Towards Optimal Sparse Inverse Covariance Selection through Non-Convex Optimization

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Abstract

We study the problem of reconstructing the graph of a sparse Gaussian Graphical Model from independent observations, which is equivalent to finding non-zero elements of an inverse covariance matrix. For a model of size $p$ and maximum degree $d$, information theoretic lower bounds established in prior works require that the number of samples needed for recovering the graph perfectly is at least $d\log p/\kappa^2$, where $\kappa$ is the minimum normalized non-zero entry of the inverse covariance matrix. Existing algorithms require additional assumptions to guarantee perfect graph reconstruction, and consequently, their sample complexity is dependent on parameters that are not present in the information theoretic lower bound. We propose an estimator, called SLICE, that consists of a cardinality constrained least-squares regression followed by a thresholding procedure. Without any additional assumptions we show that SLICE attains a sample complexity of $\frac{d^3}{\kappa^2}d\log p$, which differs from the lower bound by only a factor proportional to $1/\kappa^2$ and depends only on parameters present in the lower bound.

1. Introduction

Graphical Models (GMs) are powerful and intuitive modelling tools to represent the dependency structure of a set of random variables. In undirected graphical models, also known as Markov Random Fields (MRFs), the sparsity pattern of the graph succinctly captures the conditional independence between the variables through the \textit{separation} property. In this paper, we study Gaussian Graphical Models (GGMs) that are described on a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ with $|\mathcal{V}| = p$ and with maximum degree $d$. The probability density function of the associated multivariate Gaussian distribution is given by

$$
P(x) = \frac{\sqrt{\det(\Theta)}}{(2\pi)^{\frac{p}{2}}} \exp \left( -\frac{1}{2} \sum_{i \in \mathcal{V}} \theta_{ii} x_i^2 - \sum_{(i,j) \in \mathcal{E}} \theta_{ij} x_i x_j \right),$$

where $\Theta$ is the inverse covariance matrix, also known as the \textit{precision matrix}. For the special case of GGMs, the sparsity pattern of the precision matrix $\Theta$ is identical to that of the graph $\mathcal{G}$, i.e., $(i, j) \in \mathcal{E}$ iff $\theta_{ij} \neq 0$.

We consider the problem of reconstructing the underlying graph $\mathcal{G}$ of an unknown sparse GGM from $n$ i.i.d. samples drawn from the distribution described by Eq. (1), where samples $\{x^k_i\}_{i \in \mathcal{V}}$ are indexed by $k \in \{1, \ldots, n\}$. We are interested in finding tractable algorithms that provide an estimate $\hat{\mathcal{G}}$ of the graph $\mathcal{G}$ using as few samples as possible. Moreover we require that with high-probability the graph should be perfectly reconstructed with a given confidence, meaning that for a prescribed $\delta > 0$,

$$
P(\hat{\mathcal{G}} = \mathcal{G}) > 1 - \delta.$$  

This problem has attracted great interest due to its application in numerous fields including protein interactions (Friedman, 2004; Jones et al., 2012), gene regulatory networks (Basso et al., 2005; Menéndez et al., 2010) and neuroscience (Huang et al., 2010; Varoquaux et al., 2010).

Numerous methods have been proposed in the literature to reconstruct sparse GGMs. Meinhausen and Buhlman in (Meinshausen & Bühlmann, 2006) adopted a regression based approach and used the LASSO (Tibshirani, 1996) to estimate the neighborhood of each vertex. Yuan and Lin (Yuan & Lin, 2007) introduced the $\ell_1$ regularized log-likelihood estimator, commonly known as GRAPH LASSO, which was further explored in (d’Aspremont et al., 2008) and (Ravikumar et al., 2009). Anandkumar et al. in (Anandkumar et al., 2012) used empirical conditional covariance thresholding and proved structural consistency for...
walk-summable models. In (Cai et al., 2011), Cai, Liu and Luo introduced an $\ell_1$ regularized estimator called CLIME and later an adaptive version called ACLIME (Cai et al., 2016), that can be implemented by linear programming. With suitable assumptions, all the above methods have been shown to successfully exploit sparsity and reconstruct the underlying graph $\mathcal{G}$ perfectly with a sample complexity of $O(\log p)$.

An information theoretic lower bound for the minimum number of samples required for perfect graph reconstruction was derived in (Wang et al., 2010). The lower bound reads

$$n^* > \max \left\{ \frac{\log \left( \frac{p-d}{2} \right) - 1}{4\kappa^2} \cdot \frac{2 \left( \log \left( \frac{p}{d} \right) - 1 \right)}{\log \left( 1 + \frac{d\kappa}{1-d\kappa} \right) - \frac{d\kappa}{1+(d-1)\kappa}} \right\},$$

(3)

where the parameter $\kappa$ denotes the minimum normalized edge strength and is given by

$$\kappa = \min_{(i,j) \in E} \frac{|\theta_{ij}|}{\sqrt{\theta_{ii}\theta_{jj}}}. \quad \text{(4)}$$

The inverse square dependence on $\kappa$ in (3) appears due to the difficulty in detecting edges of low strength from their absence. Noticeably, the IT lower bound only depends on the dimension $p$, sparsity $d$, and minimum edge strength $\kappa$.

In contrast, analysis of the existing estimators in the literature always require additional assumptions to prove perfect graph reconstruction. The analysis of LASSO in (Meinshausen & Bühlmann, 2006) assumes certain incoherence properties of the matrix $\Theta$, reminiscent of the compressed sensing problem. In (Ravikumar et al., 2009), a variant of the incoherence condition is assumed, which by itself can be hard to verify. The proof of CLIME (Cai et al., 2011) and ACLIME (Cai et al., 2016) require that the eigenvalues of the precision matrix are bounded. The analysis of the conditional covariance thresholding algorithm (Anandkumar et al., 2012) was conducted only for the class of so-called walk-summable models. Due to these additional assumptions, the sample complexity of the algorithms depend on extra parameters that are not present in the IT lower bound (3). Among other quantities, all the above algorithms exhibit dependence on the condition number of $\Theta$. As a result, there is a gap between the information theoretic lower bound and the sample complexity of known algorithms. Further, due to the dependence of the sample complexity on extra parameters, it is unclear whether the lower bound is loose and fails to reflect dependence on additional parameters, or if the existing algorithms fail to achieve the same parametric dependence as the lower bound.

In this manuscript, we propose a two stage algorithm consisting of a sparse least-squares regression followed by a thresholding procedure. We call this algorithm Sparse Least-squares Inverse Covariance Estimator (SLICE). Without any additional assumption, we prove that SLICE successfully reconstructs the graph $\mathcal{G}$ perfectly with probability greater than $1 - \delta$ using $d + \frac{32}{\kappa^2} \log \left( \frac{4e^{d+1}}{\delta} \right)$ samples. The sample complexity of our algorithm is off from the lower bound only by a $O(1/\kappa^2)$ factor. More importantly, it depends only on the same set of parameters as the lower bound, thus closing the gap with respect to parametric dependence.

The first step in the algorithm adopts a regression perspective and similar to the LASSO, minimizes an empirical least squares objective for each vertex. However, instead of using an $\ell_1$ penalty we use a cardinality constraint, often referred to as an $\ell_0$ constraint, which enforces that the number of non-zero elements of the regression vector is at most $d$. The second step, based on a product and threshold procedure is unique to our algorithm and is critical to keep the sample complexity low.

The computational complexity of algorithm is dictated primarily by the computationally heavier non-convex regression step. In its bare form, this step is equivalent to an exhaustive search over all possible size $d$ neighborhoods of a vertex, resulting in a computational complexity of $O(p^{d+1})$. The problem however can be solved much faster in practice by recasting it as a Mixed Integer Quadratic Program (MIQP), an approach that has been explored previously in the compressed sensing literature (Bertsimas et al., 2016). The MIQP formulation leverages significant recent advances in mixed integer programming technology and availability of powerful commercial solvers.

Our paper is organized as follows: In Section 2 we introduce our algorithm starting with the optimization step and following with the thresholding procedure. We also present a MIQP formulation of the first step at the end of this section. In Section 3 we provide rigorous mathematical guarantees on the sample complexity required to achieve perfect graph reconstruction with our algorithm. Detailed proofs and analysis of the optimization step and the thresholding procedure can be found in Section 4 and in Section 5 respectively. Section 6 contains numerical simulations and comparisons with few popular reconstruction algorithms. Conclusion and discussions on future works can be found in Section 7. Appendix A contains detailed proofs for several technical lemmas.

2. Algorithm

In this section we describe the details of the SLICE algorithm. The loss function is constructed locally around each vertex of $\mathcal{G}$. The cardinality constraint is tantamount to an exhaustive search over all possible $d$-sparse neigh-
components are given by \( \hat{\Sigma} \), and where \( \ell \) corresponds to \( \hat{\beta} \), coefficients determine the graph structure. The estimated graph is then declared as \( \hat{G} = (V, \hat{E}) \).

2.2. Interpretation as Minimum Conditional Variance

For a given \( i \in V \), the \( \ell_0 \)-constraint in (6) is tantamount to an exhaustive search over all candidate neighborhoods of vertex \( i \), denoted by \( \hat{B}_i \), of size exactly \( d \). Note that neighborhoods of size strictly less than \( d \) can be eliminated from the search as they are strictly contained in bigger candidate neighborhoods. Thus, the optimization in (6) can be rewritten as

\[
\min_{\hat{B}_i \subseteq [p] \setminus i : |\hat{B}_i| = d} \beta_i \in \mathbb{R}^{p-1} : \text{Supp}(\beta_i) \subseteq \hat{B}_i, \quad \min_{\hat{B}_i \subseteq [p] \setminus i : |\hat{B}_i| = d} \beta_i \in \mathbb{R}^{p-1} : \text{Supp}(\beta_i) \subseteq \hat{B}_i.
\]

The corresponding optimal value is given by

\[
L_i(\hat{B}_i, \hat{\Sigma}) = L_i(\hat{\beta}_i(\hat{B}_i), \hat{\Sigma}) = \hat{\Sigma}_{i} - \hat{\Sigma}_{i\hat{B}_i} \hat{\Sigma}_{i\hat{B}_i}^{-1} \hat{\Sigma}_{i\hat{B}_i}
\]

and

\[
L_i^* (\hat{B}_i, \hat{\Sigma}) = \text{Var}(X_i | X_{\hat{B}_i}^c).
\]

Thus, the first step of the SLICE algorithm is equivalent to finding a candidate neighborhood \( \hat{B}_i \in [p] \) for vertex \( i \) that minimizes the empirical conditional variance. To see why this is a suitable objective, it is helpful to consider the limit of large number of samples, when the empirical conditional variance is replaced by the true one. In this case, any set \( \hat{B}_i \) that minimizes the conditional variance must be a superset of the neighborhood of \( i \). This follows from the observation that conditioning reduces variance in the case of multivariate Gaussians.

\[
\text{Var}(X_i | X_A) \leq \text{Var}(X_i | X_{[p] \setminus \{i\}}), \quad \forall A \subseteq [p] \setminus \{i\}, \tag{15}
\]

and using the separation property of graphical models,

\[
\text{Var}(X_i | X_{[p] \setminus \{i\}}) = \text{Var}(X_i | X_{\hat{B}_i}), \tag{16}
\]

where \( B_i \subseteq [p] \) denotes the set of neighbors of \( i \).

We remark here that (15) is a property specific to Gaussians, but can also be thought of as a special case of the more general information theoretic inequality which states
that conditioning reduces entropy. Indeed, (15) and (16) holds for any graphical model if we replace $\text{Var}(\cdot)$ by the Shannon entropy function $H(\cdot)$, and the equivalence in the gaussian case follows from

$$H(X_i | X_A) = \frac{1}{2} \log [2\pi e \text{Var}(X_i | X_A)].$$

Incidentally, minimizing conditional entropy, more popularly referred to as the pseudo-likelihood loss function has been proved to reconstruct graph structure in (Ravikumar et al., 2010) under incoherence assumption, and recently in (Lokhov et al., 2016) without any assumptions.

2.3. Computational Complexity and MIQP Formulation

Step 1 of the SLICE algorithm has a computational complexity of $O(p^d)$ since it is equivalent to an exhaustive search over all possible size $d$ neighborhood of each vertex $i \in V$. The second step can be implemented with a much lower computational complexity of $O(pd)$ leading to an overall complexity of $O(pd^2)$. Since $d = O(1)$, the algorithm is of polynomial time complexity.

However when $d$ is not small enough, performing an exhaustive search can be prohibitively expensive. Instead, the problem can be reformulated as a Mixed Integer Quadratic Program (MIQP), which in practice is significantly faster, especially when using modern mixed integer solvers such as CPLEX or GUROBI. In the context of compressive sensing and sparse regression, the use of MIQP has been explored in (Bertsimas et al., 2016) to solve an $\ell_0$ constrained quadratic objective. We present one such formulation:

$$\min_{\beta_i \in R^{p-1}} \begin{equation}
\frac{\beta_i^T \hat{\Sigma} \beta_i + 2 \hat{\Sigma}_{i\cdot} \beta_i + \hat{\Sigma}_{ii}}{s_{ij} L - \beta_{ij} \leq s_{ij} U, \forall j \neq i} \quad (18a)
\end{equation}
\begin{equation}
\sum_j s_{ij} = d \quad (18b)
\end{equation}
\begin{equation}
s_{ij} \in \{0, 1\}, \forall j \neq i. \quad (18d)
\end{equation}$$

In the above $L$ and $U$ denote known or estimated upper and lower bounds on the regression variables. For a more detailed discussion on these bounds, and formulations that avoid using such bounds, we refer the reader to (Bertsimas et al., 2016).

3. Sufficient Conditions for Structure Recovery

In this section we present our main result which states that the SLICE estimator successfully recovers the graph structure $\hat{G}$ with a number of samples that depends only on $\kappa, d$ and $p$.

**Theorem 1.** Given $\delta > 0$, the probability of perfect graph reconstruction using SLICE is lower bounded as

$$P(\hat{G} = G) > 1 - \delta,$$

provided that the number of samples satisfies

$$n - d > \frac{32}{\kappa^2} \log \left(\frac{4pd^{d+1}}{\delta}\right).$$

We prove Theorem 1 by establishing the following two results that provide guarantees for each step of the SLICE estimator.

**Proposition 1** (Optimal support contains the true support). For each $i \in V$, let $B_i \subset [p]$ be the support of the optimal solution in (6) and let $B \subset [p]$ be the neighbors of $i$. Then for any $\delta > 0$, the support $B_i$ satisfies $B_i \subseteq B$ with probability greater than $1 - \delta/2$, provided that the number of samples satisfies

$$n - d > \frac{32}{\kappa^2} \log \left(\frac{4pd^{d+1}}{\delta}\right).$$

**Proposition 2** (Post-processing Proposition). Assume that

$$n - d > \frac{64}{\kappa^2} \log \left(\frac{8dp}{\delta}\right).$$

Then with probability greater than $1 - \delta/2$, the post-processing procedure consisting of Product and Threshold terminates with exactly the correct support.

Theorem 1 follows by combining Proposition 1 and Proposition 2 and applying the union bound.

4. Proof of Proposition 1

To prove Proposition 1, it is sufficient to show that if $B_i$ is not a subset of $\hat{B}_i$ then the corresponding objective value $L_i^*(\hat{B}_i, \hat{\Sigma})$ in (12) is too large. We establish this in two steps. We first show that when $\hat{\Sigma}$ is replaced by the true underlying covariance matrix $\Sigma$ in (13), then the corresponding objective value $L_i^*(B_i, \Sigma)$ is smaller than $L_i^*(\hat{B}_i, \hat{\Sigma})$ by a factor that depends on $\kappa$, for any $|B| = d$ that does not contain $B_i$ (see Lemma 1). We then show that the ordering is preserved even with the estimation error that results when we replace $\hat{\Sigma}$ by $\hat{\Sigma}$ provided that we have sufficient number of samples as specified by Proposition 1. These statements are formalized in the following lemmas.

**Lemma 1** (Multiplicative gap in noiseless optimal solutions). Fix $i \in V$ and let $B_i \subset [p]$ be the neighbors of $i$. Let $\hat{B} \subset [p]$ be any subset such that $|\hat{B}| = d$ and $B_i \nsubseteq \hat{B}$. Then

$$L_i^*(\hat{B}, \hat{\Sigma}) \geq L_i^*(B_i, \Sigma)(1-\kappa^2)^{-1}.$$
Lemma 2 (Large deviations on \( L^*_i(\cdot, \Sigma) \)). Fix \( i \in \mathcal{V} \) and let \( 0 < \epsilon < 1 \). Then for every subset \( A \subset [p] \setminus \{i\} \) with \( |A| = d \), we have
\[
(1 - \epsilon)L^*_i(A, \Sigma) \leq L^*_i(A, \hat{\Sigma}) \leq (1 + \epsilon)L^*_i(A, \Sigma), \tag{24}
\]
with probability at least \( 1 - 2(P - 1)\epsilon e^{-(n-d)\kappa^2/8} \).

We first show that Proposition 1 follows from the above two lemmas.

**Proof of Proposition 1.** Combining Lemma 1 and Lemma 2 and using \( \epsilon = \kappa^2/2 \) we have for any \( i \in \mathcal{V} \) that the sequence of inequalities
\[
L^*_i(B_i, \hat{\Sigma}) < (1 + \epsilon)L^*_i(B_i, \Sigma) < (1 + \epsilon)(1 - \kappa^2)L^*_i(\hat{B}, \Sigma),
\]
is satisfied for all \( \hat{B} \subset [p] \setminus \{i\} : |\hat{B}| = d \). From Proposition 1 we have that for all \( \{i, u\} \). The inequality (b) follows from (4).

**Proof of Lemma 1.** From (14) we have that
\[
L^*_i(B_i, \Sigma) = \text{Var}(X_i | X_{B_i}) = \text{Var}(X_i | X_{[p]\setminus \{i\}}), \tag{26}
\]
where (a) follows from the separation property of graphical models, and (b) follows from (13). Similarly,
\[
L^*_i(\hat{B}, \Sigma) = \text{Var}(X_i | X_{\hat{B}}). \tag{27}
\]

Using the law of total variance we get that
\[
\text{Var}(X_i | X_{\hat{B}}) = \mathbb{E} \left[ \text{Var}(X_i | X_{B_i} \cup \hat{B}) | X_{\hat{B}} \right] + \text{Var} \left( \mathbb{E} \left[ X_i | X_{B_i} \cup \hat{B} \right] | X_{\hat{B}} \right)
\]
\[
= \theta_{ii}^{-1} + \text{Var} \left( \sum_{j \in B_i \cup \hat{B}} \frac{\theta_{ij}}{\theta_{ii}} X_j | X_{\hat{B}} \right)
\]
\[
= \theta_{ii}^{-1} + \theta_{ii}^{-2} \text{Var} \left( \sum_{j \in B_i \cup \hat{B}} \theta_{ij} X_j | X_{\hat{B}} \right). \tag{28}
\]

Let \( u \in B_i \setminus \hat{B} \). From above, we get
\[
\text{Var}(X_i | X_{\hat{B}}) - \text{Var}(X_i | X_{B_i}) = \theta_{ii}^{-2} \text{Var} \left( \sum_{j \in B_i \cup \hat{B}} \theta_{ij} X_j | X_{\hat{B}} \right)
\]
\[
\begin{align*}
&\geq \theta_{ii}^{-2} \text{Var} \left( \sum_{j \in B_i \cup \hat{B}} \theta_{ij} X_j | X_{[p]\setminus \{i, u\}} \right) \\
&\geq \theta_{ii}^{-2} \theta_{iu}^2 \text{Var} \left( X_u | X_{[p]\setminus \{i, u\}} \right) \\
&= \theta_{ii}^{-1} \left( \frac{\theta_{ii} \theta_{iu}}{\theta_{iu}} - 1 \right)^{-1} \\
&\geq \frac{\text{Var}(X_i | X_{B_i})}{1 - \kappa^2}. \tag{29}
\end{align*}
\]

The inequality (a) follows from the fact that conditioning reduces variance in Gaussian and observing that \( \hat{B} \subseteq [p] \setminus \{i, u\} \). The inequality (b) follows from (4).

**Proof of Lemma 2.** Fix \( i \in \mathcal{V} \) and \( A \subset [p] \setminus \{i\} \) with \( |A| = d \). Then using properties of the Wishart distribution we get that,
\[
\hat{\Sigma}_{ii} - \Sigma_{ii} \sim \sum_{\hat{A}i} \Sigma_{A_i}^{-1} \Sigma_A \sim \left( \Sigma_{ii} - \Sigma_{i,A} \Sigma_{A_i} \Sigma_A \right) \chi_{n-d}^2
\]
\[
= L^*_i(A, \Sigma) \chi_{n-d}^2. \tag{30}
\]
where \( \chi_t^2 \) denotes the standard Chi-squared distribution with \( t \) degrees of freedom. Using the Chernoff bound,
\[
\text{P}(\chi_{n-d}^2 > 1 + \epsilon) < e^{-(n-d)(\frac{\epsilon}{2} - \frac{1}{8} \log(1+\epsilon))} < e^{-(n-d)\epsilon^2/8}, \tag{31}
\]
\[
\text{P}(\chi_{n-d}^2 < 1 - \epsilon) < e^{-(n-d)(-\frac{1}{8} \log(1-\epsilon) - \frac{\epsilon}{2})} < e^{-(n-d)\epsilon^2/8}. \tag{32}
\]

The proof is completed by using the union bound for all \( A \subset [p] \setminus \{i\} \) with \( |A| = d \).

**5. Proof of Proposition 2**

In this section, we prove the post-processing proposition. From Proposition 1 we have that for all \( i \in \mathcal{V} \) the estimated neighborhoods \( \hat{B}_i \) in Step 1 of SLICE satisfies \( \hat{B}_i \subseteq B_i \). The post-processing aims at eliminating the vertices \( u \in \hat{B}_i \setminus B_i \) so that we obtain the exact neighborhood. The proof is based on showing that the estimates \( \hat{\beta}_i \) obtained in Step 1 are sufficiently accurate. For the rest of the section we assume that the statement in Proposition 1 holds.

Our proof of Proposition 2 proceeds in the following steps. First we show that the random quantities \( \beta_{ij} \) estimated in step one have the correct mean \( \mathbb{E} \left[ \beta_{ij} \right] = \frac{\theta_{ij}}{\theta_{ii}} \), and are conditionally distributed as normal random variables. Then we show that although the variance of the normal random variable \( \beta_{ij} \) is dependent on the conditioning, it can be bounded from above with high probability. The proof of Proposition 2 then follows by combining the above two steps and
showing that the estimates \( \hat{\beta}_{ij} \) are accurate enough that the product and threshold procedure finds the exact structure. These steps are contained in the following lemmas.

**Lemma 3.** Fix \( i \in \mathcal{V} \). The conditional distribution of \( \hat{\beta}_{ij} \) for any \( j \in \hat{B}_i \) is given by

\[
\hat{\beta}_{ij} \mid \hat{\Sigma}_{\hat{B}_i, \hat{B}_i} \sim \mathcal{N}\left( \frac{\Theta_{ij}}{\theta_{ii}}, \frac{1}{\theta_{ii}} \left( \hat{\Sigma}_{\hat{B}_i, \hat{B}_i} \right)_{jj} \right),
\]

where \( \mathcal{N}(\cdot, \cdot) \) denotes the normal distribution.

**Lemma 4.** For any \( \epsilon > 0 \) the random variable \( \left( \hat{\Sigma}_{\hat{B}_i, \hat{B}_i} \right)_{jj} \) satisfies the following large deviation inequality

\[
P \left( \left( \hat{\Sigma}_{\hat{B}_i, \hat{B}_i} \right)_{jj} > (1 - \epsilon)^{-1} \Theta_{jj} \right) \leq e^{-\frac{(n-d+1)\epsilon^2}{4}}.
\]

The next lemma combines the above two lemmas to prove that the estimated quantities \( \hat{\beta}_{ij} \) are close to \( \frac{\theta_{ij}}{\theta_{ii}} \).

**Lemma 5.** Fix any \( i \in \mathcal{V} \) and \( j \in \hat{B}_i \). The estimates \( \hat{\beta}_{ij} \) satisfy the following large deviation inequality

\[
P \left( \left| \hat{\beta}_{ij} - \frac{\theta_{ij}}{\theta_{ii}} \right| \geq \frac{\kappa}{4} \sqrt{\frac{\theta_{jj}}{\theta_{ii}}} \right) \leq 4e^{-\frac{(n-d+1)\kappa^2}{64}},
\]

where \( \kappa \) denotes the minimum normalized edge strength defined in (4).

We defer the proof of the above lemmas and first show that Proposition 2 follows from Lemma 5.

**Proof of Proposition 2.** Using Lemma 5 and using the union bound for all \( i \in \mathcal{V} \) and \( j \in B_i \), we get

\[
P \left( \left| \hat{\beta}_{ij} - \frac{\theta_{ij}}{\theta_{ii}} \right| \leq \frac{\kappa}{4} \sqrt{\frac{\theta_{jj}}{\theta_{ii}}} \quad \forall j \in \hat{B}_i, i \in \mathcal{V} \right)
\]

\[
\geq 1 - 4dpe^{-\frac{(n-d+1)\kappa^2}{64}}
\]

\[
\geq 1 - \delta^2.
\]

An identical argument gives

\[
|\hat{\beta}_{ij} - \hat{\beta}_{ji}| \leq \left( \frac{|\theta_{ij}|}{\sqrt{\theta_{ii}\theta_{jj}}} + \frac{\kappa}{4} \right) \left( \frac{|\theta_{ij}|}{\sqrt{\theta_{ii}\theta_{jj}}} + \frac{\kappa}{4} \right).
\]

From (39), we get that for \( (i, j) \in E \) the estimates satisfy \( \sqrt{|\hat{\beta}_{ij}||\hat{\beta}_{ji}|} \geq 3\kappa/4 > \kappa/2 \) and similarly from (40) we get that for \( (i, j) \notin E \), the estimates satisfy \( \sqrt{|\hat{\beta}_{ij}||\hat{\beta}_{ji}|} \leq \kappa/4 < \kappa/2 \). This proves that the post-processing step recovers the exact support.

\[\square\]

### 6. Numerical Simulations

In this section we explore with a simple family of GGMs the probability of reconstruction failure of various algorithms. We aim to illustrate that for fixed \( \kappa \), degree \( d \), dimension \( p \) and number of samples \( n \), the probability of failure of our algorithm does not depend on other properties of the model unlike other methods. We compare SLICE with some of the most well-known reconstruction algorithms, LASSO (Meinshausen & Bühlmann, 2006), GRAPH LASSO (Yuan & Lin, 2007) and ACCLIME (Cai et al., 2016). We consider a family of GGMs that have the same graph consisting of a triangle of three nodes with two weak links and one stronger link and a collection of independent nodes. This family of GGMs is parametrized by the following inverse covariance matrix,

\[
\Theta_{\kappa, \epsilon, \sigma} = \begin{bmatrix}
1 & \kappa & \kappa & 0 \\
\kappa & 1 - \epsilon & \kappa & 0 \\
\kappa & 1 - \epsilon & 1 & 0 \\
0 & 0 & 0 & \frac{1}{\sigma} \mathbf{I}_{(p-3) \times (p-3)}
\end{bmatrix},
\]

where \( 1 - \epsilon \) is the strength of the strong link, \( \kappa < 1 - \epsilon \) is the strength of the weak links and \( \sigma \) is the variance of the independent nodes.

The simulations are performed for a matrix of dimension, \( p = 200 \), and with a number of samples, \( n = 175 \), lower than the dimension size. The family of GGMs described by the precision matrix in Eq. (41) have a bounded maximum degree, \( d = 2 \). We repeat the reconstruction procedure 50 times with independent samples for different values of \( \sigma \in \{1, \ldots, 10^3\} \) while \( \kappa = 0.4 \) and \( \epsilon = 0.01 \) are fixed. The value of the regularizer parameters in ACCLIME, LASSO and GRAPH LASSO have been optimized to yield the best possible results for each value of \( \sigma \). Note that in practice, when the ground truth is not known, optimizing over the regularization value is challenging. This issue is inherently not present with SLICE.

For each algorithm we have compared their estimate of the
normalized link value between nodes (1,2) and (1,4),
\[
\gamma_{12} = \sqrt{\frac{\theta_{12}\theta_{21}}{\theta_{13}\theta_{32}}} , \quad \gamma_{14} = \sqrt{\frac{\theta_{14}\theta_{41}}{\theta_{13}\theta_{34}}}.
\]

ACLIME directly estimates the matrix elements \( \Theta \) but SLICE, LASSO and the iterative version of GRAPH LASSO aim to estimate ratios of the matrix elements \( \beta_{ij} \). Henceforth their estimate for the normalized link value is found through the product \( \hat{\gamma}_{ij}^2 = \hat{\beta}_{ij}\hat{\beta}_{ji} \). We declare that an algorithm fails to reconstruct the graph whenever \( \gamma_{12} < \gamma_{14} \). The reason is that if this condition is satisfied links (1,2) or/and (1,4) are incorrectly reconstructed regardless of the thresholding procedure. Note that this choice of reconstruction failure criterion is quite generous. It is very unlikely that one can devise a successful thresholding procedure solely based on the criterion \( \gamma_{12} < \gamma_{14} \) when \( \gamma_{12} \) and \( \gamma_{14} \) are close to each other. This is particularly true for several reconstructions provided by GRAPH LASSO and ACLIME as illustrated in Figure 1. However this failure criterion has the advantage to be simple and enables us to reconstruct only neighborhood while strengthening our comparisons. Note that we compare normalized link strengths \( \gamma_{ij} \) instead of matrix element ratios \( \beta_{ij} \) or matrix elements \( \theta_{ij} \). The reason is that quantities \( \gamma_{ij} \) are invariant upon rescaling of the \( \Theta \) matrix while \( \beta_{ij} \) and \( \theta_{ij} \) are not. Thus reconstruction based on thresholding the later quantities would fail for a suitable rescaling of \( \Theta \).

Simulation results of are summarized in Figure 2 where the probability of failure is plotted against the variance \( \sigma \) of the independent nodes. For \( \sigma \) close to one, the four algorithms succeed with high-probability and are able to correctly identify that there is a link (1,2) and no link between (1,4). However for larger value of \( \sigma \), the probability of failure of ACLIME, LASSO and GRAPH LASSO is close to one while SLICE remains insensitive to changes in \( \sigma \). We stress that the information theoretical bound predicts a sample complexity that is independent of \( \sigma \) but only depend on \( \kappa, d \) and \( p \) that are fixed in the simulations. With this simple example we highlight that when algorithms depend on properties not present in the information theoretical bound, the graph reconstruction can be severely impacted even by independent nodes.

7. Conclusions and Path Forward

In this paper we propose a polynomial time algorithm, called SLICE, that perfectly recovers the graph of arbitrary Gaussian graphical models. We prove that the number of samples needed to perform this task is close from being optimal and only depends on parameters present in the information theoretic lower-bound. In particular it demonstrates that, contrary to existing algorithms, the number of samples needed by SLICE neither depends on the incoherence properties of the precision matrix nor on its conditioning number. This is critical when samples are scarce or expensive and can drastically impact the reconstruction even for simple models as illustrated in this paper. In addition, although SLICE requires solving a non-convex optimization problem, we have shown that it can be efficiently implemented as a Mixed-Integer Quadratic Program leveraging recent progress made in mixed-integer solvers.

Future works will consist in improving the solving time of the non-convex optimization problem. Possible pathways include finding more efficient MIQP formulations and using greedy heuristic or the convex \( \ell_1 \) penalty to warm start the non-convex optimization. We would also like to perform a more exhaustive numerical study of the SLICE algorithm. This will involve a sample complexity comparison against state of art methods including the recently developed “Interaction Screening” algorithm (Vuffray et al., 2016) that was shown to be optimal for reconstructing discrete graphical models. Finally it would be interesting to know if the information theoretic lower bound on the sample complexity is perfectly tight with respect to scaling in all involved parameters, and if this scaling is efficiently achievable. This requires either improving the IT bound or to devise a polynomial time reconstruction algorithm that closes the gap.
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Figure 2. Detecting a triangle in a cloud of independent nodes. Empirical probability of failure averaged over 50 trial reconstructions with a fixed number of samples \( n = 175 \). The values for all algorithms except SLICE have been optimized over regularization coefficients. All algorithms fail for some larger values of \( \sigma \) except for the SLICE algorithm which shows a consistently good performance.

A. Proof of Technical Lemmas

In this section we prove Lemma 3, 4 and 5. In the process we make heavy use of the marginal and conditional probability distributions of the inverse Wishart distribution based on the properties of the Schur complement stated in the following lemma.

**Lemma 6** (Properties of Wishart and inverse Wishart). Let \( X \in \mathbb{R}^{k \times k} \sim W(V, l) \) be a random matrix distributed according to the Wishart distribution with parameter \( V > 0 \) and order \( l > k-1 \). Let \( Y = X^{-1} \) with \( Y \sim W^{-1}(V, l) \) where \( U = V^{-1} \). Let

\[
X = \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix}, \quad V = \begin{bmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{bmatrix}
\]

\[
Y = \begin{bmatrix} Y_{11} & Y_{12} \\ Y_{21} & Y_{22} \end{bmatrix}, \quad U = \begin{bmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{bmatrix}
\]

be any block matrix representation of \( X, Y, U \) and \( V \) with the same dimensions \( k_1, k_2 \) that satisfy \( k_1 + k_2 = k \). Then,

(a) The Schur complement of \( Y_{11} \) is distributed as

\[
Y_{11} - Y_{12}Y_{22}^{-1}Y_{21} = X_{11}^{-1} \sim W^{-1}(V_{11}^{-1}, l)
\]

\[
= W^{-1}(U_{11} - U_{12}U_{22}^{-1}U_{21}, l),
\]

(b) The random matrix \( Y_{22}^{-1}Y_{21} \) conditioned on \( X_{11}^{-1} \) is distributed as a matrix normal distribution

\[
Y_{22}^{-1}Y_{21} | X_{11}^{-1} \sim \mathcal{N}(U_{22}^{-1}U_{21}, X_{11}^{-1} \otimes U_{22}^{-1}).
\]

**Proof of Lemma 6.** See reference (Ouellette, 1981). □

**Proof of Lemma 3.** For any \( i \in \mathcal{V} \) let \( \tilde{\Psi}_{(iB_i)(i\hat{B}_i)} = \left( \Sigma_{(i\hat{B}_i)(i\hat{B}_i)} \right)^{-1} \) and \( \Psi_{(iB_i)(i\hat{B}_i)} = \left( \Sigma_{(i\hat{B}_i)(i\hat{B}_i)} \right)^{-1} \). Using the block matrix decomposition for matrix inverse

\[
\Psi_{(iB_i)(i\hat{B}_i)} = \Theta_{(iB_i)(i\hat{B}_i)} - \Theta_{(iB_i)D} \Theta_{DD}^{-1} \Theta_{D(i\hat{B}_i)},
\]

where \( D = [p] \setminus \{ i \cup \hat{B}_i \} \). Since \( B_i \subseteq \hat{B}_i \), we must have \( \Theta_{iD} = 0 \). Hence the matrix \( \Psi_{(iB_i)(i\hat{B}_i)} \) satisfies the following properties

\[
\Psi_{(iB_i)} = \Theta_{(iB_i)} \quad \text{and} \quad \Psi_{jj} \leq \Theta_{jj}, \quad \forall j \in B_i.
\]

From Lemma 6, part (b) we get that

\[
\beta_{ij} \mid \Sigma_{\hat{B}_iB_i} \sim \mathcal{N}\left( \frac{\Psi_{ij}}{\Psi_{ii}}, \Psi_{ii}^{-1}\left( \Sigma_{\hat{B}_i\hat{B}_i} \right)_{jj} \right)
\]

\[
\overset{(a)}{=} \mathcal{N}\left( \frac{\Theta_{ij}}{\Theta_{ii}}, \Theta_{ii}^{-1}\left( \Sigma_{\hat{B}_i\hat{B}_i} \right)_{jj} \right),
\]

where (a) follows from (46).

**Proof of Lemma 4.** From Lemma 6, the random matrix \( \Sigma_{\hat{B}_iB_i} \) is distributed according to the Wishart distribution

\[
\Sigma_{\hat{B}_iB_i} \sim W \left( \Sigma_{\hat{B}_i\hat{B}_i}, n \right).
\]

Hence

\[
\left[ \left( \Sigma_{\hat{B}_iB_i} \right)_{jj} \right]^{-1} = \Sigma_{jj} - \Sigma_{j(\hat{B}_i \setminus j)}\Sigma_{(\hat{B}_i \setminus j)(\hat{B}_i \setminus j)}\Sigma_{(\hat{B}_i \setminus j)j} \quad \overset{(a)}{=} \quad \Sigma_{jj} - \Sigma_{j(\hat{B}_i \setminus j)}\Sigma_{(\hat{B}_i \setminus j)(\hat{B}_i \setminus j)}\Sigma_{(\hat{B}_i \setminus j)j} \chi_n^2 n^{-d+1} \equiv \alpha_j \chi_n^2 n^{-d+1},
\]

where (a) follows from Lemma 6 and the constant \( \alpha_j \) can be bounded from above for every \( j \in \hat{B}_i \) as

\[
\alpha_j^{-1} = (\Sigma_{jj} - \Sigma_{j(\hat{B}_i \setminus j)}\Sigma_{(\hat{B}_i \setminus j)(\hat{B}_i \setminus j)}\Sigma_{(\hat{B}_i \setminus j)j})^{-1} = \Psi_{jj} - \Psi_{jj}^{2} \Psi_{ii}^{-1} \leq \Psi_{jj} \leq \Theta_{jj}.
\]

We bound

\[
P \left( \left[ \left( \Sigma_{\hat{B}_iB_i} \right)_{jj} \right]_j \ > \ (1 - e^{-1})\Theta_{jj} \right)
\]

\[
= P \left( \chi_n^2 n^{-d+1} \ < \ (1 - e^{-1})\Theta_{jj} \right)
\]

\[
\overset{(a)}{=} \leq e^{-(n-d+1)e^2/8},
\]

where (a) follows from (51) and (31).

**Proof of Lemma 5.** Define the event \( E = \left[ \left( \Sigma_{\hat{B}_iB_i} \right)_{jj} \leq (1 - \epsilon_1)^{-1}\Theta_{jj} \right] \). We bound the deviation of \( \beta_{ij} \) from \( \frac{\theta_{ij}}{\hat{\theta}_{ii}} \) as

\[
P \left( \left| \beta_{ij} - \frac{\theta_{ij}}{\hat{\theta}_{ii}} \right| \geq \epsilon \sqrt{\frac{\theta_{jj}}{\hat{\theta}_{ii}}} \right)
\]
Combining (54) and (55) we complete the proof.

\[
\begin{align*}
= \mathbb{P}\left( |\hat{\beta}_{ij} - \theta_{ij}| \leq \epsilon \sqrt{\frac{\theta_{ii}}{\theta_{ij}}} | E \right) \\
+ \mathbb{P}\left( |\hat{\beta}_{ij} - \theta_{ij}| \geq \epsilon \sqrt{\frac{\theta_{ii}}{\theta_{ij}}} | E^c \right)
\end{align*}
\]

where (a) follows by bounding the first term using Lemma 3 and the definition of the event \( E \), and bounding the second term by the probability of the event \( E^c \) using Lemma 4. Setting \( \epsilon = \kappa/4 \) and \( \epsilon_1 = \kappa/2 \), and a tight upper bound on the Gaussian CDF, we get

\[
\Phi^c \left( \epsilon \sqrt{1 - \epsilon_1 \sqrt{n}} \right) + e^{-(n-d+1)\epsilon_1^2/8} \leq e^{-\kappa^2 n/64} + e^{-(n-d+1)\kappa^2/32} \leq 2e^{-(n-d+1)\kappa^2/64}.
\]

Combining (54) and (55) we complete the proof.

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