Variable selection in high-dimensional linear models: partially faithful distributions and the PC-simple algorithm

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Abstract

We consider the problem of variable selection in high-dimensional linear models where the number of covariates greatly exceeds the sample size. We introduce a new concept, called partial faithfulness, and discuss how this concept can be used to infer associations between the covariates and the response. Under the assumption of partial faithfulness, we develop a simplified version of the PC algorithm (Spirtes et al., 2000), the PC-simple algorithm. This algorithm is computationally feasible even with thousands of covariates, and yields consistency for high-dimensional variable selection under rather mild conditions on the (random) design matrix. Our assumptions are of a different nature than coherence conditions for penalty-based approaches like the Lasso: we make a simple assumption on the structure of the regression coefficients to exclude adversarial cases. We provide an efficient implementation of our algorithm in the `R`-package `pcalg` and demonstrate the method on real and simulated data.

Keywords: Directed acyclic graph, Elastic net, Graphical modeling, Lasso, Regression

1 Introduction

The variable selection problem for high-dimensional models has recently attracted a lot of attention. A particular stream of research has focused on penalty-based estimators whose computation is feasible and provably correct (Meinshausen and Bühlmann, 2006; Zou, 2006; Zhao and Yu, 2006; Wainwright, 2006; Candès and Tao, 2007; van de Geer, 2008; Zhang and Huang, 2008; Meinshausen and Yu, 2009; Huang et al., 2008; Bickel et al., 2009; Wasserman and Roeder, 2009; Candès and Plan, 2009). Another important approach for estimation in high-dimensional settings, including selection of variables, has been developed within the Bayesian paradigm, see for example George and McCulloch (1993, 1997); Brown et al. (1999, 2002); Nott and Kohn (2005); Park and Casella (2008). These methods rely on MCMC techniques which are typically very expensive for truly high-dimensional problems.

In this paper, we propose a method for variable selection in linear models which is "diametrically opposed" to penalty-based schemes. Reasons to look at such a new approach include: (i) From a practical perspective, it can be very valuable to have a "diametrically opposed" method in the tool-kit for high-dimensional data analysis, raising the confidence for relevance of variables if they are selected by two or more very different methods. (ii) From a methodological and theoretical perspective, we introduce a new framework of so-called partially faithful distributions. The name "partial faithfulness" is derived from the

concept of linear faithfulness that is used in graphical models. Our partial faithfulness condition is typically weaker than linear faithfulness (see Theorem 2) and this is emphasized by the word "partial". We prove that partial faithfulness arises naturally in the context of (high-dimensional) linear models if we make a simple assumption on the structure of the regression coefficients to exclude adversarial cases (see assumption (A2) and Theorem 1).

The framework of partial faithfulness can be exploited to construct an efficient hierarchical algorithm, called the "PC-simple algorithm", which is a simplification of the PC algorithm (Spirtes et al., 2000) for estimating directed acyclic graphs. We present asymptotic consistency of the PC-simple algorithm for variable selection in high-dimensional partially faithful linear models under rather general designs (Theorem 4). The required mathematical assumptions are very different from coherence assumptions for variable selection with penalty-based methods. The PC-simple algorithm can also be viewed as a generalization of correlation screening or "sure independence screening" (Fan and Lv, 2008). Thus, as a special case, we also obtain a consistency result for correlation screening, but our reasoning and mathematical assumptions are very different from Fan and Lv (2008), as shown in Theorem 5. We illustrate the PC-simple algorithm, using our implementation in the R-package `pcalg`, on high-dimensional simulated examples and some real data on riboflavin (vitamin B2) production by the bacterium *Bacillus subtilis*.

2 Model and notation

Let $X = (X^{(1)}, \ldots, X^{(p)}) \in \mathbb{R}^p$ be a vector of covariates with $E(X) = \mu_X$ and $\mathrm{cov}(X) = \Sigma_X$. Let $\epsilon \in \mathbb{R}$ with $E(\epsilon) = 0$ and $\mathrm{var}(\epsilon) = \sigma^2 > 0$, such that ϵ is uncorrelated with $X^{(1)}, \ldots, X^{(p)}$. Let $Y \in \mathbb{R}$ be defined by the following random design linear model:

$$Y = \delta + \sum_{j=1}^{p} \beta_j X^{(j)} + \epsilon, \tag{1}$$

for some parameters $\delta \in \mathbb{R}$ and $\beta = (\beta_1, \ldots, \beta_p)^T \in \mathbb{R}^p$. Note that we assume implicitly that $E(Y^2) < \infty$ and $E\{(X^{(j)})^2\} < \infty$ for $j = 1, \ldots, p$.

We consider models in which some (or most) of the β_j's are equal to zero. Our main goal is to identify the active set

$$\mathcal{A} = \{1 \le j \le p;\ \beta_j \neq 0\}$$

based on a sample of independent observations $(X_1, Y_1), \ldots, (X_n, Y_n)$ which are distributed as (X, Y). We denote the "effective dimension" of the model, i.e., the number of nonzero β_j's, by peff:

$$\mathrm{peff} = |\mathcal{A}|.$$

We consider the following additional assumptions:

(A1) Σ_X is strictly positive definite.

(A2) The regression coefficients satisfy:

$$\{\beta_j;\ j \in \mathcal{A}\} \sim f(b)db,$$

where $f(\cdot)$ denotes a density on (a subset of) $\mathbb{R}^{\text{peff}}$ of an absolutely continuous distribution with respect to Lebesgue measure.

Note that assumption (A1) implies identifiability of the regression parameters from the joint distribution of (X, Y) since $\beta = \Sigma_X^{-1}(\text{cov}(Y, X^{(1)}) \ldots, \text{cov}(Y, X^{(p)}))^T$. Assumption (A2) says that the non-zero regression coefficients are (fixed) realizations from an absolutely continuous distribution with respect to Lebesgue measure. Once the β_j's are realized, we fix them such that they can be considered as deterministic in the linear model (1). This framework is loosely related to a Bayesian formulation treating the β_j's as independent and identically distributed random variables from a prior distribution which is a mixture of point mass at zero (for β_j's with $j \notin \mathcal{A}$) and a density with respect to Lebesgue measure (for β_j's with $j \in \mathcal{A}$). Assumption (A2) is rather mild in the following sense: the regression coefficients having values zero can arise in an arbitrary way and only the non-zero coefficients are restricted to exclude adversarial cases. Interestingly, Candès and Plan (2009) also make an assumption on the regression coefficients using the concept of random sampling in their "generic S-sparse model", but other than that, there are no immediate deeper connections between their setting and ours.

We close this section by introducing some notation that we will use throughout the paper. We denote the (i, j)th entry of a matrix Σ_X by $\Sigma_{X;i,j}$. For any set $\mathcal{S} \subseteq \{1, \ldots, p\}$, we let $|\mathcal{S}|$ denote the cardinality of $\mathcal{S}$, and we let $\mathcal{S}^C$ denote the complement of $\mathcal{S}$ in $\{1, \ldots, p\}$. For example, $\{j\}^C = \{1, \ldots, p\} \setminus \{j\}$ for $j \in \{1, \ldots, p\}$. Moreover, we let $X^{(\mathcal{S})}$ denote the set of $X^{(j)}$'s for which $j \in \mathcal{S}$, i.e., $X^{(\mathcal{S})} = \{X^{(j)};\ j \in \mathcal{S}\}$. Finally, we use $\text{parcor}(Z^{(1)}, Z^{(2)}|W)$ and $\text{parcov}(Z^{(1)}, Z^{(2)}|W)$ to denote the population partial correlation and the population partial covariance between two variables $Z^{(1)}$ and $Z^{(2)}$ given a collection of variables W.

3 Linear faithfulness and partial faithfulness

3.1 Partial faithfulness

We now introduce the concept of partial faithfulness. This concept will allow us to identify the active set $\mathcal{A}$ using a simplified version of the PC algorithm (see Section 4).

Definition 1. *(Partial faithfulness) Let $X \in \mathbb{R}^p$ be a random vector (e.g. covariates), and let $Y \in \mathbb{R}$ be a random variable (e.g. response). The distribution of (X, Y) is said to be partially faithful if for every $j \in \{1, \ldots, p\}$*

$$\begin{aligned} &\textit{parcor}(Y, X^{(j)}|X^{(\mathcal{S})}) = 0 \ \ \textit{for some } \mathcal{S} \subseteq \{j\}^C \\ &\implies \textit{parcor}(Y, X^{(j)}|X^{(\{j\}^C)}) = 0. \end{aligned}$$

Note that for the linear model (1) with assumption (A1), $\beta_j = 0$ if and only if $\text{parcor}(Y, X^{(j)}|X^{(\{j\}^C)}) = 0$. Hence, such a model satisfies the partial faithfulness assumption if for every $j \in \{1, \ldots, p\}$:

$$\text{parcor}(Y, X^{(j)}|X^{(\mathcal{S})}) = 0 \text{ for some } \mathcal{S} \subseteq \{j\}^C \implies \beta_j = 0. \tag{2}$$

Theorem 1. *Consider the linear model (1) satisfying assumptions (A1) and (A2). Then partial faithfulness holds almost surely (with respect to the distribution generating the non-zero regression coefficients, see (A2)).*

A proof is given in the Appendix. Theorem 1 says that failure of partial faithfulness has probability zero (i.e., Lebesgue measure zero). This is in the same spirit as a result by Spirtes et al. (2000, Th. 3.2) for graphical models, saying that non-faithful distributions for directed acyclic graphs have Lebesgue measure zero, but we are considering here the notion of *partial* faithfulness.

A direct consequence of partial faithfulness is as follows:

Corollary 1. *Consider the linear model (1) satisfying the partial faithfulness condition. Then the following holds for every $j \in \{1, \ldots, p\}$:*

$$\textit{parcor}(Y, X^{(j)}|X^{(\mathcal{S})}) \neq 0 \textit{ for all } \mathcal{S} \subseteq \{j\}^C \iff \beta_j \neq 0.$$

A simple proof is given in the Appendix. Corollary 1 shows that an effective variable, i.e., an element of the active set $\mathcal{A}$, has a strong interpretation in the sense that all corresponding partial correlations are different from zero when conditioning on any subset $\mathcal{S} \subseteq \{j\}^C$. In many applications, such a strong concept of association is a desirable property.

3.2 Relationship between linear faithfulness and partial faithfulness

In this section, we discuss the relationship between partial faithfulness and the concept of linear faithfulness that is used in graphical models. This discussion clarifies the meaning of partial faithfulness. It is the only section which uses concepts from graphical modeling and it may be skipped, since it is not required to understand the remainder of the paper.

We first recall the definition of linear faithfulness. The distribution of a collection of random variables $Z^{(1)}, \ldots, Z^{(q)}$ can be depicted by a directed acyclic graph (DAG) G in which each vertex represents a variable, and the directed edges between the vertices encode conditional dependence relationships. The distribution of $(Z^{(1)}, \ldots, Z^{(q)})$ is said to be *linearly faithful* to the DAG G if the following holds for all $i \neq j \in \{1, \ldots, q\}$ and $\mathcal{S} \subseteq \{1, \ldots, q\} \setminus \{i, j\}$:

$$Z^{(i)} \text{ and } Z^{(j)} \text{ are d-separated by } Z^{(S)} \text{ in } G \iff \text{parcor}(Z^{(i)}, Z^{(j)}|Z^{(S)}) = 0,$$

see, e.g., Spirtes et al. (2000, page 47). In other words, linear faithfulness to a DAG G means that all and only all zero partial correlations among the variables can be read off from G using d-separation.

Partial faithfulness is related to a weaker version of linear faithfulness. We say that the distribution of (X, Y), where $X \in \mathbb{R}^p$ is a random vector (e.g. covariates) and $Y \in \mathbb{R}$ is a random variable (e.g. response), is *linearly Y-faithful* to a DAG G if the following holds for all $j \in \{1, \ldots, p\}$ and $\mathcal{S} \subseteq \{j\}^C$:

$$X^{(j)} \text{ and } Y \text{ are d-separated by } X^{(S)} \text{ in } G \iff \text{parcor}(X^{(j)}, Y|X^{(S)}) = 0. \qquad (3)$$

Thus, linear Y-faithfulness requires that all and only all zero partial correlations between Y and the $X^{(j)}$'s can be read off from the DAG using d-separation, but it does not require

that all and only all zero partial correlations among the $X^{(j)}$'s can be read off using d-separation.

We now consider the relationship between linear faithfulness, linear Y-faithfulness and partial faithfulness. First, we note that linear faithfulness and linear Y-faithfulness are graphical concepts, in that they link a distribution to a DAG, while partial faithfulness (Definition 1) is not a graphical concept. From the definition of linear faithfulness and linear Y-faithfulness, it is clear that linear faithfulness implies linear Y-faithfulness. The following theorem relates linear Y-faithfulness to partial faithfulness.

Theorem 2. *Assume that the distribution of (X, Y) is linearly Y-faithful (see (3)) to a DAG in which Y is childless. Then partial faithfulness holds.*

A proof is given in the Appendix. We note that a distribution is typically linearly Y-faithful to several DAGs. Theorem 2 applies if Y is childless in at least one of these graphs.

We illustrate Theorem 2 by three examples. Example 1 shows a distribution where partial faithfulness does not hold. In this case, Theorem 2 does not apply, because the distribution of (X, Y) is not linearly Y-faithful to any DAG in which Y is childless. Examples 2 and 3 show distributions where partial faithfulness does hold. In Example 2, the distribution of (X, Y) is linearly Y-faithful to a DAG in which Y is childless, and hence partial faithfulness follows from Theorem 2. On the other hand, in Example 3, the distribution of (X, Y) is not linearly Y-faithful to any DAG in which Y is childless. This shows that linear Y-faithfulness to a DAG in which Y is childless is not a necessary condition for partial faithfulness.

Example 1. *Consider the following Gaussian linear model:*

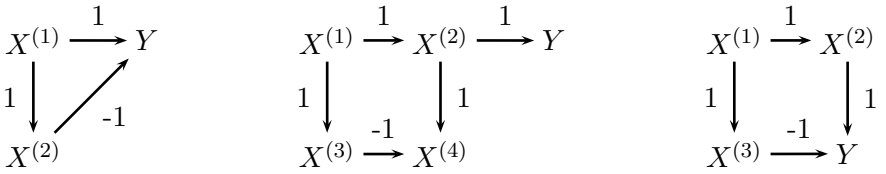
$$X^{(1)} = \varepsilon_1,\ X^{(2)} = X^{(1)} + \varepsilon_2,\ Y = X^{(1)} - X^{(2)} + \varepsilon,$$

where ε_1, ε_2 and ε are independent standard Normal random variables. This model can be represented by the linear model (1) *with $\beta_1 = 1$ and $\beta_2 = -1$. Furthermore, the distribution of $(X, Y) = (X^{(1)}, X^{(2)}, Y)$ factorizes according to the DAG in Figure 1(a).*

Note that the distribution of (X, Y) is not partially faithful, since parcor$(Y, X^{(1)}|\emptyset) =$ cor$(Y, X^{(1)}) = 0$ but parcor$(Y, X^{(1)}|X^{(2)}) \neq 0$. We now discuss why Theorem 2 does not apply. First, we note that the distribution of (X, Y) is not linearly Y-faithful to the DAG in Figure 1(a), since cor$(X^{(1)}, Y) = 0$ but $X^{(1)}$ and Y are not d-separated in the DAG by the empty set. The zero correlation between $X^{(1)}$ and Y occurs because $X^{(1)} = \varepsilon_1$ drops out of the equation for Y due to a parameter cancellation that is similar to equation (11) *in the proof of Theorem 1: $Y = X^{(1)} - X^{(2)} + \varepsilon = \varepsilon_1 - (\varepsilon_1 + \varepsilon_2) + \varepsilon = -\varepsilon_2 + \varepsilon$. The distribution of (X, Y) is linearly faithful (and hence also linearly Y-faithful) to another DAG, namely $X^{(1)} \to X^{(2)} \leftarrow Y$, but such a DAG is not allowed in Theorem 2 because Y has a child. The distribution of (X, Y) is not linearly Y-faithful to any DAG in which Y is childless, and hence Theorem 2 does not apply.*

Example 2. *Consider the following Gaussian linear model:*

$$X^{(1)} = \varepsilon_1,\ X^{(2)} = X^{(1)} + \varepsilon_2,\ X^{(3)} = X^{(1)} + \varepsilon_3,\ X^{(4)} = X^{(2)} - X^{(3)} + \varepsilon_4,\ Y = X^{(2)} + \varepsilon,$$



(a) Example 1 (b) Example 2 (c) Example 3

Figure 1: Graphical representation of the models used in Examples 1 - 3.

where $\varepsilon_1, \ldots, \varepsilon_4$ and ε are independent standard Normal random variables. This model can be represented by the linear model (1) with $\beta_1 = \beta_3 = \beta_4 = 0$ and $\beta_2 = 1$. Furthermore, the distribution of $(X, Y) = (X^{(1)}, \ldots, X^{(4)}, Y)$ factorizes according to the DAG in Figure 1(b).

Note that the distribution of (X, Y) is partially faithful, since $parcor(Y, X^{(j)}|X^{(\{j\}^C)}) \neq 0$ only for $j = 2$, and $parcor(Y, X^{(2)}|X^{(\mathcal{S})}) \neq 0$ for any $\mathcal{S} \subseteq \{1, 3, 4\}$. In this example, partial faithfulness follows from Theorem 2, since the distribution of (X, Y) is linearly Y-faithful to the DAG in Figure 1(b) and Y is childless in this DAG. Note that the distribution of (X, Y) is not linearly faithful to the DAG in Figure 1(b), since $cor(X^{(1)}, X^{(4)}) = 0$ but $X^{(1)}$ and $X^{(4)}$ are not d-separated in the DAG by the empty set. Moreover, there does not exist any other DAG to which the distribution of (X, Y) is linearly faithful. Thus, this example also illustrates that linear Y-faithfulness is strictly weaker than linear faithfulness.

Example 3. *Consider the following Gaussian linear model:*

$$X^{(1)} = \varepsilon_1,\ X^{(2)} = X^{(1)} + \varepsilon_2,\ X^{(3)} = X^{(1)} + \varepsilon_3,\ Y = X^{(2)} - X^{(3)} + \varepsilon,$$

where ε_1, ε_2, ε_3 and ε are independent standard Normal random variables. This model can be represented by the linear model (1) with $\beta_1 = 0$, $\beta_2 = 1$ and $\beta_3 = -1$. Furthermore, the distribution of $(X, Y) = (X^{(1)}, X^{(2)}, X^{(3)}, Y)$ factorizes according to the DAG in Figure 1(c).

Note that the distribution of (X, Y) is partially faithful, since $parcor(Y, X^{(j)}|X^{(\{j\}^C)}) \neq 0$ for $j \in \{2, 3\}$, and $parcor(Y, X^{(2)}|X^{(\mathcal{S})}) \neq 0$ for any $\mathcal{S} \subseteq \{1, 3\}$, and $parcor(Y, X^{(3)}|X^{(\mathcal{S})}) \neq 0$ for any $\mathcal{S} \subseteq \{1, 2\}$. However, in this case partial faithfulness does not follow from Theorem 2, since the distribution of (X, Y) is not linearly Y-faithful to the DAG in Figure 1(c), since $cor(X^{(1)}, Y) = 0$ but $X^{(1)}$ and Y are not d-separated in the DAG by the empty set. Moreover, there does not exist any other DAG to which the distribution of (X, Y) is linearly Y-faithful.

4 The PC-simple algorithm

4.1 Population version of the PC-simple algorithm

We now explore how partial faithfulness can be used for variable selection. In order to show the key ideas of the algorithm, we first assume that the population partial correlations are known. In Section 4.2 we consider the more realistic situation where the population partial correlations are unknown, and need to be estimated from data.

Recall that partial faithfulness for the linear model (1) says:

$$\text{parcor}(Y, X^{(j)}|X^{(\mathcal{S})}) = 0 \text{ for some } \mathcal{S} \subseteq \{j\}^C \implies \beta_j = 0.$$

The easiest relation is with $\mathcal{S} = \emptyset$:

$$\text{cor}(Y, X^{(j)}) = 0 \implies \beta_j = 0, \tag{4}$$

showing that the active set $\mathcal{A}$ cannot contain any j for which $\text{cor}(Y, X^{(j)}) = 0$. Hence, we can screen all marginal correlations between pairs $(Y, X^{(j)})$, $j = 1, \ldots, p$, and build a first set of candidate active variables

$$\mathcal{A}^{[1]} = \{1 \le j \le p;\ \text{cor}(Y, X^{(j)}) \neq 0\}.$$

We call this the step_1 active set or the correlation screening active set, and we know by (4) that

$$\mathcal{A} \subseteq \mathcal{A}^{[1]}. \tag{5}$$

Such correlation screening may reduce the dimensionality of the problem by a substantial or even huge amount, and due to (5), we can use other variable selection methods on the reduced set of variables $\mathcal{A}^{[1]}$.

Furthermore, we can screen partial correlations of order one by using the following relation: for $j \in \mathcal{A}^{[1]}$,

$$\text{parcor}(Y, X^{(j)}|X^{(k)}) = 0 \text{ for some } k \in \mathcal{A}^{[1]} \setminus \{j\} \implies \beta_j = 0. \tag{6}$$

That is, for checking whether the jth covariate remains in the model, we can additionally screen all partial correlations of order one. Note that we only consider partial correlations given variables in the step_1 active set $\mathcal{A}^{[1]}$. This is similar to what is done in the PC algorithm, and yields an important computational reduction while still allowing us to eventually identify the true active set $\mathcal{A}$ (see Algorithm 1 and Theorem 3). Thus, screening partial correlations of order one using (6) leads to a smaller active set

$$\mathcal{A}^{[2]} = \{j \in \mathcal{A}^{[1]};\ \text{parcor}(Y, X^{(j)}|X^{(k)}) \neq 0 \text{ for all } k \in \mathcal{A}^{[1]} \setminus \{j\}\} \subseteq \mathcal{A}^{[1]}.$$

This new step_2 active set $\mathcal{A}^{[2]}$ further reduces the dimensionality of the candidate active set, and because of (6) we still have that $\mathcal{A}^{[2]} \supseteq \mathcal{A}$.

We can continue screening of higher-order partial correlations, resulting in a nested sequence of step_m active sets

$$\mathcal{A}^{[1]} \supseteq \mathcal{A}^{[2]} \supseteq \ldots \supseteq \mathcal{A}^{[m]} \supseteq \ldots \supseteq \mathcal{A}. \tag{7}$$

A step_m active set $\mathcal{A}^{[m]}$ can be used as dimensionality reduction and any favored variable selection method can then be used for the reduced linear model with covariates corresponding to indices in $\mathcal{A}^{[m]}$. Alternatively, we can continue the algorithm until the candidate active set does not change anymore. This leads to our PC-simple algorithm (Algorithm 1).

The value m that is reached in Algorithm 1 is called m_{reach}:

$$m_{\text{reach}} = \min\{m;\ |\mathcal{A}^{[m]}| \le m\}. \tag{8}$$

The following theorem shows that the population version of the PC-simple algorithm correctly identifies the active set $\mathcal{A}$ for linear model (1) satisfying (A1) and partial faithfulness.

Algorithm 1 The population version of the PC-simple algorithm.

1: Set $m = 1$. Do correlation screening, see (4), and build the step$_1$ active set $\mathcal{A}^{[1]} = \{1 \le j \le p;\ \mathrm{cor}(Y, X^{(j)}) \neq 0\}$.
2: **repeat**
3: $m = m + 1$. Construct the step$_m$ active set:

$$\mathcal{A}^{[m]} = \{j \in \mathcal{A}^{[m-1]};\ \mathrm{parcor}(Y, X^{(j)}|X^{(\mathcal{S})}) \neq 0 \text{ for all } \mathcal{S} \subseteq \mathcal{A}^{[m-1]} \setminus \{j\} \text{ with } |\mathcal{S}| = m - 1\}.$$

4: **until** $|\mathcal{A}^{[m]}| \le m$.

Theorem 3. *For the linear model (1) satisfying (A1) and partial faithfulness, the population version of the PC-simple algorithm identifies the true underlying active set, i.e.* $\mathcal{A}^{[m_{\mathrm{reach}}]} = \mathcal{A} = \{1 \le j \le p;\ \beta_j \neq 0\}$.

A proof is given in the Appendix. We note that partial faithfulness (which is often weaker than linear faithfulness, see Section 3.2) is sufficient to guarantee correct inference of the population PC-simple algorithm. The PC-simple algorithm is similar to the PC algorithm (Spirtes et al., 2000, Section 5.4.2). But the PC algorithm considers all ordered pairs of variables in $(X^{(1)}, \ldots, X^{(p)}, Y)$, while we only consider ordered pairs $(Y, X^{(j)})$, $j \in \{1, \ldots, p\}$. The reason that we do not need to consider pairs $(X^{(j)}, X^{(k)})$ is that we are only interested in associations between Y and $X^{(j)}$. Less obvious is the fact that we can restrict ourselves to consider conditioning sets in the neighborhood of Y only (instead of both neighborhoods of Y and $X^{(j)}$ as in the PC algorithm).

4.2 Sample version of the PC-simple algorithm

For finite samples, we need to estimate partial correlations. We use the following shorthand notation:

$$\begin{aligned} \rho(Y, j|\mathcal{S}) &= \mathrm{parcor}(Y, X^{(j)}|X^{(\mathcal{S})}), & \hat{\rho}(Y, j|\mathcal{S}) &= \widehat{\mathrm{parcor}}(Y, X^{(j)}|X^{(\mathcal{S})}), \\ \rho(i, j|\mathcal{S}) &= \mathrm{parcor}(X^{(i)}, X^{(j)}|X^{(\mathcal{S})}), & \hat{\rho}(i, j|\mathcal{S}) &= \widehat{\mathrm{parcor}}(X^{(i)}, X^{(j)}|X^{(\mathcal{S})}), \end{aligned}$$

where the "hat-versions" denote sample partial correlations. The sample partial correlations can be calculated recursively: for any $k \in \mathcal{S}$ we have

$$\hat{\rho}(Y, j|\mathcal{S}) = \frac{\hat{\rho}(Y, j|\mathcal{S} \setminus \{k\}) - \hat{\rho}(Y, k|\mathcal{S} \setminus \{k\})\hat{\rho}(j, k|\mathcal{S} \setminus \{k\})}{\sqrt{\{1 - \hat{\rho}(Y, k|\mathcal{S} \setminus \{k\})^2\}\{1 - \hat{\rho}(j, k|\mathcal{S} \setminus \{k\})^2\}}}.$$

In order to test whether a partial correlation is zero, we apply Fisher's Z-transform

$$Z(Y, j|\mathcal{S}) = \frac{1}{2} \log\left(\frac{1 + \hat{\rho}(Y, j|\mathcal{S})}{1 - \hat{\rho}(Y, j|\mathcal{S})}\right). \tag{9}$$

Classical decision theory in the Gaussian case yields the following rule when using significance level α. Reject the null-hypothesis $H_0(Y, j|\mathcal{S}) :\ \rho(Y, j|\mathcal{S}) = 0$ against the two-sided alternative $H_A(Y, j|\mathcal{S}) :\ \rho(Y, j|\mathcal{S}) \neq 0$ if $\sqrt{n - |\mathcal{S}| - 3}|Z(Y, j|\mathcal{S})| > \Phi^{-1}(1 - \alpha/2)$, where

$\Phi(\cdot)$ denotes the standard normal cumulative distribution function. The Gaussian distribution serves as a reference: even in the absence of a Gaussian distribution, the rule above is a thresholding operation.

The sample version of the PC-simple algorithm is obtained by replacing the statements about $\text{parcor}(Y, X^{(j)}|X^{(\mathcal{S})}) \neq 0$ (including $\mathcal{S} = \emptyset$) in Algorithm 1 by

$$\sqrt{n - |\mathcal{S}| - 3}|Z(Y, j|\mathcal{S})| > \Phi^{-1}(1 - \alpha/2).$$

The resulting estimated set of variables is denoted by $\widehat{\mathcal{A}}(\alpha) = \widehat{\mathcal{A}}^{\hat{m}_{\text{reach}}}(\alpha)$, where $\hat{m}_{\text{reach}}$ is the estimated version of the quantity in (8). The only tuning parameter α of the PC-simple algorithm is the significance level for testing the partial correlations.

We note that the PC-simple algorithm is very different from a greedy forward (or backward) scheme: it screens many correlations or partial correlations at once and may delete many variables at once. Furthermore, it is a more sophisticated pursuit of variable screening than the marginal correlation approach in Fan and Lv (2008) or the low-order partial correlation method in Wille and Bühlmann (2006). Castelo and Roverato (2006) extended the latter and considered a limited-order partial correlation approach. However, their method does not exploit the clever trick of the PC-simple algorithm that it is sufficient to consider only conditioning sets $\mathcal{S}$ which have survived in the previous step_{m-1} active set $\mathcal{A}^{[m-1]}$. Therefore, the algorithm of Castelo and Roverato (2006) is often infeasible and has to be approximated by a Monte Carlo approach.

Since the PC-simple algorithm is a simplified version of the PC algorithm, its computational complexity is bounded above by that of the PC algorithm. The complexity of the PC algorithm is difficult to evaluate exactly, but the worst case is polynomial in p: the crude bound is $O(p^{\text{peff}})$, see Kalisch and Bühlmann (2007, formula (4)). In fact, we can easily use our PC-simple algorithm for problems where $p \approx 100 - 5'000$, as demonstrated in Section 6.

5 Asymptotic results in high dimensions

5.1 Consistency of the PC-simple algorithm

We show that the PC-simple algorithm from Section 4.2 is asymptotically consistent for variable selection, even if p is much larger than n, if we assume that the true underlying linear model is sparse.

We consider the linear model in (1). In order to simplify the asymptotic calculations, we assume a joint Gaussian distribution (see (B1) below). To capture high-dimensional behavior, we let the dimension grow as a function of sample size and thus, $p = p_n$ and also the distribution of (X, Y) (including e.g. partial correlations $\rho(\cdot, \cdot|\cdot) = \rho_n(\cdot, \cdot|\cdot)$), the regression coefficients $\beta_j = \beta_{j,n}$ and the active set $\mathcal{A} = \mathcal{A}_n$ with $\text{peff} = \text{peff}_n = |\mathcal{A}_n|$ change with n. Our assumptions are as follows.

(B1) The distribution in model (1)

$$(X, Y) \sim P_n = \mathcal{N}_{p_n+1}(\mu_{X,Y;n}, \Sigma_{X,Y;n})$$

is Gaussian and P_n satisfies assumption (A1) and the partial faithfulness condition for all n.

(B2) The dimension $p_n = O(n^a)$ for some $0 \leq a < \infty$.

(B3) The cardinality of the active set $\text{peff}_n = |\mathcal{A}_n| = |\{1 \leq j \leq p_n;\ \beta_{j,n} \neq 0\}|$ satisfies: $\text{peff}_n = O(n^{1-b})$ for some $0 < b \leq 1$.

(B4) The partial correlations $\rho_n(Y, j|\mathcal{S}) = \text{parcor}(Y, X^{(j)}|X^{(\mathcal{S})})$ satisfy:

$$\inf\Big\{|\rho_n(Y, j|\mathcal{S})|;\ 1 \leq j \leq p_n,\ \mathcal{S} \subseteq \{j\}^C \text{ with } \rho_n(Y, j|\mathcal{S}) \neq 0\Big\} \geq c_n,$$

where $c_n^{-1} = O(n^d)$ for some $0 \leq d < b/2$, and b is as in (B3).

(B5) The partial correlations $\rho_n(Y, j|\mathcal{S})$ and $\rho_n(i, j|\mathcal{S}) = \text{parcor}(X^{(i)}, X^{(j)}|X^{(\mathcal{S})})$ satisfy:

$$\sup_{n,j,\mathcal{S}\subseteq\{j\}^C} |\rho_n(Y, j|\mathcal{S})| \leq M < 1, \quad \sup_{n,i\neq j,\mathcal{S}\subseteq\{i,j\}^C} |\rho_n(i, j|\mathcal{S})| \leq M < 1.$$

The Gaussian assumption in (B1) is not crucial: Theorem 3 shows that the population case does not require a Gaussian assumption and (B1) is only made to simplify asymptotic calculations. We remark that it is virtually impossible to check assumptions (B1)-(B5) in practice, with the exception of (B2). However, this is common to assumptions made in existing methods for high-dimensional variable selection, such as the neighborhood stability condition (Meinshausen and Bühlmann, 2006), the irrepresentable condition (Zhao and Yu, 2006), or the restrictive eigenvalue assumption (Bickel et al., 2009). A more detailed discussion of assumptions (B1)-(B5) is given in Section 5.2.

Denote by $\widehat{\mathcal{A}}_n(\alpha)$ the estimated set of variables from the PC-simple algorithm in Section 4.2 with significance level α.

Theorem 4. *Consider the linear model (1) and assume (B1)-(B5). Then there exists a sequence $\alpha_n \to 0$ $(n \to \infty)$ and a constant $0 < C < \infty$ such that the PC-simple algorithm satisfies:*

$$pr[\widehat{\mathcal{A}}_n(\alpha_n) = \mathcal{A}_n] = 1 - O(\exp(-Cn^{1-2d})) \to 1 \ (n \to \infty),$$

where d is as in (B4).

A proof is given in the Appendix. A choice for the value of the tuning parameter leading to consistency is $\alpha_n = 2(1 - \Phi(n^{1/2}c_n/2))$. Note that this choice depends on the unknown lower bound of the partial correlations in (B4). This value α_n, although being a significance level of a single test, is a tuning parameter which allows to control type I and II errors over the many tests which are pursued in the PC-simple algorithm.

5.2 Discussion of the conditions of Theorem 4

There is a substantial amount of recent work on high-dimensional and computationally tractable variable selection, most of it considering (versions of) the Lasso (Tibshirani, 1996) or the Dantzig selector (Candès and Tao, 2007). Neither of these methods exploit partial faithfulness and thus, it is interesting to discuss our conditions with a view towards other established results.

First, we remark that most other works on high-dimensional variable selection make assumptions on the design matrix but allow for any sparse parameter vector β; an exception is the work by Candès and Plan (2009). In this paper, our assumption (A2) poses some restrictions on the non-zero components of β but allows for rather general designs where the Lasso is inconsistent, see Example 4 below.

For the Lasso, Meinshausen and Bühlmann (2006) proved that a so-called "neighborhood stability" condition is sufficient and almost necessary for consistent variable selection (the word "almost" refers to the fact that a strict inequality "$<$" appears in the sufficient condition whereas for necessity, the corresponding relation is a "$\leq$" relation). Zou (2006) and Zhao and Yu (2006) gave a different, but equivalent condition: in the latter work, it is called the "irrepresentable" condition. We point out that the neighborhood stability or the irrepresentable condition can quite easily fail to hold (e.g. in Example 4 below) which, due to the almost necessity of the condition, implies inconsistency of the Lasso for variable selection. The adaptive Lasso (Zou, 2006) or other two-stage Lasso and thresholding procedures (Meinshausen and Yu, 2009) yield consistent variable selection under substantially weaker conditions than the neighborhood stability or irrepresentable condition, see also Example 4 below. Such two-stage procedures rely on results for $\|\hat{\beta} - \beta\|_q$ $(q = 1, 2)$ whose optimal convergence rate to zero is guaranteed under remarkable mild assumptions (Bickel et al., 2009) (These conditions are not directly comparable with our conditions (B1)-(B5)).

Regarding our assumption (B1), the Gaussian distribution can be relaxed at the price of tightening other assumptions and a more involved proof. Note that the population version does not require a Gaussian assumption (Theorem 3). The inclusion of (A1) is rather weak since we do not require explicitly any behavior of the covariance matrix $\Sigma_X = \Sigma_{X;n}$ in the sequence of distributions P_n $(n \in \mathbb{N})$, except for strict positive definiteness for all n (but not an explicit bound on the minimal eigenvalue). The partial faithfulness condition follows from Theorem 1 if we assume (A2) in Section 2 for every n. It is also interesting to note that we require *partial* faithfulness only: dependence relations among covariates enter only indirectly via conditioning sets $\mathcal{S} \subseteq \{1, \ldots p\} \setminus \{j\}$ for a partial correlation between the response Y and some covariate $X^{(j)}$. However, as a word of caution, the results by Robins et al. (2003) indicate that uniform consistency for variable selection may fail to hold due to "nearly" partially faithful distributions. Assumption (B2) allows for an arbitrary polynomial growth of dimension as a function of sample size, i.e. high-dimensionality, while (B3) is a sparseness assumption in terms of the number of effective variables. Both (B2) and (B3) are fairly standard assumptions in high-dimensional asymptotics. Assumption (B4) imposes a constraint regarding the detectability of small non-zero partial correlations. Obviously, we cannot detect non-zero values of order $O(1/\sqrt{n})$. When $\text{peff}_n = \text{peff} < \infty$ and $b = 1$ in (B3), this is indeed what assumption (B4) says, as it requires the non-zero partial correlations to decay not faster than $n^{-1/2+\epsilon}$ for some $\epsilon > 0$. In high-dimensional models with $b < 1$ in (B3), assumption (B4) is stronger: it requires the partial correlations to decay not faster than $n^{-b/2+\epsilon}$ for some $\epsilon > 0$. Assumption (B4) is crucial for controlling the type II errors in the many tests of the PC-simple algorithm, see the proof of Theorem 4. Finally, assumption (B5) is excluding perfect collinearity: since we require all partial correlations to be bounded by a constant $M < 1$ for all $n \in \mathbb{N}$, this imposes a rather mild additional restriction on the covariance matrix $\Sigma_{X,Y} = \Sigma_{X,Y;n}$. If the dimension p is fixed (with fixed distribution P in the linear model), (B2), (B3) and (B4) hold automatically,

and (B1) and (B5) remain as the only conditions.

Although our assumptions are not directly comparable to the neighborhood stability or irrepresentable condition for the Lasso, it is easy to construct examples where the Lasso fails to be consistent while the PC-simple algorithm recovers the true set of variables, as shown by the following example.

Example 4. *Consider a Gaussian linear model as in (1) with*

$$p = 4,\ \text{peff} = 3, \sigma^2 = 1, \mu_X = (0, \ldots, 0)^T,$$
$$\Sigma_X = \begin{pmatrix} 1 & \rho_1 & \rho_1 & \rho_2 \\ \rho_1 & 1 & \rho_1 & \rho_2 \\ \rho_1 & \rho_1 & 1 & \rho_2 \\ \rho_2 & \rho_2 & \rho_2 & 1 \end{pmatrix}, \quad \rho_1 = -0.4,\ \rho_2 = 0.2,$$
$$\beta_1, \beta_2, \beta_3 \text{ fixed i.i.d. realizations from } \mathcal{N}(0,1),\ \beta_4 = 0.$$

It is shown in Zou (2006, Cor. 1) that the Lasso is inconsistent for this model. On the other hand, (B1) holds because of Theorem 1, and also (B5) is true. These are all the conditions for the PC-simple algorithm for a fixed distribution P. Hence, the PC-simple algorithm is consistent for variable selection. It should be noted though that the adaptive Lasso is also consistent for this example.

5.3 Asymptotic behavior of correlation screening

For correlation screening, see formula (5), we do not require any sparsity. We also remark that correlation screening is the same as "sure independence screening" by Fan and Lv (2008), but our reasoning, assumptions and mathematical derivations via partial faithfulness are very different. We define:

(C1) as assumption (B4) but for marginal correlations $\text{cor}(Y, X^{(j)}) = \rho_n(Y, j)$ only.

(C2) as assumption (B5) but for marginal correlations $\text{cor}(Y, X^{(j)}) = \rho_n(Y, j)$ only.

Denote by $\widehat{\mathcal{A}}_n^{[1]}(\alpha)$ the correlation screening active set estimated from data using significance level α, i.e. the first step in the sample version of the PC-simple algorithm.

Theorem 5. *Consider the linear model (1) and assume (B1), (B2), (C1) and (C2). Then there exists a sequence $\alpha_n \to 0$ $(n \to \infty)$ and a constant $0 < C < \infty$ such that:*

$$pr[\widehat{\mathcal{A}}_n^{[1]}(\alpha_n) \supseteq \mathcal{A}_n] = 1 - O(\exp(-Cn^{1-2d})) \to 1 \ (n \to \infty),$$

where $d > 0$ is as in (C1).

A proof is given in the Appendix. A possible choice of α_n is $\alpha_n = 2(1 - \Phi(n^{1/2} c_n/2))$. As pointed out above, we do not make any assumptions on sparsity. However, for non-sparse problems, many correlations may be non-zero, preventing an effective dimension reduction. In such problems, $\widehat{\mathcal{A}}^{[1]}$ can still be large, for example almost as large as the full set $\{1 \le j \le p\}$.

Under some restrictive conditions on the covariance Σ_X of the random design, Fan and Lv (2008) have shown that correlation (or sure independence) screening is overestimating

the active set $\mathcal{A}$, as stated in Theorem 5. However, Theorem 5 indicates that this result holds without any strong assumptions on Σ_X but assuming partial faithfulness instead (while Fan and Lv (2008) do not assume partial faithfulness). Hence, our result justifies correlation screening as a more general tool, extending the range of applications, than what it appears to be from the setting of Fan and Lv (2008).

6 Numerical results

6.1 ROC analysis for simulated data

We simulate data according to a Gaussian linear model as in (1) having p covariates with $\mu_X = (0, \ldots, 0)^T$ and covariance matrix $\Sigma_{X;i,j} = \rho^{|i-j|}$. In order to generate values for β, we follow (A2): a certain number peff of coefficients β_j have a value different from zero. The values of the nonzero β_j's are sampled independently from a standard normal distribution and the indices of the nonzero β_j's are evenly spaced between 1 and p. We consider a low- and a high-dimensional setting:

Low-dimensional: $p = 19$, peff $= 3$, $n = 100$; $\rho \in \{0, 0.3, 0.6\}$ with 1000 replicates

High-dimensional: $p = 499$, peff $= 10$, $n = 100$; $\rho \in \{0, 0.3, 0.6\}$ with 300 replicates

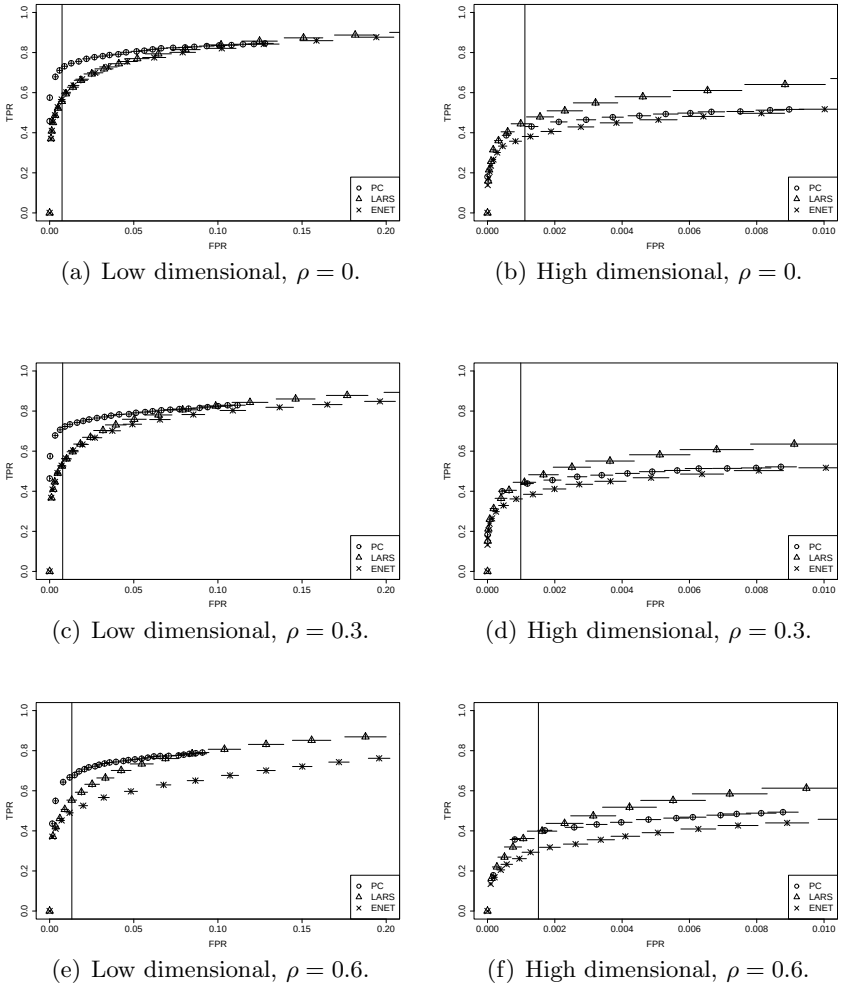
We evaluate the performance of the methods using ROC curves which measure the capacity for variable selection independently from the issue of choosing good tuning parameters. We compare the PC-simple algorithm (PC, R-package `pcalg`) with the Lasso using the LARS algorithm (Efron et al., 2004) (LARS, R-package `lars`) and with the Elastic Net (Zou and Hastie, 2005) (ENET, R-package `elasticnet`). For the latter, we vary the ℓ^1-penalty parameter only while keeping the ℓ^2-penalty parameter fixed at the default value from the R-package `elasticnet` to construct the ROC curve. In our PC-simple algorithm, the proposed default value for the tuning parameter is $\alpha = 0.05$: its performance is indicated by the intersection of the vertical lines and the ROC curves in Figure 2. We refer to Meinshausen and Bühlmann (2008) for a more principled way to choose the amount of regularization. They present a generic approach based on subsampling which can control the familywise error rate.

We first discuss the results of the low-dimensional settings (Figures 2(a), 2(c), 2(e)). For small false positive rates (FPRs, see equation (10) for the definition), our PC-simple algorithm is clearly dominating LARS and ENET. If the correlation among the covariates increases, the performance of ENET deteriorates, whereas the performances of PC-simple and LARS do not vary much. When focusing on the FPR arising from the default value for α in our method, PC-simple outperforms LARS and ENET by a large margin. Note that many application areas call for a small FPR, as discussed also in Section 6.3.

For the high-dimensional settings (Figures 2(b), 2(d), 2(f)), we see that for small FPRs, the difference between the methods is small. LARS performs best, while ENET is worst and PC-simple is somewhere in between. For larger FPRs, this effect becomes stronger. Up to the FPR which arises at the default value of $\alpha = 0.05$, PC-simple is never significantly outperformed by either LARS or ENET.

Further examples, with $p = 1000$, peff $= 5$, $n = 50$ and equi-correlated design $\Sigma_{X;i,j} = 0.5$ for $i \neq j$ and $\Sigma_{X;i,i} = 1$ for all i, are reported in Bühlmann (2008).

Finally, regarding runtimes of the different methods, the computing time of the PC-simple algorithm on 10 different (small) values of α has about the same order of magnitude as LARS or ENET for their whole solution paths. Thus, the PC-simple method is certainly feasible for high-dimensional problems.



(a) Low dimensional, $\rho = 0$.

(b) High dimensional, $\rho = 0$.

(c) Low dimensional, $\rho = 0.3$.

(d) High dimensional, $\rho = 0.3$.

(e) Low dimensional, $\rho = 0.6$.

(f) High dimensional, $\rho = 0.6$.

Figure 2: ROC curves for the simulation study in Section 6.1. The horizontal and vertical bars indicate 95% confidence intervals for the FPR and TPR, respectively. The solid vertical lines indicate the performance of the PC-simple algorithm using the default $\alpha = 0.05$.

6.2 Prediction optimal tuned methods for simulated data

We now compare the PC-simple algorithm to several existing methods when using prediction optimal tuning. It is known that the prediction-optimal tuned Lasso overestimates the true model (Meinshausen and Bühlmann, 2006). But the adaptive Lasso (Zou, 2006) and the relaxed Lasso (Meinshausen, 2007) correct Lasso's overestimation behavior and

prediction-optimal tuning for these methods yields a good amount of regularization for variable selection.

We use our PC-simple algorithm for variable selection and then use the Lasso or the adaptive Lasso to estimate the coefficients for the sub-model selected by the PC-simple algorithm. We compare this procedure to the Lasso, the adaptive Lasso and the relaxed Lasso. For simplicity, we do not show results for the elastic net (which was found to be worse in terms of ROC-curves than the Lasso, see Section 6.1).

We simulate from a Gaussian linear model as in (1) with $p = 1000$, $\text{peff} = 20$, $n = 100$ and:

$$\begin{aligned}&\mu_X = (0, \ldots, 0)^T,\ \Sigma_{X;i,j} = 0.5^{|i-j|},\ \sigma^2 = 1,\\ &\beta_1, \ldots, \beta_{20} \text{ i.i.d. } \sim \mathcal{N}(0,1), \quad \beta_{21} = \ldots = \beta_{1000} = 0,\end{aligned}$$

with 100 replicates.

We consider the following performance measures:

$$\begin{array}{ll}\|\hat{\beta} - \beta\|_2^2 = \sum_{j=1}^p (\hat{\beta}_j - \beta_j)^2 & \text{(MSE Coeff)}\\ E_X[\{X^T(\hat{\beta} - \beta)\}^2] = (\hat{\beta} - \beta)\text{cov}(X)(\hat{\beta} - \beta)^T & \text{(MSE Pred)}\\ \sum_{j=1}^p I(\hat{\beta}_j \neq 0, \beta_j \neq 0) / \sum_{j=1}^p I(\beta_j \neq 0) & \text{(true positive rate (TPR))}\\ \sum_{j=1}^p I(\hat{\beta}_j \neq 0, \beta_j = 0) / \sum_{j=1}^p I(\beta_j = 0) & \text{(false positive rate (FPR))}\end{array} \tag{10}$$

where $I(\cdot)$ denotes the indicator function.

The methods are used as follows. Prediction optimal tuning is pursued with a validation set having the same size as the training data. The Lasso is computed using the `lars`-package from `R`. For the adaptive Lasso, we first compute a prediction-optimal Lasso as initial estimator $\hat{\beta}_{init}$, and the adaptive Lasso is then computed by solving the following optimization problem:

$$\text{argmin}_{\beta \in \mathbb{R}^p}(\sum_{i=1}^n (Y_i - X_i^T \beta)^2 + \lambda \sum_{j=1}^p |\beta_j| / |\hat{\beta}_{init,j}|),$$

where λ is chosen again in a prediction-optimal way. The computations are done with the `lars`-package from `R`, using re-scaled covariates for the adaptive step. The relaxed Lasso is computed with the `relaxo`-package from `R`. Our PC-simple algorithm with the Lasso for estimating coefficients is straightforward to compute using the `pcalg`- and `lars`-packages from `R`: optimal tuning is with respect to the α-parameter for the PC-simple algorithm and the penalty parameter for Lasso. For the PC-simple algorithm with the adaptive Lasso, we first compute weights w_j as follows: if the variable has not been selected, we set $w_j = 0$; if the variable has been selected, we let w_j be the minimum value of the test statistic $\sqrt{n - 3 - |\mathcal{S}|} Z(Y, j|\mathcal{S})$ (see Section 4.2) over all iterations of the PC-simple algorithm. We then compute the adaptive Lasso by solving the following optimization problem:

$$\text{argmin}_{\beta \in \mathbb{R}^p}(\sum_{i=1}^n (Y_i - X_i^T \beta)^2 + \lambda \sum_{j=1}^p w_j^{-1} |\beta_j|),$$

i.e., the weights for the adaptive step are from the PC-simple algorithm.

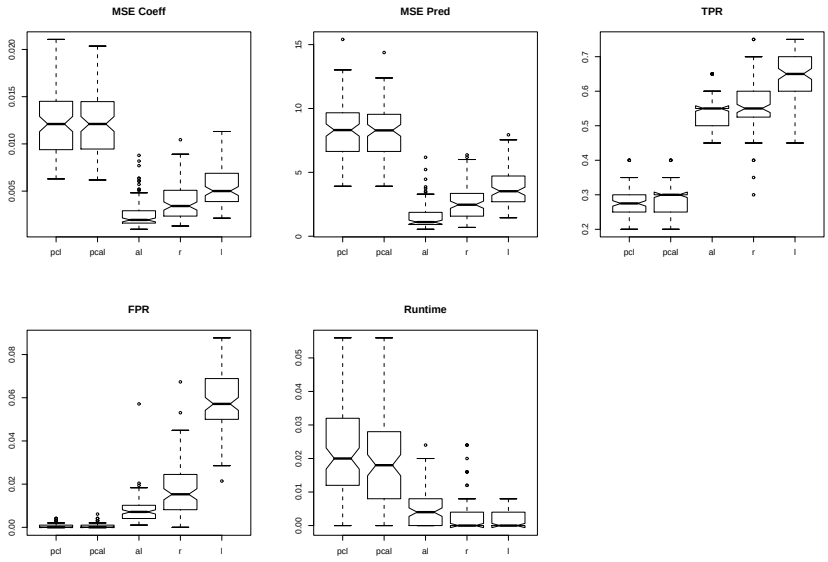


Figure 3: Boxplots of performance measures (see (10)) and runtimes for the simulation study in Section 6.2 considering the following prediction optimal tuned methods: the PC-simple algorithm with Lasso coefficient estimation (pcl), the PC-simple algorithm with adaptive Lasso (pcal), adaptive Lasso (al), relaxed Lasso (r) and Lasso (l).

Figure 3 displays the results. As expected, the Lasso is yielding too many false positives while the adaptive Lasso and the relaxed Lasso have much better variable selection properties. The PC-simple based methods clearly have the lowest FPRs while paying a price in terms of power, i.e., the TPR, and in terms of mean squared errors (MSE Coeff and MSE Pred). In many applications, a low FPR is highly desirable even when paying a price in terms of power. For example, in molecular biology where a covariate represents a gene, only a limited number of selected genes (covariates) can be experimentally validated and hence, methods with a low FPR are preferred, in the hope that most of the top-selected genes are relevant. This type of application is sketched in the next section.

6.3 Real data: riboflavin production by Bacillus subtilis

We consider a high-dimensional real data set about riboflavin (vitamin B2) production by the bacterium *B. subtilis*, kindly provided by DSM Nutritional Products. There is a continuous response variable Y which measures the logarithm of the production rate of riboflavin, and there are $p = 4088$ covariates corresponding to the logarithms of expression levels of genes. One of the main goals is to genetically modify *B. subtilis* in order to increase its production rate for riboflavin. An important step to achieve this goal is to find genes which are most relevant for the production rate. We pursue this step by variable (i.e. gene) selection in a linear model.

We use the methods PC-simple, LARS and ENET as for the simulated data in Section 6.1. We run PC-simple on the full data set, with various values of α. Then we compute LARS and ENET and choose the tuning parameters such that the same number of selected variables arise as for PC-simple. We show the results from a genetically homogeneous

group of $n = 71$ individuals.

Table 1 indicates that the variable selection results of LARS and ENET are more similar than the results of PC-simple and any of these two methods. Thus, the PC-simple algorithm seems to extract information, i.e. selects genes, in a "rather different" way than the penalized methods LARS and ENET. We view this property as very desirable: for any large-scale problem, we want to see different aspects of the problem by using different methods; and ideally, results from different methods can be combined to obtain better results than what is achievable with a single procedure. Here, we find a remarkable

α for PC-simple	selected var.	PC-LARS	PC-ENET	LARS-ENET
0.001	3	0	0	2
0.01	4	2	1	3
0.05	5	2	1	3
0.15	6	3	2	3

Table 1: Variable selection for a real data set on riboflavin production by *B. subtilis*. The columns show the number of selected variables (selected var.), the number of variables that were selected by both PC-simple and LARS (PC-LARS), the number of variables that were selected by both PC-simple and ENET (PC-ENET), and the number of variables that were selected by both LARS and ENET (LARS-ENET).

overlap of the few selected genes among $p = 4088$ candidates. In fact, it is highly significant when calibrating with a null-distribution which consists of pure random noise only.

7 Discussion

We introduce the PC-simple algorithm, a complementary approach to Lasso-type estimation, for inferring associations in a high-dimensional (but sparse) linear model where the number of covariates can greatly exceed the sample size. We show that our methods are consistent (Theorems 4-5), and we demonstrate them on real and simulated data, using the implementation in the `R`-package `pcalg`.

A key part of our approach is the introduction of the concept of partial faithfulness which is related to and typically weaker than linear faithfulness in graphical modeling, see Section 3.2. In the regression setting, we show that partial faithfulness holds generically (Theorem 1) when excluding some adversarial constellations for the non-zero regression coefficients via assumption (A2).

8 Appendix 1: Proofs

Proof of Theorem 1:
Consider the linear model (1) satisfying assumptions (A1) and (A2). In order to prove that the partial faithfulness assumption holds almost surely, it suffices to show that the following holds for all $j \in \{1, \ldots, p\}$ and $S \subseteq \{j\}^C$:

$$\beta_j \neq 0 \implies \text{parcor}(Y, X^{(j)} | X^{(S)}) \neq 0 \quad a.s.$$

(with respect to the distribution generating the β_j's).

Thus, let $j \in \{1, \ldots, p\}$ such that $\beta_j \neq 0$, and let $S \subseteq \{j\}^C$. We recall that $\text{parcor}(Y, X^{(j)}|X^{(\mathcal{S})}) = 0$ if and only if the partial covariance $\text{parcov}(Y, X^{(j)}|X^{(\mathcal{S})})$ between Y and $X^{(j)}$ given $X^{(\mathcal{S})}$ equals zero (cf. Anderson (1984, page 37, definition 2.5.2)). Partial covariances can be computed using the recursive formula given in Anderson (1984, page 43, equation (26)). This formula shows that the partial covariance is linear in its arguments, and that $\text{parcov}(\epsilon, X^{(j)}|X^{(\mathcal{S})}) = 0$ for all $j \in \{1, \ldots, p\}$ and $\mathcal{S} \subseteq \{j\}^C$. Hence,

$$\begin{aligned}
\text{parcov}(Y, X^{(j)}|X^{(\mathcal{S})}) &= \text{parcov}(\delta + \sum_{r=1}^{p} \beta_r X^{(r)} + \epsilon, X^{(j)}|X^{(\mathcal{S})}) \\
&= \sum_{r=1}^{p} \beta_r \text{parcov}(X^{(r)}, X^{(j)}|X^{(\mathcal{S})}) \\
&= \beta_j \text{parcov}(X^{(j)}, X^{(j)}|X^{(\mathcal{S})}) + \sum_{r=1, r\neq j}^{p} \beta_r \text{parcov}(X^{(r)}, X^{(j)}|X^{(\mathcal{S})}).
\end{aligned}$$

Since $\beta_j \neq 0$ by assumption, and since $\text{parcov}(X^{(j)}, X^{(j)}|X^{(\mathcal{S})}) \neq 0$ by assumption (A1), the only way for $\text{parcov}(Y, X^{(j)}|X^{(\mathcal{S})})$ to equal zero is if there is a special parameter constellation of the β_r's, such that

$$\sum_{r=1, r\neq j}^{p} \beta_r \text{parcov}(X^{(r)}, X^{(j)}|X^{(\mathcal{S})}) = -\beta_j \text{parcov}(X^{(j)}, X^{(j)}|X^{(\mathcal{S})}). \tag{11}$$

But such a parameter constellation has Lebesgue measure zero under assumption (A2). □

Proof of Corollary 1:
The implication "$\Longrightarrow$" follows from the fact that $\beta_j \neq 0$ in the linear model (1) if and only if $\text{parcor}(Y, X^{(j)}|X^{(\{j\}^C)}) \neq 0$. The other implication "$\Longleftarrow$" follows from the definition of partial faithfulness, by taking the negative of expression (2). □

Proof of Theorem 2:
Suppose that $(X, Y) = (X^{(1)}, \ldots, X^{(p)}, Y)$ is linearly Y-faithful to a DAG G in which Y is childless, i.e., any edges between Y and the $X^{(j)}$'s, $j = 1, \ldots, p$, point towards Y. We will show that this implies that the distribution of (X, Y) is partially faithful, by showing that $\text{parcor}(Y, X^{(j)}|X^{(\{j\}^C)}) \neq 0$ implies that $\text{parcor}(Y, X^{(j)}|X^{(\mathcal{S})}) \neq 0$ for all $\mathcal{S} \subseteq \{j\}^C$.

Thus, let $j \in \{1, \ldots, p\}$ such that $\text{parcor}(Y, X^{(j)}|X^{(\{j\}^C)}) \neq 0$. By linear Y-faithfulness, this implies that Y and $X^{(j)}$ are not d-separated by $X^{(\{j\}^C)}$ in the DAG G, meaning that $X^{(\{j\}^C)}$ does not block all d-connecting paths between $X^{(j)}$ and Y. Note that all paths between $X^{(j)}$ and Y must be of the form $X^{(j)} - \cdots - \ldots \cdots - X^{(r)} \to Y$, where $-$ denotes an edge of the form $\leftarrow$ or $\rightarrow$. First suppose that $r \neq j$. Then, because $X^{(r)}$ cannot be a collider on the given path (since we know that the edge from $X^{(r)}$ to Y points towards Y), the path is blocked by $X^{(r)} \in X^{(\{j\}^C)}$, and hence the path is blocked by $X^{(\{j\}^C)}$. Thus, since $X^{(\{j\}^C)}$ does *not* block all paths between $X^{(j)}$ and Y, there must be a path where $r = j$, or in other words, there must be an edge between $X^{(j)}$ and Y: $X^{(j)} \to Y$. Such a path $X^{(j)} \to Y$ cannot be blocked by any set $X^{(\mathcal{S})}$, $\mathcal{S} \subseteq \{j\}^C$. Hence, there does

not exist a set $\mathcal{S}$ that d-separates $X^{(j)}$ and Y. By linear Y-faithfulness, this implies that $\text{parcor}(X^{(j)}, Y|X^{(\mathcal{S})}) \neq 0$ for all $\mathcal{S} \subseteq \{j\}^C$. □

Proof of Theorem 3:
By partial faithfulness and equation (7), $\mathcal{A} \subseteq \mathcal{A}^{[m_{\text{reach}}]}$. Hence, we only need to show that $\mathcal{A}$ is not a strict subset of $\mathcal{A}^{[m_{\text{reach}}]}$. We do this using contra-position. Thus, suppose that $\mathcal{A} \subset \mathcal{A}^{[m_{\text{reach}}]}$ strictly. Then there exists a $j \in \mathcal{A}^{[m_{\text{reach}}]}$ such that $j \notin \mathcal{A}$. Fix such an index j. Since $j \in \mathcal{A}^{[m_{\text{reach}}]}$, we know that

$$\text{parcor}(Y, X^{(j)}|X^{(\mathcal{S})}) \neq 0 \text{ for all } \mathcal{S} \subseteq \mathcal{A}^{[m_{\text{reach}}-1]} \setminus \{j\} \quad \text{with} \quad |\mathcal{S}| \leq m_{\text{reach}} - 1. \tag{12}$$

This statement for sets $\mathcal{S}$ with $|\mathcal{S}| = m_{\text{reach}} - 1$ follows from the definition of iteration m_{reach} of the PC-simple algorithm. Sets $\mathcal{S}$ with lower cardinality are considered in previous iterations of the algorithm, and since $A^{[1]} \supseteq \mathcal{A}^{[2]} \supseteq \ldots$, all subsets $\mathcal{S} \subseteq \mathcal{A}^{[m_{\text{reach}}-1]}$ with $|\mathcal{S}| \leq m_{\text{reach}} - 1$ are considered.

We now show that we can take $\mathcal{S} = \mathcal{A}$ in (12). First, note that the supposition $\mathcal{A} \subset \mathcal{A}^{[m_{\text{reach}}]}$ and our choice of j imply that

$$\mathcal{A} \subseteq \mathcal{A}^{[m_{\text{reach}}]} \setminus \{j\} \subseteq \mathcal{A}^{[m_{\text{reach}}-1]} \setminus \{j\}.$$

Moreover, $\mathcal{A} \subset \mathcal{A}^{[m_{\text{reach}}]}$ implies that $|\mathcal{A}| \leq |\mathcal{A}^{[m_{\text{reach}}]}| - 1$. Combining this with $|\mathcal{A}^{[m_{\text{reach}}]}| \leq m_{\text{reach}}$ (see the definition of m_{reach} in (8)), yields that $|\mathcal{A}| \leq m_{\text{reach}} - 1$. Hence, we can indeed take $\mathcal{S} = \mathcal{A}$ in (12), yielding that $\text{parcor}(Y, X^{(j)}|X^{(\mathcal{A})}) \neq 0$.

On the other hand, $j \notin \mathcal{A}$ implies that $\beta_j = 0$, and hence $\text{parcor}(Y, X^{(j)}|X^{(\mathcal{A})}) = 0$. This is a contradiction, and hence $\mathcal{A}$ cannot be a strict subset of $\mathcal{A}^{[m_{\text{reach}}]}$. □

Proof of Theorem 4:
A first main step is to show that the population version of the PC-simple algorithm infers the true underlying active set $\mathcal{A}_n$, assuming partial faithfulness. We formulated this step in Theorem 3 as a separate result, and its proof is given above.

The arguments for controlling the estimation error due to a finite sample size are similar to the ones used in the proof of Theorem 1 in Kalisch and Bühlmann (2007). We proceed in two steps.

Analysis of partial correlations.
We show an exponential inequality for estimating partial correlations up to order $m_n = o(n)$. We use the following notation: $K_j^{m_n} = \{\mathcal{S} \subseteq \{0, \ldots, p_n\} \setminus \{j\}; |\mathcal{S}| \leq m_n\}$ ($j = 1, \ldots, p_n$). Then, for $m_n < n - 4$ and $0 < \gamma < 2$,

$$\sup_{\mathcal{S} \in K_j^{m_n}, 1 \leq j \leq p_n} \text{pr}[|\hat{\rho}_n(Y, j|\mathcal{S}) - \rho_n(Y, j|\mathcal{S})| > \gamma] \leq C_1 n \exp(n - m_n - 4) \log\left(\frac{4 - \gamma^2}{4 + \gamma^2}\right),$$

where $0 < C_1 < \infty$ depends on M in (B5) only. This bound appears in Kalisch and Bühlmann (2007, Corollary 1): for proving it, we require the Gaussian assumption for the distribution (without partial faithfulness) and (B5). It is now straightforward to derive an exponential inequality for the estimated Z-transformed partial correlations. We define $Z_n(Y, j|\mathcal{S}) = g(\hat{\rho}_n(Y, j|\mathcal{S}))$ and $z_n(Y, j|\mathcal{S}) = g(\rho_n(Y, j|\mathcal{S})$, where $g(\rho) = \frac{1}{2}\log(\frac{1+\rho}{1-\rho})$.

Lemma 1. *Suppose that the Gaussian assumption from (B1) and condition (B5) hold. Define $L = 1/(1-(1+M)^2/4)$, with M as in assumption (B5). Then, for $m_n < n-4$ and $0 < \gamma < 2L$,*

$$\begin{aligned} & \sup_{\mathcal{S}\in K_j^{m_n}, 1\le j\le p_n} pr[|Z_n(Y,j|\mathcal{S}) - z_n(Y,j|\mathcal{S})| > \gamma] \\ \le\ & O(n)\left(\exp((n-4-m_n)\log(\frac{4-(\gamma/L)^2}{4+(\gamma/L)^2})) + \exp(-C_2(n-m_n))\right) \end{aligned}$$

for some constant $0 < C_2 < \infty$.

We omit the proof since this is Lemma 3 in Kalisch and Bühlmann (2007).

Analysis of the PC-simple algorithm.
First, we consider a version of the PC-simple algorithm that stops after a fixed (i.e., non-random) number of m iterations (and if $m \ge \hat{m}_{\text{reach}}$, where $\hat{m}_{\text{reach}}$ is the estimation analogue of (8), we set $\widehat{\mathcal{A}}^{[m]} = \widehat{A}^{[\hat{m}_{\text{reach}}]}$). We denote this version by PC-simple(m) and the resulting estimate by $\widehat{\mathcal{A}}(\alpha, m)$.

Lemma 2. *Assume (B1)-(B5). Then, for m_n satisfying $m_n \ge m_{\text{reach},n}$ (see (8)) and $m_n = O(n^{1-b})$ (with b as in (B3)), there exists a sequence $\alpha_n \to 0$ such that*

$$pr[\widehat{\mathcal{A}}_n(\alpha_n, m_n) = \mathcal{A}_n] = 1 - O(\exp(-Cn^{1-2d})) \to 1 \ (n\to\infty) \text{ for some } 0 < C < \infty.$$

A concrete choice of α_n is $\alpha_n = 2(1-\Phi(n^{1/2}c_n/2))$, where c_n is the lower bound from (B4) (which is typically unknown).

Proof: Obviously, the population version of the PC-simple(m_n) algorithm is correct for $m_n \ge m_{\text{reach},n}$, see Theorem 3. An error can occur in the PC-simple(m_n) algorithm if there exists a covariate $X^{(j)}$ and a conditioning set $\mathcal{S} \in K_j^{m_n}$ (although the algorithm is typically only going through random subsets of $K_j^{m_n}$) where an error event $E_{j|\mathcal{S}}$ occurs; $E_{j|\mathcal{S}}$ denotes the event that "an error occurred when testing $\rho_n(Y,j|\mathcal{S}) = 0$". Thus,

$$\begin{aligned} & \text{pr[an error occurs in the PC-simple}(m_n)\text{-algorithm]} \\ \le\ & \text{pr}[\bigcup_{\mathcal{S}\in K_j^{m_n}, 1\le j\le p_n} E_{j|\mathcal{S}}] \le O(p_n^{m_n+1}) \sup_{\mathcal{S}\in K_j^{m_n}, j} \text{pr}[E_{j|\mathcal{S}}], \end{aligned} \tag{13}$$

using that the cardinality of the index set $\{\mathcal{S} \in K_j^{m_n}, 1 \le j \le p_n\}$ in the union is bounded by $O(p_n^{m_n+1})$. Now

$$E_{j|\mathcal{S}} = E^I_{j|\mathcal{S}} \cup E^{II}_{j|\mathcal{S}}, \tag{14}$$

where

$$\begin{aligned} &\text{type I error } E^I_{j|\mathcal{S}}: \ \sqrt{n-|\mathcal{S}|-3}|Z_n(Y,j|\mathcal{S})| > \Phi^{-1}(1-\alpha/2) \text{ and } z_n(Y,j|\mathcal{S}) = 0, \\ &\text{type II error } E^{II}_{j|\mathcal{S}}: \ \sqrt{n-|\mathcal{S}|-3}|Z_n(Y,j|\mathcal{S})| \le \Phi^{-1}(1-\alpha/2) \text{ and } z_n(Y,j|\mathcal{S}) \ne 0. \end{aligned}$$

Choose $\alpha = \alpha_n = 2(1-\Phi(n^{1/2}c_n/2))$, where c_n is from (B4). Then,

$$\begin{aligned} \sup_{\mathcal{S}\in K_j^{m_n}, 1\le j\le p_n} \text{pr}[E^I_{j|\mathcal{S}}] &= \sup_{\mathcal{S}\in K_j^{m_n}, j} \text{pr}[|Z_n(Y,j|\mathcal{S}) - z_n(Y,j|\mathcal{S})| > \sqrt{n/(n-|\mathcal{S}|-3)}c_n/2] \\ &\le O(n)\exp(-C_3(n-m_n)c_n^2), \end{aligned} \tag{15}$$

for some $0 < C_3 < \infty$, using Lemma 1 and the fact that $\log(\frac{4-\delta^2}{4+\delta^2}) \leq -\delta^2/2$ for $0 < \delta < 2$. Furthermore, with the choice of $\alpha = \alpha_n$ above,

$$\begin{aligned} & \sup_{\mathcal{S} \in K_j^{m_n}, 1 \leq j \leq p_n} \text{pr}[E_{j|\mathcal{S}}^{II}] = \sup_{\mathcal{S} \in K_j^{m_n}, j} \text{pr}[|Z_n(Y, j|\mathcal{S})| \leq \sqrt{n/(n - |\mathcal{S}| - 3)} c_n/2] \\ \leq & \sup_{\mathcal{S} \in K_j^{m_n}, j} \text{pr}[|Z_n(Y, j|\mathcal{S}) - z_n(Y, j|\mathcal{S})| > c_n(1 - \sqrt{n/(n - |\mathcal{S}| - 3)}/2)], \end{aligned}$$

because $\inf_{\mathcal{S} \in K_j^{m_n}, j}\{|z_n(Y, j|\mathcal{S})|;\ z_n(Y, j|\mathcal{S}) \neq 0\} \geq c_n$ since $|g(\rho)| = |\frac{1}{2}\log(\frac{1+\rho}{1-\rho})| \geq |\rho|$ for all ρ and using assumption (B4). This shows the crucial role of assumption (B4) in controlling the type II error. By invoking Lemma 1 we then obtain:

$$\sup_{\mathcal{S} \in K_j^{m_n}, j} \text{pr}[E_{j|\mathcal{S}}^{II}] \leq O(n) \exp(-C_4(n - m_n)c_n^2) \tag{16}$$

for some $0 < C_4 < \infty$. Now, by (13)-(16) we get

$$\begin{aligned} & \text{pr}[\text{an error occurs in the PC-simple}(m_n)\text{-algorithm}] \\ \leq & \ O(p_n^{m_n+1} n \exp(-C_5(n - m_n)c_n^2)) \\ \leq & \ O(n^{a(m_n+1)+1} \exp(-C_5(n - m_n)n^{-2d})) \\ = & \ O\left(\exp\left(a(m_n + 1)\log(n) + \log(n) - C_5(n^{1-2d} - m_n n^{-2d})\right)\right) = o(1), \end{aligned}$$

because n^{1-2d} dominates all other terms in the argument of the exp-function, due to $m_n = O(n^{1-b})$ and the assumption in (B4) that $d < b/2$. This completes the proof. □

Lemma 2 leaves some flexibility for choosing m_n. The PC-algorithm yields a data-dependent stopping level $\hat{m}_{\text{reach},n}$, that is, the sample version of (8).

Lemma 3. *Assume (B1)-(B5). Then,*

$$pr[\hat{m}_{\text{reach},n} = m_{\text{reach},n}] = 1 - O(\exp(-Cn^{1-2d})) \to 1 \ (n \to \infty)$$

for some $0 < C < \infty$, with d is as in (B4).

Proof: Consider the population version of the PC-simple algorithm, with stopping level m_{reach} as defined in (8). Note that $m_{\text{reach}} = m_{\text{reach},n} = O(n^{1-b})$ under assumption (B3). The sample PC-simple(m_n) algorithm with stopping level in the range of $m_{\text{reach}} \leq m_n = O(n^{1-b})$, coincides with the population version on a set A having probability $P[A] = 1 - O(\exp(-Cn^{1-2d}))$, see the last formula in the proof of Lemma 2. Hence, on the set A, $\hat{m}_{\text{reach},n} = m_{\text{reach}}$. □

Lemma 2 and 3 together complete the proof of Theorem 4.

Proof of Theorem 5:
By definition, $\mathcal{A}_n \subseteq \mathcal{A}^{[1]}$, where $\mathcal{A}^{[1]}$ is the set of variables from correlation screening.

Denote by $Z_n(Y, j)$ the quantity as in (9) with $\mathcal{S} = \emptyset$ and by $z_n(Y, j)$ its population analogue, i.e., the Z-transformed population correlation. An error occurs when screening

the jth variable if $Z_n(Y,j)$ has been tested to be zero but in fact $z_n(Y,j) \neq 0$. We denote such an error event by E_j^{II}. Note that

$$\sup_{1\leq j\leq p_n} \mathrm{pr}[E_j^{II}] \leq O(n)\exp(-C_1 n c_n^2),$$

for some $0 < C_1 < \infty$, see formula (16) above (we do not use any sparsity assumption for this derivation; we do invoke (C1) which requires a lower bound on non-zero marginal correlations). Thus, the probability of an error occurring in the correlation screening procedure is bounded by

$$\begin{aligned} \mathrm{pr}[\cup_{1\leq j\leq p_n} E_j^{II}] &= O(p_n n)\exp(-C_1 n c_n^2) = O(\exp((1+a)\log(n) - C_1 n^{1-2d})) \\ &= O(\exp(-C_2 n^{1-2d})) \end{aligned}$$

for some $0 < C_2 < \infty$. This completes the proof. □

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