SPARSE ESTIMATION IN ISING MODEL VIA PENALIZED MONTE CARLO METHODS

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Abstract. We consider a problem of model selection in high-dimensional binary Markov random fields. The usefulness of the Ising model in studying systems of complex interactions has been confirmed in many papers. The main drawback of this model is the intractable norming constant that makes estimation of parameters very challenging. In the paper we propose a Lasso penalized version of the Monte Carlo maximum likelihood method. We prove that our algorithm, under mild regularity conditions, recognizes the true dependence structure of the graph with high probability. The efficiency of the proposed method is also investigated via simulation studies.

1. Introduction

A Markov random field is an undirected graph \((V,E)\), where \(V = \{1, \ldots, d\}\) is a set of vertices and \(E \subset V \times V\) is a set of edges. The structure of this graph describes conditional independence among subsets of a random vector \(Y = (Y(1), \ldots, Y(d))\), where a random variable \(Y(s)\) is associated with a vertex \(s \in V\). Finding interactions between random variables is a central element of many branches of science, for example biology, genetics, physics or social network analysis. The goal of the current paper is to recognize the structure of a graph on the basis of a sample consisting of \(n\) independent graphs. We consider the high-dimensional setting, i.e. the number of vertices \(d\) can be comparable or larger than the sample size \(n\). It is motivated by contemporary applications of Markov random fields in the above-mentioned places, for instance gene microarray data.

The Ising model (Ising, 1925) is an important example of a mathematical model that is often used to explain relations between discrete random variables. In the literature one can find many papers that argue for its effectiveness in recognizing the structure of a graph (Ravikumar et al., 2010; Höfling and Tibshirani, 2009; Guo et al., 2010; Xue et al., 2012; Jalali et al., 2011). This model also plays a key role in our paper. On the other hand, the Ising model is an example of an intractable constant model that is the joint distribution of \(Y\) is known only up to a norming constant and this constant cannot be calculated in practice.

Thus, there are two main difficulties in the considered model. The first one is the high-dimensionality of the problem. The second one is the intractable norming constant. To overcome the first obstacle we apply a well-known Lasso method (Tibshirani, 1996). The properties of this method in model selection are deeply studied in many papers that mainly investigate linear models or generalized linear models (Bickel et al., 2009; Bühlmann and van de Geer, 2011; Huang and Zhang, 2012; van de Geer, 2008; Ye and Zhang, 2010; Zhao and Yu, 2006; Zhou, 2009). However, it is not difficult to find papers that describe properties of Lasso estimators in more complex models, for instance Markov random fields (Bühlmann and van de Geer,

Key words and phrases. Ising model, Monte Carlo Markov chain, Markov random field, model selection, Lasso penalty.
There are many approaches trying to overcome the second obstacle that is the intractable norming constant. For instance, in Ravikumar et al. (2010) one proposes to perform $d$ regularized logistic regression problems. This idea is based on the fact that the norming constant reduces, if one considers the conditional distribution instead of the joint distribution in the Ising model. This simple fact is at the heart of the pseudolikelihood approach (Besag, 1974) that is replacing the likelihood (that contains the norming constant) by the product of conditionals (that do not contain the norming constant). This idea is widely applied in the literature (Höfling and Tibshirani, 2009; Guo et al., 2010; Xue et al., 2012; Jalali et al., 2011) to study model selection properties of high-dimensional Ising models. However, this approach works well only if the pseudolikelihood is a good approximation of the likelihood. In general, it depends on the true structure of a graph. Namely, if this structure of the graph is sufficiently simple (examples of different structures can be found in section 5), then the product of conditionals should be close to the joint distribution. However, in practice this knowledge is unavailable. Therefore, in the current paper we propose another approach to the norming constant problem that relates to Markov chain Monte Carlo (MCMC) methods. Namely, the norming constant is approximated using the importance sampling technique. The advantage of this method over the pseudolikelihood is that it does not depend on the unknown complexity of the estimated graph. Roughly speaking, the size of a sample used in importance sampling should be sufficiently large to have good approximation of the likelihood.

The MCMC method is a well-known approach to overcome the problem with the intractable norming constant in classical (low-dimensional) estimation of graphs. For instance, their properties are investigated in influential papers Geyer and Thompson (1992); Geyer (1994). However, to the best of our knowledge they have not been studied (theoretically and practically) in high-dimensional Markov random fields previously. Thus, the main contribution of the paper is investigating their properties in model selection in the high-dimensional scenario and comparing them with the existing methods that are mentioned above. Model selection for undirected graphical models means finding the existing edges in the "sparse" graph that is a graph having relatively few edges (comparing to the total number of possible edges $\frac{d(d-1)}{2}$ and the sample size $n$).

The paper is organized as follows: in the next section we describe the Ising model and our approach to the problem that relates to minimization of the penalized MCMC approximation of the likelihood. The literature concerning this topic is also discussed. In section 3 we state main theoretical results. Details of practical implementation are given in section 4, while the results of simulation studies are presented in section 5. The conclusions can be found in section 6. Finally, the proofs are postponed to appendices A and B.

2. Model description and related works

In this section we introduce the Ising model and the proposed method. It also contains a review of the literature relating to this problem.

2.1. Ising Model and undirected graphs. Let $(V, E)$ be an undirected graph that consists of a set of vertices $V$ and a set of edges $E$. The random vector $Y = (Y(1), Y(2), \ldots, Y(d))$, that takes values in $Y$, is associated with this graph. In the paper we consider a special case
of the Ising model that $Y(s) \in \{-1, 1\}$ and the joint distribution of $Y$ is given by the formula

$$p(y|\theta^*) = \frac{1}{C(\theta^*)} \exp \left( \sum_{r<s} \theta^*_{rs} y(r) y(s) \right),$$

where the sum in (1) is taken over such pairs of indices $(r, s) \in \{1, \ldots, d\}^2$ that $r < s$. The vector $\theta^* \in \mathbb{R}^{d(d-1)/2}$ is a true parameter and $C(\theta^*)$ is a norming constant, i.e.

$$C(\theta^*) = \sum_{y \in \mathcal{Y}} \exp \left( \sum_{r<s} \theta^*_{rs} y(r) y(s) \right).$$

The norming constant is a finite sum but it consists of $2^d$ elements that makes it intractable even for a moderate size of $d$.

For convenience, we denote $J(y) = (y(r) y(s))_{r<s}$, so

$$p(y|\theta^*) = \frac{1}{C(\theta^*)} \exp \left[ (\theta^*)' J(y) \right].$$

**Remark 1.** The model (1) is a simplified version of the Ising model, for instance we omit an external field in (1). We have decided to restrict to the model containing only parameters $\theta^*_{rs}$, because interactions between random variables is what we focus on in the current paper. However, our results can be extended rather easily.

The Ising model has the following property: vertices $r$ and $s$ are not connected by an edge (i.e. $\theta^*_{rs} = 0$) means that variables $Y(r)$ and $Y(s)$ are conditionally independent given the other vertices. Therefore, we recognize the structure of the graph (its edges) by estimating the parameter $\theta^*$. Assume that $Y_1, \ldots, Y_n$ are independent random vectors from the model (1). Then the negative log-likelihood is

$$\ell_n(\theta) = -\frac{1}{n} \sum_{i=1}^n \theta' J(Y_i) + \log C(\theta).$$

The second term in (2) contains the norming constant so we cannot use (2) to estimate $\theta^*$. To overcome this problem one usually replaces the negative log-likelihood by its approximation and estimates $\theta^*$ using the minimizer of this approximation. We describe two main approaches that follow this idea.

The first method is the pseudolikelihood approach (Besag, 1974). It uses the following approximation of the density

$$p(y|\theta) = \prod_{s=1}^d p(y(s)|y(s-1), \ldots, y(1), \theta)$$

$$\approx \prod_{s=1}^d p(y(s)|y(-s), \theta),$$

where $y(-s) = (y(1), \ldots, y(s-1), y(s+1), \ldots, y(d))$. It is easy to verify that conditional distributions in (3) does not depend on the norming constant. Moreover, they are the same as in the standard model of logistic regression, in which all but one components of the vector $y$ play the role of covariates. However, it is clear that the quality of the approximation in (3) depends on the structure of the graph. Problems with efficiency of the pseudolikelihood method have been described in Besag (1977); Geyer and Thompson (1992) or Wu and Huffer (1997) in the context of spatial statistics.
The second approximation of (2) relates to Monte Carlo (MC) methods. Suppose that \( h(y) \) is an importance sampling distribution and note that

\[
C(\theta) = \sum_{y \in \mathcal{Y}} \exp \left[ \theta^T J(y) \right] = \sum_{y \in \mathcal{Y}} \frac{\exp \left[ \theta^T J(y) \right]}{h(y)} h(y) = \mathbb{E}_{Y \sim h} \frac{\exp \left[ \theta^T J(Y) \right]}{h(Y)}
\]

for each \( \theta \). Therefore, an MC approximation of the norming constant is

\[
\frac{1}{m} \sum_{k=1}^{m} \frac{\exp \left[ \theta^T J(Y_k) \right]}{h(Y_k)} \to C(\theta),
\]

where \( Y^1, \ldots, Y^m \) is a sample drawn from \( h \) or, which is more realistic and is considered in the current paper, \( Y^1, \ldots, Y^m \) is a Markov chain with \( h \) being a density of its stationary distribution. From LLN for Markov chains (Roberts and Rosenthal, 2004) we have

\[
\frac{1}{m} \sum_{k=1}^{m} \frac{\exp \left[ \theta^T J(Y_k) \right]}{h(Y_k)} \to C(\theta),
\]

when \( m \to \infty \) and \( \theta \) is fixed. Thus, the MCMC approximation of (2) is

\[
\ell_m^n(\theta) = -\frac{1}{n} \sum_{i=1}^{n} \theta^T J(Y_i) + \log \left( \frac{1}{m} \sum_{k=1}^{m} \frac{\exp \left[ \theta^T J(Y_k) \right]}{h(Y_k)} \right).
\]

A natural choice of the importance sampling distribution is \( h(y) = p(y|\psi) \) for some parameter \( \psi \). It leads to

\[
\ell_m^n(\theta) = -\frac{1}{n} \sum_{i=1}^{n} \theta^T J(Y_i) + \log \left( \frac{1}{m} \sum_{k=1}^{m} \frac{\exp \left[ (\theta - \psi)^T J(Y_k) \right]}{h(Y_k)} \right) + \log(C(\psi)).
\]

The last term in (7), that contains the unknown constant \( C(\psi) \), does not depend on \( \theta \), so it can be ignored while minimizing (7).

Our goal is selecting the true model (recognizing edges of a graph) in the high-dimensional setting. It means that the number of vertices \( d \) can be large. In fact, it can be much greater than the sample size, i.e. \( d = d_n \gg n \). To estimate the vector \( \theta^* \) we use penalized empirical risk minimization. The natural choice of the penalty would be the \( l_0 \)-penalty but it makes the procedure nonconvex and computationally expensive even for moderate values of \( d \). To avoid such problems we use the Lasso penalty and minimize a function

\[
\ell_m^n(\theta) + \lambda_m^n |\theta|_1,
\]

where \( |\theta|_1 = \sum_{r<s} |\theta_{rs}| \) and \( \lambda_m^n > 0 \) is a smoothing parameter that is a balance between minimizing the MCMC approximation and the penalty. We denote the minimizer of (8) by \( \hat{\theta}_n^m \). Notice that the function (8) that we minimize is convex in \( \theta \), because the Lasso penalty as well as the MCMC approximation (7) are convex function in \( \theta \). The latter follows from the fact that the Hessian of \( \ell_m^n(\theta) \), that is given explicitly in (19), is a weighted covariance matrix with positive weights that sum up to one. Convexity of the problem is important from the practical and theoretical point of view. First, every minimum of a convex function is the global minimum, so there are no local minimum problems. Second, convexity is also utilized in the proofs of the results contained in the paper.
2.2. Related works. Model selection in the high-dimensional Ising model is a popular topic and many papers investigating this problem using different methods can be found in the literature (Banerjee et al., 2008; Bresler et al., 2008; Lee et al., 2006; Ravikumar et al., 2010; Höfling and Tibshirani, 2009; Guo et al., 2010; Xue et al., 2012; Jalali et al., 2011). The significant part of them uses the pseudolikelihood approximation with the Lasso penalty. For instance, Ravikumar et al. (2010) applies it by considering $d$ logistic regression problems. They prove that this algorithm is model selection consistent, if some regularity conditions are satisfied. These conditions are similar to the “irrepresentable conditions” (Zhao and Yu, 2006) that are sufficient to prove an analogous property in the linear model. The pseudolikelihood method with the Lasso as a “joint” procedure is proposed in Höfling and Tibshirani (2009). Moreover, in the same paper one also proposes an “exact” algorithm that minimizes the negative log-likelihood with the Lasso penalty. However, this procedure also bases on the pseudolikelihood approximation. Model selection consistency of the latter algorithm has not been studied yet. The former procedure has this property that is showed in Guo et al. (2010) provided that conditions similar to Ravikumar et al. (2010) are satisfied. In Xue et al. (2012) the Lasso penalty is replaced by the SCAD penalty (Fan and Li, 2001) and theoretical properties of this algorithm are studied. In Jalali et al. (2011) one replaces restrictive irrepresentable conditions by weaker restricted strong convexity and smoothness conditions (Negahban et al., 2009) and proves model selection consistency of an algorithm that joints ideas from Ravikumar et al. (2010) and Zhang (2009). Namely, it performs $d$ separate logistic regression problems with the forward-backward greedy approach.

We have already mentioned weakness of the pseudolikelihood method as an approximation of the likelihood. Therefore, in the current paper we apply the MCMC method to overcome the intractable norming constant problem. Our experimental study (presented in section 5) confirms that estimators based on the MCMC approximation performs better in model selection than their pseudolikelihood analogs, unless the considered model has a simple structure. Obviously, in practice it cannot be verified beforehand. Our theoretical results are similar to those described in the previous paragraph that is we prove model selection consistency. But, in general, our assumptions are weaker than their analogs from the above-mentioned papers. The detailed comparison is given after Corollary 1 in Section 3. The obvious drawback of our approach is the need of additional simulations to obtain the MCMC sample. It makes our procedure computationally more complex, but at the same time more accurate in selecting the true model.

2.3. Notation. In further parts of the paper we need few notations. Most of them are collected in this subsection.

For simplicity, we write $\hat{\theta}$ and $\lambda$ instead of $\hat{\theta}_m$ and $\lambda_m$, respectively. Besides, we denote the number of estimated parameters in the model by $d = d(d - 1)/2$. Nonzero coordinates of $\theta^*$ are collected in the set $T$, and $T^c$ is a completion of $T$. Besides, $d_0 = |T|$ denotes the number of elements of the set $T$.

For a vector $a$ we denote its $l_\infty$-norm by $|a|_\infty = \max_k |a_k|$ and $a^{\otimes 2} = aa'$. The vector $a_T$ is the same as the vector $a$ on $T$ and zero otherwise. The $l_\infty$-norm of a matrix $\Sigma$ is denoted by $|\Sigma|_\infty = \max_{k,l} |\Sigma_{kl}|$.

Let us consider a Markov chain on space $S$ with transition kernel $P(x, \cdot)$ and stationary distribution $\pi$. We define the Hilbert space $L^2(\pi)$ as a space of functions that $\pi(f^2) < \infty$ and the inner product is given as $\langle f, g \rangle = \int_S f(x)g(x)\pi(dx)$. The linear operator $P$ on $L^2(\pi)$...
associated with transition kernel $P(x, \cdot)$ is defined as follows

$$Pf(x) = \int_S f(y)P(x,dy).$$

We say that the Markov chain has a spectral gap $1 - \kappa$ if and only if

$$\kappa = \sup \{ |\rho| : \rho \in Spec(P) \setminus \{1\} \},$$

where $Spec(\cdot)$ denotes the spectrum of an operator in $L^2(\pi)$. For reversible chains the spectral gap property is equivalent to geometric ergodicity of the chain, see (Kontoyiannis and Meyn, 2012; Roberts and Rosenthal, 1997).

In the paper we focus on the Gibbs sampler for the Ising model. However, theoretical results remain true for other MCMC algorithms as long as the spectral gap property is satisfied. The random scan Gibbs sampler for the Ising model is defined as follows: given $Y^{k-1}$, first we sample uniformly index $r$ and we draw $Y^k(r)$ from the distribution

$$P(Y^k(r) = 1) = \frac{\exp\{\psi'J(Y^+)^{(+)}\}}{\exp\{\psi'J(Y^+)^{(+)}\} + \exp\{\psi'J(Y^-)^{(-)}\}},$$

where $Y^+(s) = Y^-(s) = Y^{k-1}(s)$ for $s \neq r$ and $Y^+(r) = 1, Y^-(r) = -1$. For $s \neq r$ we set $Y^k(s) = Y^{k-1}(s)$.

Suppose that $Y^1, \ldots, Y^m$ is a Markov chain on $Y$ generated by a random scan Gibbs sampler, with stationary distribution with the density $h$ and the initial measure $\nu$ with the density $q$. Since the state space is finite and the chain is reversible then there exists a spectral gap $1 - \kappa$. Actually, $\kappa$ is the second greatest absolute value of eigenvalues of the transition matrix. We will need three quantities related to this Markov chain:

$$\beta_1 = \sqrt{\sum_{y \in Y} \frac{q^2(y)}{h(y)}} , \quad \beta_2 = \frac{1 - \kappa}{1 + \kappa} , \quad M = \max_{y \in Y} \frac{\exp((\theta^*)'J(y))}{h(y)C(\theta^*)}.$$

Roughly speaking, these three values can be viewed as: $\beta_1$ - how close the initial density is to the stationary one, $\beta_2$ - how fast the chain "mixes", $M$ - how close the importance sampling density is to the true density $1$.

### 3. Main results

In this section we state key results of the paper. In the first one (Theorem 1) we show that the estimation error of the minimizer of the MCMC approximation with the Lasso penalty can be controlled. In the second result (Corollary 1) we prove model selection consistency for the thresholded Lasso estimator (Zhou, 2009).

First, we introduce the cone invertibility factor that plays an important role in investigating properties of Lasso estimators. It is defined analogously to Ye and Zhang (2010); Huang and Zhang (2012); Huang et al. (2013) that concerns linear regression, generalized linear models and the Cox model, respectively. It is also closely related to the compatibility condition (van de Geer, 2008) or the restricted eigenvalues (Bickel et al., 2009). Thus, for $\xi > 1$ and the set $T$ we define a cone as

$$C(\xi, T) = \{ \theta : |\theta_T|_1 \leq \xi |\theta_T|_1 \}.$$

For a nonnegative definite matrix $\Sigma$ the cone invertibility factor is

$$F(\xi, T, \Sigma) = \inf_{0 \neq \theta \in C(\xi, T)} \frac{\theta' \Sigma \theta}{|\theta_T|_1 |\theta|_\infty}.$$
Cone invertibility factors of Hessians of two functions are crucial in our argumentation. The first function is the expectation of the negative log-likelihood (2), i.e.

\[ \mathbb{E} \ell_n(\theta) = -\theta' \mathbb{E} J(Y) + \log C(\theta) \]

and the second one is the MCMC approximation (6). We denote them as

\[ F(\xi, T) = \inf_{0 \neq \theta \in C(\xi, T)} \frac{\theta' \nabla^2 \log C(\theta) \theta}{|\theta_T|_1 |\theta|_\infty} \]

and

\[ \hat{F}(\xi, T) = \inf_{0 \neq \theta \in C(\xi, T)} \frac{\theta' \nabla^2 \ell_n(\theta) \theta}{|\theta_T|_1 |\theta|_\infty}, \]

respectively. Notice that only the values of \( \nabla^2 \log C(\theta) \) and \( \nabla^2 \ell_n(\theta) \) at the true parameter \( \theta^* \) are taken into consideration in (12) and (13).

Now we can state main results of the paper.

**Theorem 1.** Let \( \varepsilon > 0, \xi > 1 \) and \( \alpha(\xi) = 2 + \frac{\xi}{\xi - 1} \). If

\[ n \geq \frac{8(1 + \xi)^4 \alpha^2(\xi) \beta_0 M^2 \log (2\tilde{d}/\varepsilon)}{F^2(\xi, T)} \]

and

\[ m \geq \frac{64(1 + \xi)^4 \alpha^2(\xi) \beta_0 M^2 \log [2\tilde{d}(\tilde{d} + 1)\beta_1 / \varepsilon]}{F^2(\xi, T) \beta_2}, \]

then with probability at least \( 1 - 4\varepsilon \) we have the inequality

\[ |\hat{\theta} - \theta^*|_\infty \leq \frac{2\varepsilon \xi \alpha(\xi) \lambda}{(\xi + 1)(\alpha(\xi) - 2)F(\xi, T)}, \]

where

\[ \lambda = \frac{\xi + 1}{\xi - 1} \max \left( \frac{2 \log (2\tilde{d}/\varepsilon)}{n}, 8M \sqrt{\log \left( \frac{(2\tilde{d} + 1)\beta_1 / \varepsilon}{m\beta_2} \right)} \right). \]

**Corollary 1.** Suppose that conditions (14) and (15) are satisfied. Let \( \theta_{min}^r = \min_{r<s} |\theta_{rs}| \) and \( R_n^m \) denote the right-hand side of the inequality (16). Consider the Lasso estimator with a threshold \( \delta > 0 \) that is the set of nonzero coordinates of the final estimator is defined as \( \tilde{T} = \{ (r, s) : |\tilde{\theta}_{rs}| > \delta \} \). If \( \theta_{min}^r / 2 > \delta \geq R_n^m \), then

\[ P \left( \tilde{T} = T \right) \geq 1 - 4\varepsilon \]

The main results of the paper describe properties of estimators that are obtained by minimization of the MCMC approximation (6) with the Lasso penalty. Theorem 1 states that the estimation error of the Lasso estimator can be controlled. Roughly speaking, the estimation error is small, if the initial sample size and the MCMC sample size are large enough, the model is sparse and the cone invertibility factor \( F(\xi, T) \) is not too close to zero. The influence of the model parameters \( (n, d, \tilde{d}_0) \) as well as Monte Carlo parameters \( (m, \beta_1, \beta_2, M) \) on the results are explicitly stated. It is worth to emphasize that our results work in the high-dimensional scenario, i.e. the number of vertices \( d \) can be (much) greater than the sample size \( n \) provided that the model is sparse. Indeed, the condition (14) is satisfied even if \( d \sim O(e^{n^{c_1}}), \tilde{d}_0 \sim O(n^{c_2}) \) and \( c_1 + 2c_2 < 1 \). The condition (15), that relates to the MCMC sample size, is also reasonable. The number \( \beta_1 \) depends on the initial and stationary distributions. In general, its relation to the number of vertices is exponential. However, in (15)
it appears with the logarithm. Moreover, \( \beta_1 \) is also reduced using so called burn-in time, i.e. the beginning of the Markov chain trajectory is discarded. Next, the number \( \beta_2 \) is related to the spectral gap of a Markov chain. Under mild conditions the inverse of \( \beta_2 \) depends polynomially on \( d \), and under strong regularity conditions it can be reduced to \( O(d \log d) \) as in Mossel and Sly (2013). Finally, there is also the number \( M \) in the condition (15) that relates to the distance between the stationary distribution \( h(\cdot) \) and \( p(\cdot|\theta^*) \). Stating the explicit relation between \( M \) and the model seems to be difficult. However, the algorithm, that we propose to calculate \( \hat{\theta} \), is designed in such a way to minimize the impact of \( M \) on the results. The detailed implementation of the algorithm is given in section 4.

The estimation error of the Lasso estimator in Theorem 1 is measured in \( l_\infty \)-norm. Similarly to Huang et al. (2013), it can be extended to the general \( l_q \)-norm, \( q \geq 1 \). We omit it, because (16) is sufficient to obtain the second main result of the paper (Corollary 1). It states that the thresholded Lasso estimator is model selection consistent, if, additionally to (14) and (15), the nonzero parameters are not too small and the threshold is appropriately chosen.

We have already mentioned that there are many approaches to the high-dimensional Ising model. The significant part of them refers to the pseudolikelihood method. Now we compare conditions that are sufficient to prove model selection consistency in the current paper to those basing on the pseudolikelihood approximation in Ravikumar et al. (2010); Guo et al. (2010); Xue et al. (2012); Jalali et al. (2011). If we simplify regularity conditions in Theorem 1, Corollary 1 and forget about Monte Carlo parameters in (15), then we have:

(a) the cone invertibility factor condition is satisfied,
(b) the sample size should be sufficiently large, that is \( n > d^2_0 \log d \),
(c) the nonzero parameters should be sufficiently large, that is \( \theta^*_{\min} > \sqrt{\log d} \frac{d}{n} \).

In Ravikumar et al. (2010, Corollary 1) and Guo et al. (2010, Theorem 2) one needs stronger irrepresentable condition in (a), \( d_0 \) in the third power in (b) and additional factor \( \sqrt{d_0} \) in (c). To be precise, in Ravikumar et al. (2010) one considers \( d \) separate procedures, so their conditions do not depend on \( d_0 \) but on the maximum neighbourhood size that is smaller than \( d_0 \).

In Xue et al. (2012, Corollary 3.1 (2)) model selection consistency of Lasso estimators is proved with stronger conditions than ours. Namely, they are similar to Ravikumar et al. (2010) and Guo et al. (2010) but \( d_0 \) is reduced in the condition (c). Moreover, they also consider the pseudolikelihood approximation with the SCAD penalty and shows that the condition (a) seems to be superfluous in this case, see Xue et al. (2012, Corollary 3.1 (1)). However, using the SCAD penalty they minimize a nonconvex function to obtain an estimator, so they have to prove that the computed (local) minimizer is the desired theoretic local solution. Their approach can be viewed as a sequence of weighted Lasso problems, so they need auxiliary Lasso procedures to behave well. Therefore, the irrepresentable condition is assumed (Xue et al., 2012, Corollary 3.2).

The conditions sufficient for model selection consistency that are stated in Jalali et al. (2011, Theorem 2) are comparable to ours but also more restrictive. Instead of the condition (a) they consider a similar requirement called the restricted strong convexity condition. It is completed by the restricted strong smoothness condition. Moreover, in the the lower bound in the condition (c) they need an additional factor \( \sqrt{d_0} \) as well as the upper bound for \( \theta^*_{\min} \).

In the proof of Theorem 1 we use methods that are well-known while investigating properties of Lasso estimators as well as some new argumentation. The main novelty (and difficulty) is the use of the Monte Carlo sample that contains dependent vectors. The first part of our argumentation consists of two steps:
- the first step can be viewed as "deterministic". We apply methods that were developed in Ye and Zhang (2010); Huang and Zhang (2012); Huang et al. (2013) and strongly exploit convexity of the considered problem. These auxiliary results are stated in Lemma 1 and Lemma 2 in Appendix A.

- the second step is "stochastic". We state a probabilistic inequality that bounds the $l_\infty$-norm of the derivative of the MCMC approximation (6) at $\theta^*$, that is

$$\nabla \ell_n^m(\theta^*) = -\frac{1}{n} \sum_{i=1}^{n} J(Y_i) + \frac{\sum_{k=1}^{m} w_k(\theta^*) J(Y^k)}{\sum_{k=1}^{m} w_k(\theta^*)},$$

where

$$w_k(\theta) = \frac{\exp[\theta' J(Y^k)]}{h(Y^k)}, \quad k = 1, \ldots, m.$$  

Notice that (18) contains independent random variables $Y_1, \ldots, Y_n$ from the initial sample and the Markov chain $Y^1, \ldots, Y^m$ from the MC sample. Therefore, to obtain the exponential inequalities for the $l_\infty$-norm of (18), which are given in Lemma 3 and Corollary 2 in Appendix A, we apply the MCMC theory. In particular, we frequently use the following Hoeffding’s inequality for Markov chains (Miasojedow, 2014, Theorem 1.1).

**Theorem 2.** Let $Y^1, \ldots, Y^m$ be a Gibbs sampler defined in Subsection 2.3. Moreover, let $g : \mathcal{Y} \to \mathbb{R}$ be a bounded function and $\mu = \mathbb{E}_{Y \sim h(Y)}$ be a stationary mean value. Then for every $t > 0, m \in \mathbb{N}$ and an initial distribution $\varrho$

$$P \left( \left| \frac{1}{m} \sum_{k=1}^{m} g(Y^k) - \mu \right| > t \right) \leq 2 \beta_1 \exp \left( -\frac{\beta_2 m t^2}{|g|_\infty} \right),$$

where $|g|_\infty = \sup_{y \in \mathcal{Y}} |g(y)|$ and $\beta_1, \beta_2$ are defined in (10).

The second part of our argumentation relates to the fact that the Hessian of the MCMC approximation at $\theta^*$, that is

$$\nabla^2 \ell_n^m(\theta^*) = \frac{\sum_{k=1}^{m} w_k(\theta^*) J(Y^k)}{\sum_{k=1}^{m} w_k(\theta^*)} - \left[ \frac{\sum_{k=1}^{m} w_k(\theta^*) J(Y^k)}{\sum_{k=1}^{m} w_k(\theta^*)} \right] \otimes 2,$$

is random variable. Similar problems were considered in several papers investigating properties of Lasso estimators in the high-dimensional Ising model (Ravikumar et al., 2010; Guo et al., 2010; Xue et al., 2012) or the Cox model (Huang et al., 2013). We overcome this difficulty by bounding from below the cone invertibility factor $\tilde{F}(\xi, T)$ by nonrandom $F(\xi, T)$. Therefore, we need to prove that Hessians of (11) and (6) are close. It is obtained again using the MCMC theory in Lemma 4 and Corollary 3 in Appendix A.

Finally, the proofs of Theorem 1 and Corollary 1 are stated in Appendix B.

### 4. Details of implementation

In this section we describe in detail practical implementation of the algorithm analyzed in the previous section. The solution of the problem (8) depends on the choice of $\lambda$ in the penalty term and the parameter $\psi$ in the instrumental distribution. Finding “optimal” $\lambda$ and $\psi$ is difficult in practice. To overcome this problem we compute a sequence of minimizers
(\hat{\theta}_i)_i$ such that \( \hat{\theta}_i \) corresponds to \( \lambda = \lambda_i \) and the sequence \( (\lambda_i)_i \) is decreasing. We start with the greatest value \( \lambda_0 \) for which the entire vector \( \hat{\theta} \) is zero. For each value of \( \lambda_i, i > 0 \), we set \( \psi = \hat{\theta}_{i-1} \) and use the MCMC approximation (8) with \( Y^1, \ldots, Y^m \) given by a Gibbs sampler with the stationary distribution \( p(y|\hat{\theta}_{i-1}) \). This scheme exploits warm starts and leads to a more stable algorithm. The important property of this approach is that the chosen \( \psi = \hat{\theta}_{i-1} \) is usually close to \( \hat{\theta}_i \), because differences between consecutive \( \lambda_i \)'s are small. In our studies the final estimator \( \hat{\theta} \) is the element of the sequence \( (\hat{\theta}_i)_i \) that recognizes the true model in the best way (in general, we would use cross-validation or one of the information criteria). One believes that the final estimator \( \hat{\theta} = \hat{\theta}_1 \) is close to \( \theta^* \), therefore the chosen \( \psi = \hat{\theta}_{i-1} \) should also be similar to \( \theta^* \) that makes \( M \) in (10) close to one. Finally, notice that conditionally on the previous step our algorithm fits to the framework described in subsection 2.1.

The function \( \ell_n^m(\theta) \) is convex, so we can use proximal gradient algorithms to compute \( \hat{\theta}_i \) as a solution of (8) for a given \( \lambda_i \) and \( \psi \). Precisely, we use the FISTA algorithm with backtracking from Beck and Teboulle (2009). The whole procedure is summarized in Algorithm 1.

**Algorithm 1** MCMC Lasso for Ising model

Let \( \lambda_0 > \lambda_1 > \cdots > \lambda_K \) and \( \psi = 0 \).

for \( i = 1 \) to \( K \) do

Simulate \( Y^1, \ldots, Y^m \) using a Gibbs sampler with the stationary distribution \( p(y|\psi) \).

Run the FISTA algorithm to compute \( \hat{\theta}_i \) as

\[
\arg \min_{\theta} \{ \ell_n^m(\theta) + \lambda_i|\theta|_1 \}.
\]

Set \( \psi = \hat{\theta}_i \).

end for

The computational cost of a single step of the Gibbs sampler is dominated by computing probability (9), which is of the order \( O(r) \), where \( r \) is the maximal degree of vertices in a graph related to the stationary distribution. In the paper we focus on estimation of sparse graphs, so the proposed \( \lambda_i \)'s have to be sufficiently large to make \( \hat{\theta}_i \)'s sparse. Therefore, the degree \( r \) is rather small and the computational cost of generating \( Y^1, \ldots, Y^m \) is of order \( O(m) \). Next, we need to compute \( \ell_n^m(\theta) \) and its gradient. For an arbitrary Markov chain the cost of these computation is of the order \( O(d^2m) \). But when we use single site updates as in the Gibbs sampler we can reduce it to \( O(dm) \) by remembering which coordinate of \( Y^k \) where updated. Indeed, if we know that only the \( r \) coordinates are updated in the step \( Y^k \rightarrow Y^{k+1} \), then

\[
\theta' J(Y^{k+1}) = \theta' J(Y^k) + \sum_{s \in \mathcal{V}_{<r}} \left( \theta_{sr} [Y^{k+1}(s)Y^{k+1}(r) - Y^k(s)Y^k(r)] \right) + \sum_{s \in \mathcal{V}_{>r}} \left( \theta_{sr} [Y^{k+1}(s)Y^{k+1}(r) - Y^k(s)Y^k(r)] \right).
\]

Finally, it is well-known that FISTA (Beck and Teboulle, 2009) achieve accuracy \( \epsilon \) in \( O(\epsilon^{-\frac{1}{2}}) \) steps. So, the total cost of computing the solution for single \( \lambda_i \) with precision \( \epsilon \) is of order \( O(\epsilon^{-\frac{1}{2}}md) \). The further reduction of the cost can be obtained using sparsity of \( \hat{\theta}_{i-1} \) in computing \( \ell_n^m(\theta) \) and its gradient, and introducing active variables inside the FISTA algorithm.

In section 5 we compare estimators based on the MCMC approximation with the one based on the pseudolikelihood (both with the Lasso penalty). The latter was introduced in
Höfling and Tibshirani (2009) and we use the proximal gradient algorithm to compute it. It is worth to notice that the cost of computing the pseudolikelihood approximation and its gradient is of order $O(d^2n)$, because the pseudolikelihood is not a function of the sufficient statistic.

5. Simulated data

To illustrate the performance of the proposed method we simulate data sets in three scenarios:

M1 The first 5 vertices are correlated, while the remaining vertices are independent: $\theta^*_{rs} = \pm \vartheta$ for $r < s$ and $s = 2, 3, 4, 5$, other $\theta^*_{rs} = 0$. We consider two cases $\vartheta = 1$ and $\vartheta = 2$, and the signs are chosen randomly. Thus, the model dimension in this problem is 10.

M2 The first 10 vertices have the “chain structure”, and the rest are independent: $\theta^*_{r-1,r} = \pm 1$ for $r \leq 10$. Again the signs are chosen randomly and the model dimension is 10.

M3 There are two independent blocks of correlated vertices (each of the length 4): $\theta^*_{rs} = \pm 2$ for $r < s$, $s = 2, 3, 4$ and for $5 \leq r < s$, $s = 6, 7, 8$. The signs are chosen randomly and the model dimension is 12.

Table 1. The performance of the pseudolikelihood and the MCMC approximation with the Lasso (bottom) and the thresholded Lasso (top) for $M1$ with $\vartheta = 1$.
The model $M1$ corresponds to the case that the dependence structure is relatively complex and the approximation by the pseudolikelihood can behave badly. The model $M2$ has a chain structure, so it is known that the pseudolikelihood approximation works well. Finally, the last scenario is a compromise between first two models.

For each of model we draw 20 configuration of signs, so we get 20 vectors $\theta^*$ for each model. We consider the following cases: $d = 20, 50$ and $n = 50, 100, 200, 500, 1000$. For each configuration of the model, the number of vertices $d$ and the number of observation $n$ we sample 20 replications of data sets. For sampling a data set we use a final configuration of independent Gibbs sampler of the length $10^6$.

Based on preliminary runs we set $m = 10^5$. Our choice of $\lambda$ and the threshold is related to Theorem 1 and Corollary 1. For models $M1$ and $M3$ we run the algorithm with $\lambda = c_1 \sqrt{\log(d(d-1)/n)}$ with $c_1$ being a sequence from 1 to 4 with the difference 0.25. In the model $M2$ this penalty was too small, so we increase the range of $c_1$ to 8. For the thresholded Lasso we use a threshold of the form $c_2 \sqrt{\log(d(d-1)/n)}$ with $c_2$ being a sequence of consecutive numbers from 0 up to 0.16 by 0.04. For each $c_1$ for the Lasso and a pair of parameters $(c_1, c_2)$ for the thresholded Lasso we compute the frequency of finding exactly the

| $d$ | $n$ | $Pseudolikelihood$ | $MCMC$ |
|-----|-----|---------------------|--------|
|     |     | True Model  | $c_1$ | $c_2$ | True Model  | $c_1$ | $c_2$ |
| 20  | 50  | 0.5075     | 3.5   | 0.00  | 0.5425     | 2.0   | 0.00  |
| 100 |     | 0.4950     | 3.5   | 0.00  | 0.5475     | 2.0   | 0.00  |
| 200 |     | 0.5200     | 1.0   | 0.20  | 0.5475     | 2.0   | 0.00  |
| 500 |     | 0.5325     | 3.0   | 0.04  | 0.5800     | 1.0   | 0.12  |
| 1000|     | 0.5700     | 3.0   | 0.00  | 0.6500     | 1.0   | 0.16  |
| 50  | 50  | 0.5050     | 3.5   | 0.00  | 0.5400     | 2.0   | 0.00  |
| 100 |     | 0.4825     | 3.5   | 0.00  | 0.5450     | 2.0   | 0.00  |
| 200 |     | 0.4625     | 1.0   | 0.20  | 0.5450     | 2.0   | 0.00  |
| 500 |     | 0.5300     | 2.5   | 0.04  | 0.5550     | 2.5   | 0.00  |
| 1000|     | 0.5263     | 3.0   | 0.00  | 0.6404     | 1.0   | 0.20  |

| $d$ | $n$ | $Pseudolikelihood$ | $MCMC$ |
|-----|-----|---------------------|--------|
|     |     | True Model  | $c_1$ | $c_2$ | True Model  | $c_1$ |
| 20  | 50  | 0.5075     | 3.5   |       | 0.5425     | 2.0   |
| 100 |     | 0.4950     | 3.5   |       | 0.5475     | 2.0   |
| 200 |     | 0.4625     | 3.5   |       | 0.5475     | 2.0   |
| 500 |     | 0.5175     | 3.0   |       | 0.5500     | 2.0   |
| 1000|     | 0.5700     | 3.0   |       | 0.5750     | 2.0   |
| 50  | 50  | 0.5050     | 3.5   |       | 0.5400     | 2.0   |
| 100 |     | 0.4825     | 3.5   |       | 0.5450     | 2.0   |
| 200 |     | 0.4600     | 3.5   |       | 0.5450     | 2.0   |
| 500 |     | 0.5125     | 4.0   |       | 0.5550     | 2.5   |
| 1000|     | 0.5263     | 3.0   |       | 0.5526     | 2.5   |

Table 2. The performance of the pseudolikelihood and the MCMC approximation with the Lasso (bottom) and the thresholded Lasso (top) for $M1$ with $\vartheta = 2$. 

true model, and we choose a pair that maximizes it. Next, we proceed in the same way with the pseudolikelihood instead of the MCMC approximation.

Results for the first model are summarized in Table 1 and Table 2 for $\vartheta = 1$ and $\vartheta = 2$, respectively. We observe that in this model the MCMC approximation outperforms the pseudolikelihood approximation. The dominance of MCMC is especially evident for $\vartheta = 1$, but in the case $\vartheta = 2$ it is also significant. Moreover, looking at the Table 1 we notice that thresholding does not improve the quality of procedures in model selection. However, for $\vartheta = 2$ and large $n$ the improvement is observed.

In Table 3 we present results for the second model. The dependence structure is simple, so the pseudolikelihood approximation is accurate. Therefore, model selection of estimators based on the pseudolikelihood is very good. Nevertheless, the MCMC approximation with the Lasso (for large $n$) and the thresholded Lasso behaves similarly to the pseudolikelihood analogue. Besides, thresholded Lasso estimators for both methods work better than Lasso estimators (especially for small $n$).

Results for the third model are presented in Table 4. For large sample sizes both methods work well, but the MCMC approximation performs better for small sample sizes. The improvement related to thresholding is also observed.

Table 3. The performance of the pseudolikelihood and the MCMC approximation with the Lasso (bottom) and the thresholded Lasso (top) for $M_2$. 

| d  | n  | Pseudolikelihood | MCMC |
|----|----|------------------|------|
|    |    | True Model | $c_1$ | $c_2$ | True Model | $c_1$ | $c_2$ |
| 20 | 50 | 0.3725 | 1.0 | 0.12 | 0.1825 | 1 | 0.12 |
| 100|    | 0.9050 | 1.0 | 0.24 | 0.7300 | 1 | 0.24 |
| 200|    | 1.0000 | 2.5 | 0.20 | 0.9700 | 1 | 0.36 |
| 500|    | 1.0000 | 4.0 | 0.16 | 1.0000 | 4 | 0.32 |
| 1000|   | 1.0000 | 3.5 | 0.24 | 1.0000 | 4 | 0.36 |
| 50 | 50 | 0.2000 | 2.5 | 0.00 | 0.1175 | 1 | 0.08 |
| 100|    | 0.8300 | 2.0 | 0.08 | 0.6125 | 1 | 0.20 |
| 200|    | 0.9975 | 1.0 | 0.28 | 0.9300 | 1 | 0.32 |
| 500|    | 1.0000 | 4.0 | 0.16 | 0.9950 | 3 | 0.36 |
| 1000|  | 1.0000 | 4.0 | 0.20 | 0.9950 | 4 | 0.08 |

| d  | n  | Pseudolikelihood | MCMC |
|----|----|------------------|------|
|    |    | True Model | $c_1$ |
| 20 | 50 | 0.2300 | 2.5 |
| 100|    | 0.7375 | 4.0 |
| 200|    | 0.7800 | 4.0 |
| 500|    | 0.9735 | 6.0 |
| 1000|   | 0.9980 | 8.0 |
| 50 | 50 | 0.2000 | 2.5 |
| 100|    | 0.6975 | 3.5 |
| 200|    | 0.8825 | 4.0 |
| 500|    | 0.9920 | 6.0 |
| 1000|  | 1.0000 | 7.5 |
Table 4. The performance of the pseudolikelihood and the MCMC approximation with the Lasso (bottom) and the thresholded Lasso (top) for $M3$.

| $d$ | $n$ | Pseudolikelihood | MCMC |
|-----|-----|------------------|------|
|     |     | True Model | $c_1$ | $c_2$ | True Model | $c_1$ | $c_2$ |
| 20  | 50  | 0.6850  | 3.5   | 0.00  | 0.7525  | 2.0   | 0.00  |
| 100 |     | 0.8875  | 2.0   | 0.08  | 0.7525  | 2.0   | 0.00  |
| 200 |     | 0.9975  | 3.0   | 0.04  | 0.9800  | 1.0   | 0.12  |
| 500 |     | 1.0000  | 3.5   | 0.00  | 1.0000  | 2.0   | 0.00  |
| 1000|     | 1.0000  | 3.5   | 0.00  | 1.0000  | 2.5   | 0.00  |
| 50  | 50  | 0.7000  | 3.0   | 0.00  | 0.7500  | 1.5   | 0.04  |
| 100 |     | 0.7400  | 1.5   | 0.12  | 0.7525  | 2.0   | 0.00  |
| 200 |     | 0.9875  | 2.5   | 0.08  | 0.8450  | 1.0   | 0.12  |
| 500 |     | 1.0000  | 4.0   | 0.00  | 1.0000  | 1.0   | 0.24  |
| 1000|     | 1.0000  | 3.5   | 0.00  | 1.0000  | 2.0   | 0.16  |

6. Conclusions

In the paper we consider a problem of structure learning of binary Markov random fields. We base estimation of model parameters on the Lasso penalized Monte Carlo approximation of the likelihood. In the theoretical part of the paper we show that the proposed procedure recognizes the true dependence structure with high probability. The regularity conditions that we need are not restrictive and are weaker than assumptions used in the pseudolikelihood approach. Moreover, the theoretical results are completed by simulation experiments. They confirm that the quality of the pseudolikelihood approximation depends strongly on the complexity of the graph structure, while the MCMC approximation is able to find the true model without regard for it.

The results of the current paper can be easily extended to other discrete Markov random fields. There are also some non-trivial issues that are not discussed in the paper, for instance how the parameter $\lambda$ should be chosen in practice (cross-validation, information criteria etc.). The evaluation of the prediction error of the procedure is also a difficult problem as well as investigating the model (1) with predictors. Clearly, these all problems need detailed studies.
Acknowledgements

Błażej Miasojedow and Wojciech Rejchel are supported by Polish National Science Center grants no. 2015/17/D/ST1/01198 and no. 2014/12/S/ST1/00344, respectively.

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Appendix A. Auxiliary results

In this section we formulate lemmas that are needed to prove main results of the paper. The roles that they play are described in detail at the end of section 3. The first lemma is borrowed from Huang et al. (2013, Lemma 3.1).

Lemma 1. Let \( \hat{\theta} = \theta - \theta^* \), \( z^* = |\nabla \ell_m(\theta^*)|_\infty \) and

\[
D(\hat{\theta}, \theta) = (\hat{\theta} - \theta)' \left[ \nabla \ell_m(\hat{\theta}) - \nabla \ell_m(\theta) \right].
\]

Then

\[
(\lambda - z^*)|\hat{\theta}_T|_1 \leq D(\hat{\theta}, \theta) + (\lambda - z^*)|\hat{\theta}_T|_1 \leq (\lambda + z^*)|\hat{\theta}_T|_1.
\]

Besides, for arbitrary \( \xi > 1 \) on the event

\[
\Omega_1 = \left\{ |\nabla \ell_m(\theta^*)|_\infty \leq \frac{\xi - 1}{\xi + 1} \lambda \right\}
\]

the random vector \( \tilde{\theta} \) belongs to the cone \( C(\xi, T) \).
Proof. The proof is the same as the proof of Huang et al. (2013, Lemma 3.1). It is quoted here to make the paper complete.

Convexity of the MCMC approximation $\ell_n^m(\theta)$ easily implies the first inequality in (20). The same property combined with convexity of the Lasso penalty gives us that zero has to belong to the subgradient of (8) at the minimizer $\hat{\theta}$, i.e.

\[
\begin{align*}
\nabla_r \ell_n^m(\hat{\theta}) &= -\lambda \text{sign}(\hat{\theta}_r), & \text{if } \hat{\theta}_r \neq 0 \\
|\nabla_r \ell_n^m(\hat{\theta})| &\leq \lambda, & \text{if } \hat{\theta}_r = 0,
\end{align*}
\]

where we use $\nabla \ell_n^m(\theta) = \left(\nabla_r \ell_n^m(\theta)\right)_{r < s}$ and $\text{sign}(t) = 1$ for $t > 0$, $\text{sign}(t) = -1$ for $t < 0$, $\text{sign}(t) = 0$ for $t = 0$. Using (22) and properties of the $l_1$-norm we obtain that

\[
D(\hat{\theta}, \theta^*) = \sum_{(r,s) \in T} \hat{\theta}_{rs} \nabla_r \ell_n^m(\theta^* + \hat{\theta}) + \sum_{(r,s) \in T^c} \hat{\theta}_{rs} \nabla_r \ell_n^m(\theta^* + \hat{\theta}) - \hat{\theta}^r \ell_n^m(\theta^*)
\]

\[
\leq \lambda \sum_{(r,s) \in T} |\hat{\theta}_{rs}| - \lambda \sum_{(r,s) \in T^c} |\hat{\theta}_{rs}| + |\hat{\theta}| \xi
\]

\[
\leq \lambda |\hat{\theta}| |\xi - 1| + z^* |\hat{\theta}| |\xi + 1| + z^* |\hat{\theta}| |\xi - 1|
\]

Thus, the second inequality in (20) is also established. To prove the last claim of the lemma notice that on the event $\Omega_1$ we obtain from (20)

\[
|\hat{\theta}| |\xi - 1| \leq \frac{\lambda + z^*}{\lambda - z^*} |\hat{\theta}| |\xi + 1| \leq \xi |\hat{\theta}| |\xi - 1|
\]

$\square$

The second lemma is an adaptation of Huang et al. (2013, Theorem 3.1) to our problem.

Lemma 2. Let $\xi > 1$. Moreover, let us denote $\tau = \frac{\xi + 1}{\xi} F(\xi, T)$ and an event

\[
\Omega_2 = \left\{ \tau < e^{-1} \right\}
\]

Then $\Omega_1 \cap \Omega_2 \subset A$, where

\[
A = \left\{ |\hat{\theta} - \theta^*| \leq \frac{2\xi \eta \lambda}{(\xi + 1) F(\xi, T)} \right\},
\]

where $\eta < 1$ is the smaller solution of the equation $\eta e^{-\eta} = \tau$.

Proof. Suppose we are on the event $\Omega_1 \cap \Omega_2$. Denote again $\hat{\theta} = \hat{\theta} - \theta^*$ and notice that $\theta = \frac{\hat{\theta}}{|\hat{\theta}|} \in C(\xi, T)$ by Lemma 1. Consider the function

\[
g(t) = \theta^* \nabla \ell_n^m(\theta^* + t \theta) - \theta^* \nabla \ell_n^m(\theta^*)
\]

for each $t \geq 0$. This function is nondecreasing, because $\ell_n^m(\cdot)$ is convex. Thus, we obtain $g(t) \leq g(|\hat{\theta}|_1)$ for every $t \in (0, |\hat{\theta}|_1)$. On the event $\Omega_1$ and from Lemma 1 we have that

\[
|\hat{\theta}|_1 \leq \frac{2\lambda}{\xi + 1} |\theta|_1.
\]

In further argumentation we consider all nonnegative $t$ satisfying (25) that is an interval $[0, \bar{t}]$ for some $\bar{t} > 0$. Proceeding similarly to the proof of Huang et al. (2013, Lemma 3.2) we obtain

\[
t^2 |\nabla \ell_n^m(\theta^* + t \theta) - \nabla \ell_n^m(\theta^*)| \geq t^2 \exp(-\gamma t) \theta^* \nabla^2 \ell_n^m(\theta^*) \theta,
\]

where $\gamma > 0$ is the parameter of the function $\ell_n^m(\cdot)$.
where \( \gamma_{t \theta} = t \max_k, l |\theta' J(Y^k) - \theta' J(Y^l)| \leq 2t \), because \( J(Y^k) = (Y^k(r) Y^k(s))_{rs} \) and \( |\theta|_1 = 1 \). Therefore, the right-hand side in (26) can be lower bounded by
\[ (27) \quad t^2 \exp(-2t') \ell_m^m(\theta^\ast) \theta. \]
Using the definition of \( \bar{F}(\xi, T) \), the fact that \( \theta \in \mathcal{C}(\xi, T) \), the bound (27) and (25) we obtain
\[
\begin{align*}
t \exp(-2t) \frac{\bar{F}(\xi, T)|\theta|_T^2}{d_0} & \leq t \exp(-2t') \theta' \ell_m^m(\theta^\ast) \theta \\
& \leq \theta' [\nabla \ell_m^m(\theta^\ast + t\theta) - \nabla \ell_m^m(\theta^\ast)] \\
& \leq 2 \lambda \xi |\theta_T|_1 - \frac{2 \lambda}{\xi + 1} |\theta_T|_1 \\
& \leq \frac{\lambda}{(\xi + 1)} |\theta_T|_1^2 / 2.
\end{align*}
\]
So, every \( t \) satisfying (25) has to fulfill the inequality \( 2t \exp(-2t) \leq \tau \). In particular, \( 2 \tilde{t} \exp(-2\tilde{t}) \leq \tau \). We are on \( \Omega_2 \), so it implies that \( 2 \tilde{t} \leq \eta \), where \( \eta \) is the smaller solution of the equation \( \eta \exp(-\eta) = \tau \). We know also that \( |\theta|_1 \leq t \), so
\[
|\theta|_1 \exp(-\eta) \leq \tilde{t} \exp(-2\tilde{t}) \leq \frac{\tilde{t} \exp(-2\tilde{t}) \theta' \ell_m^m(\theta^\ast) \theta}{\bar{F}(\xi, T)|\theta_T|_1|\theta|_\infty} \\
\leq \frac{\theta' [\nabla \ell_m^m(\theta^\ast + \tilde{t}\theta) - \nabla \ell_m^m(\theta^\ast)]}{\bar{F}(\xi, T)|\theta_T|_1|\theta|_\infty} \\
\leq \frac{2 \lambda \xi}{(\xi + 1) \bar{F}(\xi, T)|\theta|_\infty},
\]
where we have used bounds (27) and (25). Using the equality \( |\theta|_\infty = \frac{|\theta|_\infty}{|\theta|_1} \), we finish the proof.

**Lemma 3.** For every natural \( n, m \) and positive \( t \)
\[
P(|\nabla \ell_m^m(\theta^\ast)|_\infty \leq t) \geq 1 - 2 \tilde{t} \exp(-nt^2/8) - \beta_1 \exp \left( -\frac{m \beta_2}{4M^2} \right) - 2 \tilde{d} \beta_1 \exp \left( -\frac{t^2 m \beta_2}{64M^2} \right).
\]

**Proof.** We can rewrite \( \nabla \ell_m^m(\theta^\ast) \) as
\[
(28) \quad \nabla \ell_m^m(\theta^\ast) = - \left( \frac{1}{n} \sum_{i=1}^n J(Y_i) - \frac{\nabla C(\theta^\ast)}{C(\theta^\ast)} \right) + \frac{1}{m} \sum_{k=1}^m w_k(\theta^\ast) \left[ J(Y^k) - \frac{\nabla C(\theta^\ast)}{C(\theta^\ast)} \right]
\]
Notice that the first therm in (28) depends only on the initial sample \( Y_1, \ldots, Y_n \) and is an average of i.i.d random variables. The second term depends only on the MCMC sample \( Y_1, \ldots, Y^m \). We start the analysis with the former one. Using Hoeffding’s inequality we obtain for each natural \( n \), positive \( t \) and a pair of indices \( r < s \)
\[
P \left( \left| \frac{1}{n} \sum_{i=1}^n J_r(Y_i) - \frac{\nabla r \ast C(\theta^\ast)}{C(\theta^\ast)} \right| > t/2 \right) \leq 2 \exp(-nt^2/8).
\]
Therefore, by the union bound we have
\[
(29) \quad P \left( \left| \frac{1}{n} \sum_{i=1}^n J(Y_i) - \frac{\nabla C(\theta^\ast)}{C(\theta^\ast)} \right|_\infty > t/2 \right) \leq 2 \tilde{d} \exp(-nt^2/8).
\]
Next, we investigate the second expression in (28). Its denominator is an average that depends on the Markov chain. To handle it we can use Theorem 2 in section 3. Notice that 
\[
\frac{\exp[h(y)]}{h(y)} \leq MC(\theta^*) \text{ for every } y \text{ and } E_{Y \sim h} \frac{\exp[h(Y)]}{h(Y)} = C(\theta^*). \]
Therefore, for every positive \( m, n \)
\[
P \left( \frac{1}{m} \sum_{k=1}^{m} w_k(\theta^*) \geq C(\theta^*)/2 \right) \geq 1 - \beta_1 \exp \left( -\frac{m\beta_2}{4M^2} \right).
\]
Finally, we bound the \( l_\infty \)-norm of the numerator of the second term in (28). We fix a pair of indices \( r < s \). It is not difficult to calculate that
\[
E_{Y \sim h} \left[ \exp \left( (\theta^*)^t J(Y) \right) \right] \left( J_{rs}(Y) - \frac{\nabla_{rs} C(\theta^*)}{C(\theta^*)} \right) = 0
\]
and for every \( y \)
\[
\frac{\exp((\theta^*)^t J(y))}{h(y)} \left| J_{rs}(y) - \frac{\nabla_{rs} C(\theta^*)}{C(\theta^*)} \right| \leq 2MC(\theta^*).
\]
From Theorem 2 we obtain for every positive \( t \)
\[
\left| \frac{1}{m} \sum_{k=1}^{m} w_k(\theta^*) \left[ J_{rs}(Y^k) - \frac{\nabla_{rs} C(\theta^*)}{C(\theta^*)} \right] \right| \geq tC(\theta^*)/4
\]
with probability at least \( 1 - 2\beta_1 \exp \left( -\frac{t^2m\beta_2}{4M^2} \right) \). Using union bounds we estimate the numerator of the second expression in (28). This fact and (30) imply that for every positive \( t \) and natural \( n, m \) with probability at least \( 1 - \beta_1 \exp \left( -\frac{m\beta_2}{4M^2} \right) - 2\tilde{d}\beta_1 \exp \left( -\frac{t^2m\beta_2}{4M^2} \right) \) we have
\[
\left| \frac{1}{m} \sum_{k=1}^{m} w_k(\theta^*) \left[ J(Y^k) - \frac{\nabla C(\theta^*)}{C(\theta^*)} \right] \right| \leq t/2.
\]
Taking (29) and (31) together we finish the proof.

\[\square\]

**Corollary 2.** Let \( \varepsilon > 0, \xi > 1 \) and
\[
\lambda = \frac{\xi + 1}{\xi - 1} \max \left( 2\sqrt{\frac{2\log(2d/\varepsilon)}{n}}, 8M \sqrt{\frac{\log \left( (2\tilde{d} + 1)\beta_1/\varepsilon \right)}{m\beta_2}} \right).
\]

Conditions (14) and (15) imply
\[
P(\Omega_1) \geq 1 - 2\varepsilon.
\]

**Proof.** We take \( t = \frac{\xi - 1}{\xi + 1} \lambda \) in Lemma 3. \[\square\]

**Lemma 4.** For every \( n, m \) and positive \( t \)
\[
P \left( \left| \nabla^2 \ell_n^m (\theta^*) - \nabla^2 \log C(\theta^*) \right|_\infty \leq t \right) \geq 1 - 2\beta_1 \exp \left( -\frac{m\beta_2}{4M^2} \right) - 2\tilde{d}(\tilde{d} + 1)\beta_1 \exp \left( -\frac{t^2m\beta_2}{256M^2} \right).
\]
Proof. To estimate the $l_\infty$-norm of the matrix difference in (32) we bound $l_\infty$-norms of two matrices:

$$\sum_{k=1}^{m} \frac{w_k(\theta^*)J(Y^k)\otimes 2}{\sum_{k=1}^{m} w_k(\theta^*)} - \frac{\nabla^2 C(\theta^*)}{C(\theta^*)} = \frac{1}{m} \sum_{k=1}^{m} w_k(\theta^*) \left[ J(Y^k)\otimes 2 - \frac{\nabla^2 C(\theta^*)}{C(\theta^*)} \right]$$

and

$$\left[ \left( \frac{1}{m} \sum_{k=1}^{m} w_k(\theta)J(Y^k) \right) \otimes 2 - \left( \frac{\nabla C(\theta^*)}{C(\theta^*)} \right)^\otimes 2 \right].$$

The denominator of the right-hand side of (33) has been estimated in the proof of Lemma 3, so we bound the numerator. We can calculate that

$$\mathbb{E}_{Y \sim h} \left[ \frac{\exp((\theta^*)^\prime J(Y))}{h(Y)} \left( J(Y)\otimes 2 - \frac{\nabla^2 C(\theta^*)}{C(\theta^*)} \right) \right] = 0$$

and for every $y$ and two pairs of indices $r < s, r' < s'$ we have

$$\frac{\exp((\theta^*)^\prime J(y))}{h(Y)} \left| J_{rs}(y)J_{r's'}(y) - \frac{\nabla_{rs,s'}C(\theta^*)}{C(\theta^*)} \right| \leq 2MC(\theta^*).$$

Using the union bound and (30) we upper-bound the $l_\infty$-norm of the right-hand side of (33) by $t/2$ with probability at least

$$1 - \beta_1 \exp \left( -\frac{m\beta_2}{4M^2} \right) - 2d\beta_1 \exp \left( -\frac{t^2m\beta_2}{64M^2} \right).$$

The last step of the proof is handling with the $l_\infty$-norm of (34). This expression can be upper-bounded by

$$\left| \sum_{k=1}^{m} \frac{w_k(\theta)J(Y^k)}{\sum_{k=1}^{m} w_k(\theta)} \right| \frac{\nabla C(\theta^*)}{C(\theta^*)} \left( \frac{\left| \sum_{k=1}^{m} w_k(\theta)J(Y^k) \right|}{\sum_{k=1}^{m} w_k(\theta)} \right) \left| \frac{\nabla C(\theta^*)}{C(\theta^*)} \right|_{\infty}.$$ 

The first term in (35) has been bounded with high probability in the proof of Lemma 3. The remaining two can be easily estimated by one. Therefore, for every positive $t$ the $l_\infty$-norm of (34) is not greater than $t/2$ with probability at least

$$1 - \beta_1 \exp \left( -\frac{m\beta_2}{4M^2} \right) - 2d\beta_1 \exp \left( -\frac{t^2m\beta_2}{256M^2} \right).$$

Putting together this fact and the bound of (33) we finish the proof. \(\square\)

**Corollary 3.** If (15), then for every $\varepsilon > 0$ the following inequality

$$\bar{F}(\xi, T) \geq F(\xi, T) - 16\bar{d}_0(1 + \xi)^2M \sqrt{\log \left[ \frac{2d(\bar{d} + 1)\beta_1/\varepsilon}{m\beta_2} \right] \frac{\log [2d(\bar{d} + 1)\beta_1/\varepsilon]}{m\beta_2}}$$

has probability at least $1 - 2\varepsilon$. 
Proof. We take
\[ t = 16M \sqrt{\frac{\log [2d(\bar{d} + 1)\beta_1 / \varepsilon]}{m\beta_2}} \]
in Lemma 4 and use Huang et al. (2013, Lemma 4.1 (ii)). □

Appendix B. Proofs of main results

Proof of Theorem 1. Fix \( \varepsilon > 0, \xi > 1 \) and denote \( \gamma = \gamma(\xi) = \frac{\alpha(\xi) - 2}{\alpha(\xi)} \in (0,1) \). First, from Corollary 2 we know that \( P(\Omega_1) \geq 1 - 2\varepsilon \). Using the condition (15) we obtain that
\[
F(\xi, T) - 16\bar{d}_0(1 + \xi)2M \sqrt{\frac{\log [2d(\bar{d} + 1)\beta_1 / \varepsilon]}{m\beta_2}} \geq \gamma F(\xi, T).
\]
Therefore, from Corollary 3 we have that \( P(\bar{F}(\xi, T) \geq \gamma F(\xi, T)) \geq 1 - 2\varepsilon \). It is not difficult to calculate that
\[
\frac{(1 + \xi)d_0 \lambda}{\gamma F(\xi, T)} \leq e^{-1},
\]
so we have also \( P(\Omega_2) \geq 1 - 2\varepsilon \). To finish the proof we use Lemma 2 (with \( \eta = 1 \) for simplicity) and again bound \( \bar{F}(\xi, T) \) from above by \( \gamma F(\xi, T) \) in the event \( A \) defined in (24).

Proof of Corollary 1. The proof is a simple consequence of the uniform bound (16) obtained in Theorem 1. Indeed, for an arbitrary pair of indices \((r, s) \notin T\) we obtain
\[
|\hat{\theta}_{rs}| = |\hat{\theta}_{rs} - \theta^*_rs| \leq R^m_n,
\]
so \((r, s) \notin \hat{T} \). Analogously, if we take a pair \((r, s) \in T\), then
\[
|\hat{\theta}_{rs}| \geq |\theta^*_rs| - |\theta_{rs} - \theta^*_rs| > 2\delta - R^m_n \geq \delta.
\]
□

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