Abstract

We explore if it is possible to learn a directed acyclic graph (DAG) from data without imposing explicitly the acyclicity constraint. In particular, for Gaussian distributions, we frame structural learning as a sparse matrix factorization problem and we empirically show that solving an $\ell_1$-penalized optimization yields to good recovery of the true graph and, in general, to almost-DAG graphs. Moreover, this approach is computationally efficient and is not affected by the explosion of combinatorial complexity as in classical structural learning algorithms.

1 Introduction

A vast literature exists on learning DAGs from data. Usually algorithms are classified as constrained based or score based [Scutari et al., 2019]. Score-based methods optimize some score function over the space of DAGs, usually employing some heuristic such as greedy search. Constraint-based methods, such as the PC algorithm [Spirtes et al., 1993, Colombo and Maathuis, 2014], use instead conditional independence testing to prune edges from the graph and apply sets of rules to direct some of the remaining edges and find an estimate of the Markov equivalence class [Chickering, 1995]. Recently, Zheng et al. [2018, 2020] proposed the use of optimization techniques to estimate DAG structures by writing the acyclicity condition of a directed graph as a smooth constraints for the weighted adjacency matrix. All the methods available in the literature for structure recovery of DAGs

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impose somehow the acyclicity condition. We propose instead to consider the estimation of DAGs as a general sparse matrix-factorization problem for the inverse covariance matrix arising from linear structural equation models [Drton 2018, Spirtes 1995, Richardson 1997]. We estimate such sparse matrix-factorization solving an \( \ell_1 \)-penalized minus log-likelihood minimization using a straightforward proximal gradient method. The proposed method takes inspiration from optimization-based algorithms for structure recovery such as the graphical lasso [Friedman et al. 2007] and especially the method proposed in Varando and Hansen 2020 where covariance matrices are parametrized as solutions of, eventually sparse, Lyapunov equations. In Section 4 we perform a simulation study and observe that the proposed method is competitive with classical approaches from the literature on the recovery of the true graph, while being generally faster.

A fortran implementation of the method, together with examples of its usage within R and python, is available at github.com/gerardovarando/nodag.

2 Linear structural equation models

A linear structural equation model (SEM) with independent Gaussian noise is a statistical model for a \( p \)-dimensional random vector \( X \) defined as the solution of

\[
X = \Lambda^t X + \epsilon,
\]

where we assume that \( \epsilon \) is a \( p \)-dimensional zero-mean independent Gaussian noise and \( \Lambda \in \mathbb{R}^{p \times p} \). If \( I - \Lambda \) is invertible, equation (1) implies the covariance parametrization [Drton 2018]

\[
\text{Var}(X) = (I - \Lambda)^{-t} \Omega (I - \Lambda)^{-1}
\]

where \( \Omega = \text{Var}(\epsilon) \) is a diagonal positive definite matrix. The connection between Gaussian Bayesian networks and the system of equations (1) is immediate if we assume that the matrix \( \Lambda \) has a sparsity structure compatible with a given directed acyclic graph \( G \).

Inverting equation (2) we obtain the factorization of the inverse covariance matrix as

\[
\text{Var}(X)^{-1} = (I - \Lambda)\Omega^{-1}(I - \Lambda)^t = AA^t,
\]
with \( A = (I - \Lambda)\Omega^{-1/2} \) having the same off-diagonal sparsity pattern as \( \Lambda \).

Parametrizing the multivariate Gaussian distribution with the inverse covariance matrix, we can define the linear structural equation model with independent Gaussian noise, and associate graph \( G \), as the family of normal distributions \( \mathcal{N}(\mu, \Sigma) \) with \( \Sigma^{-1} \) in

\[
\mathcal{M}_G = \{ AA^t \text{ s.t. } A \in \mathbb{R}^{p \times p} \text{ invertible and } A_{ij} = 0 \text{ if } i \not\rightarrow j \text{ in } G \}
\]

In particular when the graph \( G \) is acyclic the set of inverse covariance matrices \( \mathcal{M}_G \) corresponds to Gaussian Bayesian network models.

### 2.1 Markov equivalence classes

It is known that in general is not possible to recover completely the graph \( G \) from observational data, since different graphs give rise to the same statistical model, in which case we say that the two graphs are equivalent [Heckerman et al., 1994]. The equivalence classes obtained considering the quotient of the space of directed graphs with respect to the above equivalence are called Markov equivalence classes. In particular, if the graph \( G \) is a DAG its Markov equivalence class consists of all DAGs having the same skeleton and exactly the same \( \psi \)-structures [Andersson et al., 1997, Heckerman et al., 1994]. A completely partially directed acyclic graph (CPDAG) can be used to represent the Markov equivalence class for DAGs [Andersson et al., 1997]. A CPDAG is a partially directed graph where directed edges represent edges that have the same directions in all DAGs belonging to the Markov class, while undirected edges are drawn where there exists DAGs in the Markov equivalence class with different directions for a given edge.

### 3 Structure recovery

Considering the factorization of the precision matrix \( (3) \) it is immediate to consider the following minimization problem for the \( \ell_1 \)-penalized minus log-likelihood

\[
\begin{align*}
\text{minimize} & \quad -2 \log \det(A) + \text{trace}(A^t \hat{R} A) + \lambda \| A \|_1 \\
\text{subject to} & \quad A \in \mathbb{R}^{p \times p} \text{ invertible}
\end{align*}
\]
where $\hat{R}$ is the empirical correlation matrix estimated from the data.

Solving the above problem, we estimate a sparse factorization of the inverse covariance matrix and the estimated graph can be read directly from the non-zero entries of the minimizer.

**Remark 1** The proposed structural estimation is a general estimation for linear SEM, including models with cycles. We focus on the recovery of DAGs mainly because the literature on learning acyclic graphs is more extensive and more methods are available.

### 3.1 Solving the optimization

Various methods can be used to solve problem (4), we present here a very simple approach using a proximal gradient method [Bach et al., 2012; Parikh and Boyd 2014] similar to the algorithm proposed in Varando and Hansen [2020].

The proximal gradient is a method applicable to minimization problems where the objective function has a decomposition into a sum of two functions of which one is differentiable. In particular, the objective function of problem (4) can be written as $f(A) + g(A)$ where $f(A) = -2 \log \det(A) + \text{trace}(A^T \hat{R} A)$ and $g(A) = ||A||_1$, with $f$ differentiable.

The proximal gradient algorithm consists of iterations of the form

$$A^{(k)} = S_{\lambda}(A^{(k)} - s \nabla f)$$

where the soft-thresholding $S_t(A)_{ij} = \text{sign}(A_{ij}) (|A_{ij}| - t)_+$ is the proximal operator for the $\ell_1$-penalization and $\nabla f(A) = 2\hat{R}A - 2A^{-1}$. At each iteration the step size $s$ is selected using the line search proposed in Beck and Teboulle [2010].

A complete description of the algorithm and its implementation is given in the Appendix A.

**Example 1** We simulate 1000 synthetic observations from a Gaussian Bayesian network with associated DAG given in Figure 1 (a). The graph estimated solving the optimization problem (4) is shown in Figure 1 (b). We can observe that all the v-structures in the true DAG are correctly recovered. Nevertheless, the estimated graph is not a valid DAG since it contains the directed cycle 7 ↔ 8.
Figure 1: True DAG (a) and estimated graph with $\lambda = 0.2$ (b).

4 Simulations

We perform a simulation study to explore how the proposed method behaves with respect to the recovery of the true graph. Data is generated from Gaussian Bayesian networks with known structure similarly to Colombo and Maathuis [2014], in particular random DAGs with $p \in \{5, 10, 20, 50, 100\}$ nodes are generated with independent probability of edges $\frac{k}{p}$, $k = 1, 2, 3, 4$. Coefficients for the linear regression of each variable on its parents are independent realizations of a uniform distribution between 0.1 and 1, and the noise distribution is either standard Gaussian or exponential with rate parameter equal to 1. For each combination of $p$, $k$ and noise distribution we generate 20 DAGs and subsequently sample $n = 100, 1000, 10000$ observations from the induced structural equation models.

We apply our proposed method (nodag) by solving the optimization problem (4) with $\lambda = 0.1, 0.2, 0.3$. For comparison, we consider three classical structural-recovery algorithms: the order independent PC [Colombo and Maathuis 2014], the greedy equivalent search [Chickering 2003], and an hill-climbing search. The PC algorithm (pc) and the greedy equivalent search (ges) are implemented in the pcalg R package [Kalisch et al.].
while the hill-climbing search with tabu (tabu) is available in the bnlearn R package [Scutari, 2010]. For the pc method we use the Gaussian conditional independence test via Fisher’s Z and various significance levels (0.01, 0.005 and 0.001). Both ges and tabu methods optimize the Bayesian information criterion, as default in their implementations. For the tabu we also fix the maximum cardinality of the parent set to 10 to limit the computational complexity.

The pc algorithm and the greedy equivalent search estimate a representation of the Markov equivalence class while the hill-climbing search and the proposed nodag method estimate a directed graph.

4.1 Results
Similarly to Colombo and Maathuis [2014] we evaluate the estimated graphs using the F1 score (f1), false positive rate (fpr) and true positive rate (tpr) with respect to the true skeleton recovery. Figure 2 shows the average metrics for the skeleton recovery for the different algorithms. We observe that the nodag method obtains, in general, comparable results to the literature algorithms, while performing clearly better in the small sample size with respect to skeleton recovery and slightly worse in the large sample size and small graphs.

Evaluating edge directions is more tricky, since different DAGs with the same skeleton can be Markov equivalent (see Section 2.1), and moreover algorithms can output estimated directed or partially directed graphs. We chose to report structural Hamming distance to both the true DAG (shd-graph) and the true CPDAG (shd-cpdag) in Figure 3. We can see that the proposed method is on average superior to other algorithms with respect to the recovery of the true DAG. As for the skeleton recovery, nodag performs worst in the large sample and small system dimensions. As we showed in Example 1 the graphs estimated by nodag have, sometimes, a double edge $i \leftrightarrow j$, and we have observed that this happens especially when the true CPDAG have the corresponding undirected edge $i \sim j$.

In general the value of the penalization coefficient $\lambda$ obtaining the optimal results is, as expected, dependent on the sample size, but on average it does not seem to be too much sensitive.
In Figure 4 we report the average execution time\(^1\) for the different methods. The \texttt{nodag} method is shown to outperform all the other methods from a computational speed prospective, especially for large sample and system sizes.

5 Protein signaling network

As an example of real-data application we consider the dataset from Sachs et al. [2005] largely used [Friedman et al., 2007; Meinshausen et al., 2016; Zheng et al., 2018; Varando and Hansen, 2020] in the graphical models and causal discovery literature.

Data consist of observations of phosphorylated proteins and phospholipids \((p = 11)\) from cells under different conditions \((n = 7466)\).

We estimate the graph representing the protein-signaling network with our \texttt{nodag} method with \(\lambda = 0.2\) (Figure 5). The \texttt{nodag} method estimates a graph without cycles and with 12 edges of which 4 are also present in the consensus network [Sachs et al., 2005]. Tow estimated edges, jnk \(\rightarrow\) pkc and mek \(\rightarrow\) raf, appear with reversed direction in the consensus network while others (jnk \(\rightarrow\) p38, akt \(\rightarrow\) erk, akt \(\rightarrow\) mek) appear in the graph estimated from other methods in the literature [Meinshausen et al., 2016; Varando and Hansen, 2020].

6 Discussion

We have framed the problem of learning DAGs in the larger class of linear structural equation models and we have shown that a simple approach based on optimization techniques and without any acyclicity constraints is able to obtain similar recovery performances than state-of-the-art algorithms, see Figures 2 and 3.

The proposed \texttt{nodag} is also considerably faster than classical constraint-based and score-based methods (Figure 4). By avoiding the acyclicity constraint we are able to use a standard proximal gradient algorithm over a matrix \(A \in \mathbb{R}^{p \times p}\) and thus the computational cost of the method depends only on the size of the system \((p)\) and not on the sparsity level or the sample size.

\(^1\)Simulations performed on a standard laptop with 8Gb of RAM and an i5-8250U CPU
Figure 2: Average F1 score, true positive rate and false positive rate for the recovery of the skeleton. Different algorithms in different colours, the proposed nodag method with solid lines and algorithms from the literature dashed. Results for nodag-0.1 are not shown for $n = 100$ to improve readability.
Figure 3: Average structural hamming distances with respect to the true CPDAG (shd-cpdag) and to the true DAG (shd-graph). Different algorithms in different colours, the proposed nodag method with solid lines and algorithms from the literature dashed. The distance with respect to the empty graph is shown with black dotted lines. Results for nodag-0.1 are not shown for n = 100 to improve readability.
Moreover, the output of the nodag method parametrizes the inverse covariance matrix and thus provides an estimation of the parameters of the model, contrary to constraint-based algorithms. In particular, from the estimation of the $A$ matrix is possible to recover an estimate of the coefficient matrix $\Lambda$ in equation (3).

6.1 Feature directions

The nodag method estimates linear SEM without acyclicity constraints and thus it would be interesting to empirically test its performance in the recovery of SEM with cycles.

As for lasso [Friedman et al., 2010], graphical lasso [Friedman et al., 2007] and other $\ell_1$-penalized methods [Varando and Hansen, 2020] it is straightforward to extend the method to estimate the regularization path for a sequence of decreasing $\lambda$ values and thus being able to perform data-driven selection for the regularization coefficient. The good computational complexity make it feasible to combine the proposed algorithm with stability selection.
Figure 5: Graph estimated as the support of $A^*$ from solving the optimization problem (4) with $\lambda = 0.2$. In blue edges that are present in the conventionally accepted network [Sachs et al., 2005].
methods Meinshausen and Bühlmann [2010] and, by not imposing acyclicity, it allows to simply average matrices estimated from bootstrapped or sub-sampled data.

Finally, from a strictly computational point of view, it would be interesting to explore ways to speed up both the computations and the convergence of Algorithm 1. The sparsity of matrix $A$ in Algorithm 1 could probably be used to speed up or avoid the computation of its LU decomposition, this would in turn decrease the cost-per-iteration. Accelerated gradient-like methods could be applied to improve the speed of convergence [Beck and Teboulle, 2009], thus reducing the number of iterations needed to converge.

6.2 Reproducibility

The code and instructions to reproduce the examples, the simulation study and the real-world application are available at [https://github.com/gherardovarando/nodag_experiments](https://github.com/gherardovarando/nodag_experiments).

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A Algorithm implementation

Algorithm 1 details the pseudocode of the proposed proximal method to solve problem 4. Each iteration of the algorithm consists basically in the gradient computation and the line search loop where the gradient descent and the proximal operator are applied for decreasingly small step sizes until the descent and the Beck and Teboulle [2010] conditions are met. The algorithm terminates when the difference of the objective function computed in the last two iterations is less than a specified tolerance ($\varepsilon$) or when the maximum number of iterations ($M$) has been reached. The LU factorization of $A$, used to compute both the log-determinant and the inverse, is performed with the LAPACK implementation [Anderson et al., 1999] using partial pivoting.

The fortran code implementing algorithm 1 is available at [github.com/gherardovarando/nodag](https://github.com/gherardovarando/nodag).
**Algorithm 1** Proximal gradient algorithm for minimization of ℓ₁-penalized minus log-likelihood

**input:** \( \hat{R} \) the empirical correlation matrix,
\[ M \in \mathbb{N}, \varepsilon > 0, \lambda > 0, \alpha \in (0, 1) \]

1: initialize \( k = 0, A = L = U = I \)
2: \[ f = \sum_{i=1}^{p} \hat{R}_{ii} \]
3: \[ g = 0 \]
4: **repeat**
5: increase iteration counter \( k = k + 1 \)
6: compute \( A^{-1} \) using the LU decomposition
7: obtain the gradient \( D = 2 \hat{R}A - 2A^{-1} \)
8: copy \( A \) into \( A' \)
9: \[ f' = f, \quad g' = g \]
10: \[ s = 1 \]
11: **loop**
12: \[ A = A' - sD \]
13: soft thresholding \( A \) at level \( s\lambda \)
14: \( L, U = \) LU decomposition of \( A \)
15: compute \( \hat{R}A \)
16: \[ f = -2 \sum_{i=1}^{p} \log(U_{ii}) + \sum_{i,j=1}^{p} A_{ij} \left( \hat{R}A \right)_{ij} \]
17: \[ g = \lambda ||A||_1 \]
18: \[ \nu = \sum_{i,j=1}^{p} \frac{1}{2} (A_{ij} - A'_{ij})^2 + (A_{ij} - A'_{ij})D_{ij} \]
19: if \( f \leq f' + \nu \) and \( f + g \leq f' + g' \) then
20: break
21: else
22: \[ s = \alpha s \]
23: end if
24: **end loop**
25: \[ \delta = (f' + g' - f - g) \]
26: **until** \( k > M \) or \( \delta < \varepsilon \)

**output:** \( A, f, \delta, k \)

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