraphs and strong interactions between nodes.
6 Conclusion

In the paper we have presented a method for jointly learning the structure and the parameters of an undirected MRF from the data. Our method is useful when there are strong correlations between nodes in the graph or when the true graph is not too sparse. If the true graph is very sparse, our algorithm efficiently finds the estimate without performing the cutting-plane step. We showed how to incorporate the class of cycle-inequalities into the algorithm, which are particularly valuable as they can be separated efficiently and added as needed to improve the solution. Furthermore, our algorithm can be efficiently combined with the algorithm for projection onto the $\ell_1$ ball in cases when the parameters are constrained to lie in the $\ell_1$ ball.

We have analyzed convergence rate of an estimate based on maximizing a penalized surrogate likelihood in high-dimensional settings. We have given a rate that depends on the number of non-zero elements of the best parameter for the surrogate likelihood. Such analysis provides insight into the performance of the method in high-dimensional setting, when both $p$ and $n$ are allowed to grow.

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