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

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SUMMARY
We consider variable selection in high-dimensional linear models where the number of covariates greatly exceeds the sample size. We introduce the new concept of partial faithfulness and use it to infer associations between the covariates and the response. Under partial faithfulness, we develop a simplified version of the PC algorithm (Spirtes et al., 2000), the PC-simple algorithm, which is computationally feasible even with thousands of covariates and provides consistent variable selection under conditions on the random design matrix that are of a different nature than coherence conditions for penalty-based approaches like the Lasso. Simulations and application to real data show that our method is competitive compared to penalty-based approaches. We provide an efficient implementation of the algorithm in the R-package pcalg.

Some key words: Directed acyclic graph; Elastic net; Graphical modeling; Lasso, Regression

1. INTRODUCTION
Variable selection in 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 & Bühlmann, 2006; Zou, 2006; Zhao & Yu, 2006; Candès & Tao, 2007; van de Geer, 2008; Zhang & Huang, 2008; Wainwright, 2009; Meinshausen & Yu, 2009; Huang et al., 2008; Bickel et al., 2009; Wasserman & Roeder, 2009; Candès & Plan, 2009). Another important approach for estimation in high-dimensional settings, including variable selection, has been developed within the Bayesian paradigm, see for example George & McCulloch (1993, 1997); Brown et al. (1999, 2002); Nott & Kohn (2005); Park & Casella (2008). These methods rely on Markov chain Monte Carlo 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 fundamentally different from penalty-based schemes. Reasons to look at such an approach include: (i) From a practical perspective, it is valuable to have a very different method in the tool-kit for high-dimensional data analysis, raising the confidence for relevance of variables if they are selected by more than a single method. (ii) From a methodological and theoretical perspective, we introduce the new framework of partial faithfulness. Partial faithfulness is related to, and typically weaker than, the concept of linear faithfulness used in graphical models, hence the name partial faithfulness. We prove that partial faithfulness arises naturally in the context of linear models if we make a simple assumption on the structure of the regression coefficients to exclude adversarial cases, see assumption (C2) and Theorem 1.
Partial faithfulness can be exploited to construct an efficient hierarchical testing algorithm, called the PC-simple algorithm, which is a simplification of the PC algorithm (Spirtes et al., 2000) for estimating directed acyclic graphs. The letters PC stand for the first names of Peter Spirtes and Clarke Glymour, the inventors of the PC algorithm. We prove consistency of the PC-simple algorithm for variable selection in high-dimensional partially faithful linear models under assumptions on the design matrix that are very different from coherence assumptions for penalty-based methods. The PC-simple algorithm can also be viewed as a generalization of correlation screening or sure independence screening (Fan & Lv, 2008). Thus, as a special case, we obtain consistency for correlation screening under different assumptions and reasoning than Fan & Lv (2008). We illustrate the PC-simple algorithm, using our implementation in the \texttt{pcalg}, on high-dimensional simulated examples and a real data set on riboflavin 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 $\text{cov}(X) = \Sigma_X$. Let $\epsilon \in \mathbb{R}$ with $E(\epsilon) = 0$ and $\text{var}(\epsilon) = \sigma^2 > 0$, such that $\epsilon$ is uncorrelated with $X^{(1)}, \ldots, X^{(p)}$. Let $Y \in \mathbb{R}$ be defined by the following random design linear model:

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

(1)

for some parameters $\delta \in \mathbb{R}$ and $\beta = (\beta_1, \ldots, \beta_p)^T \in \mathbb{R}^p$. 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 $\beta_j$s are equal to zero. Our goal is to identify the active set

$$A = \{ j = 1, \ldots, p; \beta_j \neq 0 \}$$

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, that is, the number of nonzero $\beta_j$s, by $\text{peff} = |A|$. We define the following additional conditions:

(C1) $\Sigma_X$ is strictly positive definite.

(C2) The regression coefficients satisfy

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

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

Assumption (C1) is a condition on the random design matrix. It is needed for 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 (C2) says that the non-zero regression coefficients are realizations from an absolutely continuous distribution with respect to Lebesgue measure. Once the $\beta_j$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 $\beta_j$s as independent and identically distributed random variables from a prior distribution which is a mixture of a point mass at zero for $\beta_j$s with $j \notin A$ and a density with respect to Lebesgue
measure for $\beta_j$s with $j \in \mathcal{A}$. Assumption (C2) is mild in the following sense: the zero coefficients can arise in an arbitrary way and only the non-zero coefficients are restricted to exclude adversarial cases. Interestingly, Candès & 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. Theorem 1 shows that assumptions (C1) and (C2) imply partial faithfulness, and partial faithfulness is used to obtain the main results in Theorems 3, 4 and 5. Assumption (C2), however, is not a necessary condition for these results.

We use the following notation. For a set $\mathcal{S} \subseteq \{1, \ldots, p\}$, $|\mathcal{S}|$ denotes its cardinality, $\mathcal{S}^C$ is its complement in $\{1, \ldots, p\}$, and $X(\mathcal{S}) = \{X(j); \ j \in \mathcal{S}\}$. Moreover, $\rho(Z^{(1)}, Z^{(2)} \mid W)$ and $\text{parcov}(Z^{(1)}, Z^{(2)} \mid W)$ 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 define partial faithfulness, the concept that will allow us to identify the active set $\mathcal{A}$ using a simplified version of the PC algorithm.

**Definition 1.** Let $X \in \mathbb{R}^p$ be a random vector, and let $Y \in \mathbb{R}$ be a random variable. The distribution of $(X, Y)$ is said to be partially faithful if the following holds for every $j \in \{1, \ldots, p\}$: if $\rho(Y, X^{(j)} \mid X(\mathcal{S})) = 0$ for some $\mathcal{S} \subseteq \{j\}^C$ then $\rho(Y, X^{(j)} \mid X(\mathcal{S})^C) = 0$.

For the linear model (1) with assumption (C1), $\beta_j = 0$ if and only if $\rho(Y, X^{(j)} \mid X(\mathcal{S})^C) = 0$. Hence, such a model satisfies the partial faithfulness assumption if for every $j \in \{1, \ldots, p\}$:

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

**Theorem 1.** Consider the linear model (1) satisfying assumptions (C1) and (C2). Then partial faithfulness holds almost surely with respect to the distribution generating the non-zero regression coefficients.

A proof is given in the Appendix. 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 typically weaker 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 $j \in \{1, \ldots, p\}$:

$$\rho(Y, X^{(j)} \mid X(\mathcal{S})) \neq 0 \text{ for all } \mathcal{S} \subseteq \{j\}^C \text{ if and only if } \beta_j \neq 0.$$

A simple proof is given in the Appendix. Corollary 1 shows that, under partial faithfulness, variables in the active set $\mathcal{A}$ have a strong interpretation in the sense that all corresponding partial correlations are different from zero when conditioning on any subset $\mathcal{S} \subseteq \{j\}^C$.

#### 3-2. Relationship between linear faithfulness and partial faithfulness

To clarify the meaning of partial faithfulness, this section discusses the relationship between partial faithfulness and the concept of linear faithfulness used in graphical models. This is the only section that uses concepts from graphical modeling, and 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 \(G\) 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 \(G\) if the following holds for all \(i \neq j \in \{1, \ldots, q\}\) and \(S \subseteq \{1, \ldots, q\} \setminus \{i, j\}:
\[
Z^{(i)} \text{ and } Z^{(j)} \text{ are d-separated by } Z^{(S)} \text{ in } G \text{ if and only if } \rho(Z^{(i)}, Z^{(j)} | Z^{(S)}) = 0,
\]
see, e.g., Spirtes et al. (2000, page 47). In other words, linear faithfulness to \(G\) means that all and only all zero partial correlations among the variables can be read off from \(G\) using d-separation, a graphical separation criterion explained in detail in Spirtes et al. (2000).

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 and \(Y \in \mathbb{R}\) is a random variable, is linearly \(Y\)-faithful to \(G\) if the following holds for all \(j \in \{1, \ldots, p\}\) and \(S \subseteq \{j\}^C:\n\]
\[
X^{(j)} \text{ and } Y \text{ are d-separated by } X^{(S)} \text{ in } G \text{ if and only if } \rho(X^{(j)}, Y | X^{(S)}) = 0. \tag{3}\]

Thus, linear \(Y\)-faithfulness to \(G\) means that all and only all zero partial correlations between \(Y\) and the \(X^{(j)}\)s can be read off from \(G\) 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. Linear faithfulness and linear \(Y\)-faithfulness are graphical concepts, in that they link a distribution to a directed acyclic graph, while partial faithfulness 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 to a directed acyclic graph in which \(Y\) is childless. Then partial faithfulness holds.

A proof is given in the Appendix. A distribution is typically linearly \(Y\)-faithful to several directed acyclic graphs. 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 directed acyclic graph 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 directed acyclic graph in which \(Y\) is childless, and hence partial faithfulness follows from Theorem 2. In Example 3, the distribution of \((X, Y)\) is not linearly \(Y\)-faithful to any directed acyclic graph in which \(Y\) is childless, showing that this is not a necessary condition for partial faithfulness.

**Example 1.** Consider the following Gaussian linear model:
\[
X^{(1)} = \varepsilon_1, \quad X^{(2)} = X^{(1)} + \varepsilon_2, \quad Y = X^{(1)} - X^{(2)} + \varepsilon, \tag{4}
\]
where \(\varepsilon_1, \varepsilon_2\) and \(\varepsilon\) 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 \((X, Y)\) is linearly \(Y\)-faithful to a directed acyclic graph according to the graph in Figure 1(a).

The distribution of \((X, Y)\) is not partially faithful, since \(\rho(Y, X^{(1)} | \emptyset) = 0\) but \(\rho(Y, X^{(1)} | X^{(2)}) \neq 0\). Theorem 2 does not apply, because the distribution of \((X, Y)\) is not linearly \(Y\)-faithful to any directed acyclic graph in which \(Y\) is childless. For instance, the distribution of \((X, Y)\) is not linearly \(Y\)-faithful to the graph in Figure 1(a), since \(\rho(X^{(1)}, Y | \emptyset) = 0\) but \(X^{(1)}\).
and $Y$ are not d-separated 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 (A1) 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 the graph $X^{(1)} \rightarrow X^{(2)} \leftarrow Y$, but this graph is not allowed in Theorem 2 because $Y$ has a child.

Such failure of partial faithfulness can also be caused by hidden variables. To see this, consider the following Gaussian linear model:

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

where $\varepsilon_1, \varepsilon_2, \varepsilon_3$ and $\varepsilon$ are independent standard Normal random variables. The distribution of $(X^{(1)}, X^{(2)}, X^{(3)}, Y)$ factorizes according to the DAG $X^{(1)} \rightarrow X^{(2)} \leftarrow X^{(3)} \rightarrow Y$, and is linearly faithful to this DAG. Hence, the distribution of $(X^{(1)}, X^{(2)}, X^{(3)}, Y)$ is partially faithful by Theorem 2. If, however, variable $X^{(3)}$ is hidden, so that we only observe $(X^{(1)}, X^{(2)}, Y)$, then the distribution of $(X^{(1)}, X^{(2)}, Y)$ has exactly the same conditional independence relationships as the distribution arising from (4). Hence, the distribution of $(X^{(1)}, X^{(2)}, Y)$ is not partially faithful.

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

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

where $\varepsilon_1, \ldots, \varepsilon_4$ and $\varepsilon$ 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 graph in Figure 1(b).

The distribution of $(X, Y)$ is partially faithful, since $\rho(Y, X^{(j)} \mid X^{(j)}) \neq 0$ only for $j = 2$, and $\rho(Y, X^{(2)} \mid X^{(S)}) \neq 0$ for any $S \subseteq \{1, 3, 4\}$. In this example, partial faithfulness follows from Theorem 2, since the distribution of $(X, Y)$ is linearly $Y$-faithful to the graph in Figure 1(b) and $Y$ is childless in this graph. The distribution of $(X, Y)$ is not linearly faithful to the graph in Figure 1(b), since $\text{cor}(X^{(1)}, X^{(4)}) = 0$ but $X^{(1)}$ and $X^{(4)}$ are not d-separated by the empty set. Moreover, there does not exist any other directed acyclic graph to which the distribution of $(X, Y)$ is linearly faithful. Hence, 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 $\varepsilon_1, \varepsilon_2, \varepsilon_3$ and $\varepsilon$ 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 graph in Figure 1(c).

The distribution of $(X, Y)$ is partially faithful, since $\rho(Y, X^{(j)} \mid X^{(j)}) \neq 0$ for $j \in \{2, 3\}$, $\rho(Y, X^{(2)} \mid X^{(S)}) \neq 0$ for any $S \subseteq \{1, 3\}$, and $\rho(Y, X^{(3)} \mid X^{(S)}) \neq 0$ for any $S \subseteq \{1, 2\}$. 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 graph in Figure 1(c), since $\text{cor}(X^{(1)}, Y) = 0$ but $X^{(1)}$ and $Y$ are not d-separated by the empty set. Moreover, there does not exist any other directed acyclic graph 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 partial correlations are estimated from data.

First, using $S = \emptyset$ in expression (2) yields that $\beta_j = 0$ if $\text{cor}(Y, X^{(j)}) = 0$ for some $j \in \{1, \ldots, p\}$. This shows 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

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

(5)

We call this the step 1 active set or the correlation screening active set, and we know by partial faithfulness that

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

(6)

Such correlation screening may reduce the dimensionality of the problem by a substantial amount, and due to (6), we could use other variable selection methods on the reduced set of variables $\mathcal{A}^{[1]}$.

Furthermore, for each $j \in \mathcal{A}^{[1]}$ expression (2) yields that

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

(7)

That is, for checking whether the $j$th covariate remains in the model, we can additionally screen all partial correlations of order one. 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 $\mathcal{A}$. Thus, screening partial correlations of order one using (7) leads to a smaller active set

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

This new step 2 active set $\mathcal{A}^{[2]}$ further reduces the dimensionality of the candidate active set, and because of (7) we still have that $\mathcal{A}^{[2]} \supseteq \mathcal{A}$. We can continue screening higher-order partial correlations, resulting in a nested sequence of step $m$ active sets

$$\mathcal{A}^{[1]} \supseteq \mathcal{A}^{[2]} \supseteq \cdots \supseteq \mathcal{A}^{[m]} \supseteq \cdots \supseteq \mathcal{A}.$$  

(8)

A step $m$ active set $\mathcal{A}^{[m]}$ could be used as dimension reduction together with any favored variable selection method in 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 the PC-simple algorithm, shown in pseudocode in Algorithm 1.
Algorithm 1 The population version of the PC-simple algorithm.

1: Set $m = 1$. Do correlation screening, and build the step$_1$ active set
   \[ A^{[1]} = \{j = 1, \ldots, p; \text{cor}(Y, X^{(j)}) \neq 0\} \] as in (5).
2: repeat
3: \hspace{1em} $m = m + 1$. Construct the step$_m$ active set:
   \[ A^{[m]} = \{j \in A^{[m-1]}; \rho(Y, X^{(j)} \mid X^{(S)}) \neq 0 \]
   \hspace{1em} for all $S \subseteq A^{[m-1]} \setminus \{j\}$ with $|S| = m - 1$.\]
4: until $|A^{[m]}| \leq m$.

The value $m$ that is reached in Algorithm 1 is called $m_{\text{reach}}$:
\[ m_{\text{reach}} = \min\{m; |A^{[m]}| \leq m\}. \] (9)

The following theorem shows correctness of the population version of the PC-simple algorithm.

**Theorem 3.** For the linear model (1) satisfying (C1) and partial faithfulness, the population version of the PC-simple algorithm identifies the true underlying active set, i.e., $A^{[m_{\text{reach}}]} = A = \{j = 1, \ldots, p; \beta_j \neq 0\}$.

A proof is given in the Appendix. Theorem 3 shows that partial faithfulness, which is often weaker than linear faithfulness, is sufficient to guarantee correctness 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 there are two important differences. First, the PC algorithm considers all ordered pairs of variables in $(X^{(1)}, \ldots, X^{(p)}), Y)$, while we only consider ordered pairs $(Y, X^{(j)})$, $j \in \{1, \ldots, p\}$, since we are only interested in associations between $Y$ and $X^{(j)}$. Second, the PC algorithm considers conditioning sets in the neighborhoods of both $Y$ and $X^{(j)}$, while we only consider conditioning sets in the neighborhood of $Y$.

### 4.2. Sample version of the PC-simple algorithm

For finite samples, the partial correlations must be estimated. We use the following shorthand notation:
\[ \rho(Y, j \mid S) = \rho(Y, X^{(j)} \mid X^{(S)}), \hspace{1em} \hat{\rho}(Y, j \mid S) = \hat{\rho}(Y, X^{(j)} \mid X^{(S)}), \]
\[ \rho(i, j \mid S) = \rho(X^{(i)}, X^{(j)} \mid X^{(S)}), \hspace{1em} \hat{\rho}(i, j \mid S) = \hat{\rho}(X^{(i)}, X^{(j)} \mid X^{(S)}), \]
where the hat-versions denote sample partial correlations. These can be calculated recursively, since for any $k \in S$ we have
\[ \hat{\rho}(Y, j \mid S) = \frac{\hat{\rho}(Y, j \mid S \setminus \{k\}) - \hat{\rho}(Y, k \mid S \setminus \{k\})\hat{\rho}(j, k \mid S \setminus \{k\})}{\{1 - \hat{\rho}(Y, k \mid S \setminus \{k\})^2\}\{1 - \hat{\rho}(j, k \mid S \setminus \{k\})^2\}^{1/2}}. \]

In order to test whether a partial correlation is zero, we apply Fisher’s $Z$-transform
\[ Z(Y, j \mid S) = \frac{1}{2} \log \left( \frac{1 + \hat{\rho}(Y, j \mid S)}{1 - \hat{\rho}(Y, j \mid S)} \right). \] (10)

Classical decision theory in the Gaussian case yields the following rule. Reject the null-hypothesis $H_0(Y, j \mid S): \rho(Y, j \mid S) = 0$ against the two-sided alternative $H_A(Y, j \mid S): \rho(Y, j \mid S) \neq 0$ if $(n - |S| - 3)^{1/2}|Z(Y, j \mid S)| > \Phi^{-1}(1 - \alpha/2)$, where $\alpha$ is the significance level and $\Phi(\cdot)$ is the standard Normal cumulative distribution function. Even in the absence of Gaussianity, the rule above is a reasonable thresholding operation.
The sample version of the PC-simple algorithm is obtained by replacing the statements about \( \rho(Y, X^{(j)} | X^{(S)}) \neq 0 \) in Algorithm 1 by

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

The resulting estimated set of variables is denoted by \( \hat{\mathcal{A}}(\alpha) = \hat{\mathcal{A}}^\text{reach}(\alpha) \), where \( \hat{\mathcal{A}}^\text{reach} \) is the estimated version of the quantity in (9). The only tuning parameter \( \alpha \) of the PC-simple algorithm is the significance level for testing the partial correlations.

The PC-simple algorithm is very different from a greedy scheme, since 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 & Lv (2008) or the low-order partial correlation method in Wille & Bühlmann (2006). Castelo & 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 \( S \) which have survived in the previous step of active set \( \mathcal{A}^{[m-1]} \). Therefore, the algorithm of Castelo & Roverato (2006) is often infeasible and must 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. This is difficult to evaluate exactly, but a crude bound is \( O(p^{\text{peff}}) \), see Kalisch & Bühlmann (2007, formula (4)). Section 6 shows that we can easily use the PC-simple algorithm in problems with thousands of covariates.

5. ASYMPTOTIC RESULTS IN HIGH DIMENSIONS

5-1. Consistency of the PC-simple algorithm

We now show that the PC-simple algorithm is consistent for variable selection, even if \( p \) is much larger than \( n \). We consider the linear model in (1). 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 \((X, Y)\), 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:

\begin{itemize}
  \item[(D1)] The distribution \( P_n \) of \((X, Y)\) is multivariate Normal and satisfies (C1) and the partial faithfulness condition for all \( n \).
  \item[(D2)] The dimension \( p_n = O(n^a) \) for some \( 0 \leq a < \infty \).
  \item[(D3)] The cardinality of the active set \( \text{peff}_n = |\mathcal{A}_n| = |\{j = 1, \ldots, p_n; \ \beta_{j,n} \neq 0\}| \) satisfies:
    \[
    \text{peff}_n = O(n^{1-b}) \quad \text{for some} \ 0 < b \leq 1.
    \]
  \item[(D4)] The partial correlations \( \rho_n(Y, j | S) = \rho(Y, X^{(j)} | X^{(S)}) \) satisfy:
    \[
    \inf \left\{ |\rho_n(Y, j | S)|; \ j = 1, \ldots, p_n, S \subseteq \{j\}^C, |S| \leq \text{peff}_n \text{ with } \rho_n(Y, j | S) \neq 0 \right\} \geq c_n,
    \]
    where \( c_n^{-1} = O(n^d) \) for some \( 0 \leq d < b/2 \), and \( b \) is as in (D3).
  \item[(D5)] The partial correlations \( \rho_n(Y, j | S) \) and \( \rho_n(i, j | S) = \rho(X^{(i)}, X^{(j)} | X^{(S)}) \) satisfy:
    \[
    (i) \sup_{n, j, S \subseteq \{j\}^C, |S| \leq \text{peff}_n} |\rho_n(Y, j | S)| \leq M < 1,
    \]
    \[
    (ii) \sup_{n, i \neq j, S \subseteq \{i, j\}^C, |S| \leq \text{peff}_n} |\rho_n(i, j | S)| \leq M < 1.
    \]
\end{itemize}

Assumption (D1) is made to simplify asymptotic calculations, and it is not needed in the population case. Unfortunately, it is virtually impossible to check assumptions (D1)-(D5) in practice,
with the exception of (D2). However, this is common to assumptions for high-dimensional variable selection, such as the neighborhood stability condition (Meinshausen & Bühlmann, 2006), the irrepresentable condition (Zhao & Yu, 2006), or the restrictive eigenvalue assumption (Bickel et al., 2009). A more detailed discussion of assumptions (D1)-(D5) is given in Section 5-2.

Letting \( \hat{A}_n(\alpha) \) denote the estimated set of variables from the PC-simple algorithm in Section 4-2 with significance level \( \alpha \), we obtain the following consistency result:

**Theorem 4.** Consider the linear model (1) and assume (D1)-(D5). Then there exists a sequence \( \alpha_n \to 0 \ (n \to \infty) \) and a constant \( C > 0 \) such that the PC-simple algorithm satisfies

\[
\Pr\{ \hat{A}_n(\alpha_n) = A_n \} = 1 - O\{ \exp(-Cn^{1-2d}) \} \to 1 \ (n \to \infty),
\]

where \( d \) is as in (D4).

A proof is given in the Appendix. The value \( \alpha_n \), although being the 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. A possible choice yielding consistency is \( \alpha_n = 2\{ 1 - \Phi(n^{1/2}c_n/2) \} \). This choice depends on the unknown lower bound of the partial correlations in (D4).

### 5-2. Discussion of the conditions of Theorem 4

There is much 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 & Tao, 2007). Neither of these methods exploit partial faithfulness. Hence, it is interesting to discuss our conditions with a view towards these other established results.

For the Lasso, Meinshausen & Bühlmann (2006) proved that a so-called neighborhood stability condition is sufficient and almost necessary for consistent variable selection, where the word almost refers to the fact that a strict inequality with the relation \( < \) appears in the sufficient condition whereas for necessity, there is a \( \leq \) relation. Zou (2006) and Zhao & Yu (2006) gave a different, but equivalent condition. In the latter work, it is called the irrepresentable condition. The adaptive Lasso (Zou, 2006) or other two-stage Lasso and thresholding procedures (Meinshausen & Yu, 2009) yield consistent variable selection under weaker conditions than the neighborhood stability or irrepresentable condition, see also Example 4 below. Such two-stage procedures rely on bounds for \( \| \hat{\beta} - \beta \|_q \ (q = 1, 2) \) whose convergence rate to zero is guaranteed under possibly weaker restricted eigenvalue assumptions on the design (Bickel et al., 2009) than what is required by the irrepresentable or neighborhood stability condition. All these different assumptions are not directly comparable with our conditions (D1)-(D5).

Assumption (D2) allows for an arbitrary polynomial growth of dimension as a function of sample size, while (D3) is a sparseness assumption in terms of the number of effective variables. Both (D2) and (D3) are fairly standard assumptions in high-dimensional asymptotics. More critical are the partial faithfulness requirement in (D1), and the conditions on the partial correlations in (D4) and (D5).

We interpret these conditions with respect to the design \( X \) and the conditional distribution of \( Y \) given \( X \). Regarding the random design, we assume (C1) and (D5,(ii)). Requiring (C1) is rather weak, since it does not impose constraints on the 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 \( n \). Condition (D5,(ii)) excludes perfect collinearity, where the fixed upper bound on partial correlations places some additional restrictions on the design. Regarding the conditional distribution of \( Y \) given \( X \), we require partial faithfulness. This becomes more explicit by invoking Theorem 1: partial faithfulness follows by assuming condition (C2) in Section 2 for every \( n \), which involves
the regression coefficients only. Conditions (D4) and (D5,(i)) place additional restrictions on
both the design $X$ and the conditional distribution of $Y$ given $X$.

Assumption (D4) is used for controlling the type II errors in the many tests of the PC-simple
algorithm, see the proof of Theorem 4. This assumption is slightly stronger than requiring that all
non-zero regression coefficients are larger than a detectability-threshold, which has been previ-
ously used for analyzing the Lasso in Meinshausen & Bühlmann (2006), Zhao & Yu (2006) and
Meinshausen & Yu (2009). Clearly, assumptions on the design $X$ are not sufficient for consistent
variable selection with any method and some additional detectability assumption is needed. Our
assumption (D4) is restrictive, as it does not allow small non-zero low-order partial correlations.
Near partial faithfulness (Robins et al., 2003), where small partial correlations would imply that
corresponding regression coefficients are small, would be a more realistic framework in practice.
However, this would make the theoretical arguments much more involved, and we do not pursue
this in this paper.

Although our assumptions are not directly comparable to the neighborhood stability or irrep-
resentable 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 $p = 4$, $\text{peff} = 3$, $\sigma^2 = 1$, $\mu_X = (0, \ldots, 0)^T$

$$\Sigma_X = \begin{pmatrix}
1 & \rho_1 & \rho_2 \\
\rho_1 & 1 & \rho_2 \\
\rho_2 & \rho_2 & 1
\end{pmatrix}, \quad \rho_1 = -0.4, \quad \rho_2 = 0.2,$$

where $\beta_1, \beta_2, \beta_3$ are fixed i.i.d. realizations from $\mathcal{N}(0, 1)$ and $\beta_4 = 0$.

It is shown in Zou (2006, Cor. 1) that the Lasso is inconsistent for variable selection in this
model. On the other hand, (D1) holds because of Theorem 1, and also (D5) is true. Since the
dimension $p$ is fixed, (D2), (D3) and (D4) hold automatically. 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.

We can slightly modify Example 4 to make it high-dimensional. Consider $\text{peff} = 3$ active vari-
ables, with design and coefficients as in Example 4. Moreover, consider $p_n - \text{peff}$ noise co-
variates which are independent from the active variables, with $p_n$ satisfying (D2). Let the design
satisfy (C1) and (D5,(ii)), for example by taking the noise covariates to be mutually independent.
Then assumptions (D1)-(D5) hold, implying consistency of the PC-simple algorithm, while the
Lasso is inconsistent.

### 5.3. Asymptotic behavior of correlation screening

Correlation screening is equivalent to sure independence screening of Fan & Lv (2008), but our
assumptions and reasoning via partial faithfulness are very different from the work of Fan & Lv.
Denote by $A_n^{[1]}(\alpha)$ the correlation screening active set, estimated from data, using significance
level $\alpha$, obtained from the first step of the sample version of the PC-simple algorithm. We do not
require any sparsity conditions for consistency. We define:

- (E1) as assumption (D4) but for marginal correlations $\text{cor}(Y, X^{(j)}) = \rho_n(Y, j)$ only.
- (E2) as assumption (D5) but for marginal correlations $\text{cor}(Y, X^{(j)}) = \rho_n(Y, j)$ only.
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Theorem 5. Consider the linear model (1) and assume (D1), (D2), (E1) and (E2). Then there exists a sequence $\alpha_n \to 0$ ($n \to \infty$) and a constant $C > 0$ such that:

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

where $d > 0$ is as in (E1).

A proof is given in the Appendix. A possible choice for $\alpha_n$ 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 and $\widehat{A}^{[1]}$ can still be large, for example almost as large as the full set $\{1, \ldots, p\}$.

Under some restrictive conditions on the covariance $\Sigma_X$ of the random design, Fan & Lv (2008) have shown that correlation screening, or sure independence screening, is overestimating the active set $\mathcal{A}_n$ as stated in Theorem 5. Theorem 5 shows that this result also holds under very different assumptions on $\Sigma_X$ when partial faithfulness is assumed in addition. Hence, our result justifies correlation screening as a more general tool than what it appears to be from the setting of Fan & Lv (2008), thereby extending the range of applications.

6. Numerical results

6.1. Analysis for simulated data

We simulate data according to a Gaussian linear model as in (1) with $\delta = 0$ and $p$ covariates with $\mu_X = (0, \ldots, 0)^T$ and covariance matrix $\Sigma_{X_{ij}} = \rho^{[i-j]}$, where $\Sigma_{X_{ij}}$ denotes the $(i, j)$th entry of $\Sigma$. In order to generate values for $\beta$, we follow (C2): a certain number $p_{\text{eff}}$ of coefficients $\beta_j$ have a value different from zero. The values of the nonzero $\beta_j$s are sampled independently from a standard normal distribution and the indices of the nonzero $\beta_j$s are evenly spaced between 1 and $p$. We consider two settings:

- low-dimensional: $p = 19$, $p_{\text{eff}} = 3$, $n = 100$; $\rho \in \{0.0, 0.3, 0.6\}$ with 1000 replicates
- high-dimensional: $p = 499$, $p_{\text{eff}} = 10$, $n = 100$; $\rho \in \{0.0, 0.3, 0.6\}$ with 300 replicates

We evaluate the performance of the methods using receiver operating characteristic curves which measure the accuracy for variable selection independently from the issue of choosing good tuning parameters. We compare the PC-simple algorithm to the Lasso (Efron et al., 2004) and Elastic Net (Zou & Hastie, 2005), using the R-packages pcalg, lars and elasticnet, respectively. For Elastic Net, we vary the $\ell^1$-penalty parameter only while keeping the $\ell^2$-penalty parameter fixed at the default value from the R-package.

In the low-dimensional settings shown in Figures 2(a), 2(c), 2(e), the PC-simple algorithm clearly dominates the Lasso and Elastic Net for small false positive rates, which are desirable in many applications. When focusing on the false positive rate arising from the default value for $\alpha=0.05$ in the PC-simple algorithm, indicated by the vertical lines, the PC-simple algorithm outperforms the Lasso and Elastic Net by a large margin. If the correlation among the covariates increases, the performance of Elastic Net deteriorates, whereas the performances of the PC-simple algorithm and the Lasso do not vary much.

In the high-dimensional settings shown in Figures 2(b), 2(d), 2(f), the difference between the methods is small for small false positive rates. The Lasso performs best, Elastic Net is worst, and the PC-simple algorithm is somewhere in between. For larger false positive rates, the differences become more pronounced. Up to the false positive rate corresponding to the default value of $\alpha=0.05$, the PC-simple algorithm is never significantly outperformed by either the Lasso or Elastic Net.
We refer to the working paper "Stability selection" by N. Meinshausen and P. Bühlmann for a more principled way to choose the tuning parameter $\alpha$. Further examples, with $p = 1000$, $\text{peff} = 5$, $n = 50$ 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).

The computing time of the PC-simple algorithm on 10 different values of $\alpha$ has about the same order of magnitude as the Lasso or Elastic Net for their whole solution paths. Hence, the PC-simple algorithm is certainly feasible for high-dimensional problems.

![Graphs showing ROC curves for different scenarios](image)

(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, $\rho = 0.6$.

Fig. 2. Receiver operating characteristic curves for the simulation study in Section 6.1. The solid line corresponds to the PC-simple algorithm, the dashed line to the Lasso and the dotted line to Elastic Net. 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 & Bühlmann, 2006). The adaptive Lasso (Zou, 2006) and the relaxed Lasso
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(Meinshausen, 2007) correct Lasso’s overestimating behavior and prediction-optimal tuning for these methods yields a good amount of regularization for variable selection.

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

$$\delta = 0, \quad \mu_X = (0, \ldots, 0)^T, \quad \Sigma_{X;i,j} = 0.5|i-j|, \quad \sigma^2 = 1,$$

$$\beta_1, \ldots, \beta_{20} \text{i.i.d.} \sim \mathcal{N}(0, 1), \quad \beta_{21} = \ldots = \beta_{1000} = 0,$$

using 100 replicates. We consider the following performance measures:

$$\|\hat{\beta} - \beta\|_2^2 = \sum_{j=1}^p (\hat{\beta}_j - \beta_j)^2 \quad \text{(MSE Coeff)}$$

$$E_X\{X^T(\hat{\beta} - \beta)\}^2 = (\hat{\beta} - \beta)\text{cov}(X)(\hat{\beta} - \beta)^T \quad \text{(MSE Pred)}$$

$$\frac{\sum_{j=1}^p I(\hat{\beta}_j \neq 0, \beta_j \neq 0)}{\sum_{j=1}^p I(\beta_j \neq 0)} \quad \text{(true positive rate)}$$

$$\frac{\sum_{j=1}^p I(\hat{\beta}_j \neq 0, \beta_j = 0)}{\sum_{j=1}^p I(\beta_j = 0)} \quad \text{(false positive rate)}$$

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

We apply the 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 Elastic Net, since this method was found to be worse in terms of receiver operating characteristic curves than the Lasso, see Section 6.1.

Prediction optimal tuning is pursued with a validation set having the same size as the training data. For the adaptive Lasso, we first compute a prediction-optimal Lasso as initial estimator $\hat{\beta}_{\text{init}}$, and the adaptive Lasso is then computed by solving the following optimization problem:

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

where $w_j^{-1} = |\hat{\beta}_{\text{init},j}|^{-1}$ and $\lambda$ is again chosen in a prediction-optimal way. The computations are done with the R-package lars, using re-scaled covariates for the adaptive step. The relaxed Lasso is computed with the R-package relaxo. The PC-simple algorithm with the Lasso for estimating coefficients is computed using the R-packages pcalg and lars, using optimal tuning with respect to the $\alpha$-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 $(n - 3 - |S|)^{1/2}Z(Y, j \mid S)$ over all iterations of the PC-simple algorithm. With these weights $w_j$, we then compute the adaptive Lasso as defined above.

The results are shown in Figure 3. As expected, the Lasso yields 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 false positive rates, but pay a price in terms of the true positive rate and mean squared errors. In many applications, a low false positive rate 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 can be experimentally validated. Hence, methods with a low false positive rate are preferred, in the hope that most of the top-selected genes are relevant, as sketched in the next section.

6.3. Real data: riboflavin production by Bacillus subtilis

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

We use data from a genetically homogeneous group of $n = 71$ individuals. We run the PC-simple algorithm on the full data set for various values of $\alpha$. Next, we compute the Lasso and Elastic Net, choosing the tuning parameters such that they select the same number of variables as the PC-simple algorithm.

Table 1 shows that there is overlap between the selected variables of the three different methods. This overlap is highly significant when calibrating with a null-distribution which consists of random noise. On the other hand, we see that the variable selection results of the Lasso and Elastic Net are more similar than the results of the PC-simple algorithm and either of these methods. Hence, the PC-simple algorithm seems to select genes in a different way than the penalty-based methods Lasso and Elastic Net. This is a desirable finding, since for any large-scale problem, we want to see different aspects of the problem by using different methods. Ideally, results from different methods can then be combined to obtain results that are better than what is achievable by a single procedure.

APPENDIX

Proofs

Proof of Theorem 1. Consider the linear model (1) satisfying assumptions (C1) and (C2). In order to prove that the partial faithfulness assumption holds almost surely, it suffices to show that the following
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| $\alpha$ for PC-simple | Selected | PC-Lasso | PC-Enet | Lasso-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 2 to 5 show the number of variables selected by the PC-simple algorithm, the number of variables selected by both the PC-simple algorithm and the Lasso, the number of variables selected by both the PC-simple algorithm and Elastic Net, and the number of variables that were selected by both the Lasso and Elastic Net.

holds for all $j \in \{1, \ldots, p\}$ and $S \subseteq \{j\}^C$; $\beta_j \neq 0$ implies that $\rho(Y, X^{(j)} | X^{(S)}) \neq 0$ almost surely with respect to the distribution generating the $\beta_j$s.

Thus, let $j \in \{1, \ldots, p\}$ such that $\beta_j \neq 0$, and let $S \subseteq \{j\}^C$. We recall that $\rho(Y, X^{(j)} | X^{(S)}) = 0$ if and only if the partial covariance $\text{parcov}(Y, X^{(j)} | X^{(S)})$ between $Y$ and $X^{(j)}$ given $X^{(S)}$ equals zero as can be seen in 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 $\text{parcov}(\epsilon, X^{(j)} | X^{(S)}) = 0$ for all $j \in \{1, \ldots, p\}$ and $S \subseteq \{j\}^C$. Hence,

$$\text{parcov}(Y, X^{(j)} | X^{(S)}) = \text{parcov}(\delta + \sum_{r=1}^{p} \beta_r X^{(r)} + \epsilon, X^{(j)} | X^{(S)})$$

$$= \sum_{r=1}^{p} \beta_r \text{parcov}(X^{(r)}, X^{(j)} | X^{(S)})$$

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

Since $\beta_j \neq 0$ by assumption, and since $\text{parcov}(X^{(j)}, X^{(j)} | X^{(S)}) \neq 0$ by assumption (C1), the only way for $\text{parcov}(Y, X^{(j)} | X^{(S)})$ to equal zero is if there is a special parameter configuration of the $\beta_j$s, such that

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

(A1)

But such a parameter constellation has Lebesgue measure zero under assumption (C2).

Proof of Corollary 1. The implication from the left to the right hand side follows from the fact that $\beta_j \neq 0$ in the linear model (1) if and only if $\rho(Y, X^{(j)} | X^{(j)^C}) \neq 0$. The other direction 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 directed acyclic graph $G$ 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 $\rho(Y, X^{(j)} | X^{(j)^C}) \neq 0$ implies that $\rho(Y, X^{(j)} | X^{(S)}) \neq 0$ for all $S \subseteq \{j\}^C$.

Thus, let $j \in \{1, \ldots, p\}$ such that $\rho(Y, X^{(j)} | X^{(j)^C}) \neq 0$. By linear $Y$-faithfulness, this implies that $Y$ and $X^{(j)}$ are not d-separated by $X^{(j)^C}$ in $G$, meaning that $X^{(j)^C}$ does not block all d-connecting paths between $X^{(j)}$ and $Y$. All paths between $X^{(j)}$ and $Y$ must be of the form $X^{(j)} \rightarrow \cdots \rightarrow X^{(r)} \rightarrow Y$, where $\leftarrow$ 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 \(Y\). Such a path \(X^{(j)} \rightarrow Y\) cannot be blocked by any set \(X(S)\), \(S \subseteq \{j\} C\). Hence, there does not exist a set \(S\) that d-separates \(X^{(j)}\) and \(Y\). By linear \(Y\)-faithfulness, this implies that \(\rho(X^{(j)}, Y | X(S)) \neq 0\) for all \(S \subseteq \{j\} C\).

Proof of Theorem 3. By partial faithfulness and equation (8), \(A \subseteq A^{[m_{\text{reach}}]}\). Hence, we only need to show that \(A\) is not a strict subset of \(A^{[m_{\text{reach}}]}\). We do this using contra-position. Thus, suppose that \(A \subset A^{[m_{\text{reach}}]}\) strictly. Then there exists a \(j \in A^{[m_{\text{reach}}]}\) such that \(j \notin A\). Fix such an index \(j\). Since \(j \in A^{[m_{\text{reach}}]}\), we know that

\[
\rho(Y, X^{(j)} | X(S)) \neq 0 \text{ for all } S \subseteq A^{[m_{\text{reach}}]} \setminus \{j\} \quad \text{with} \quad |S| \leq m_{\text{reach}} - 1. \quad (A2)
\]

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

We now show that we can take \(S = A\) in (A2). First, the supposition \(A \subset A^{[m_{\text{reach}}]}\) and our choice of \(j\) imply that

\[
A \subseteq A^{[m_{\text{reach}}]} \setminus \{j\} \subseteq A^{[m_{\text{reach}}]} \setminus \{j\}.
\]

Moreover, \(A \subset A^{[m_{\text{reach}}]}\) implies that \(|A| \leq |A^{[m_{\text{reach}}]}| - 1\). Combining this with \(|A^{[m_{\text{reach}}]}| \leq m_{\text{reach}}\) yields that \(|A| \leq m_{\text{reach}} - 1\). Hence, we can indeed take \(S = A\) in (A2), yielding that \(\rho(Y, X^{(j)} | X(A)) \neq 0\).

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

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 \(A_n\), assuming partial faithfulness. We formulated this step as a separate result in Theorem 3.

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 & Bühlmann (2007). We proceed in two steps, analyzing first partial correlations and then the PC-simple algorithm.

We show an exponential inequality for estimating partial correlations up to order \(m_n = o(n)\). We use the following notation: \(K_{m_n}^n = \{S \subseteq \{0, \ldots, n\} \setminus \{j\}; |S| \leq m_n\} (j = 1, \ldots, p_n)\). We require more general versions of assumptions (D4) and (D5) where the cardinality of the condition sets are bounded by the number \(m_n\):

(D4\(_{m_n}\)) The partial correlations \(\rho_n(Y, j | S) = \rho(Y, X^{(j)} | X(S))\) satisfy:

\[
\inf \left\{ |\rho_n(Y, j | S)|; j = 1, \ldots, p_n, S \subseteq \{j\} C, |S| \leq m_n\text{ with } \rho_n(Y, j | S) \neq 0 \right\} \geq c_n,
\]

where \(c_n^{-1} = O(n^d)\) for some \(0 \leq d < b/2\), and \(b\) is as in (D3).

(D5\(_{m_n}\)) The partial correlations \(\rho_n(Y, j | S)\) and \(\rho_n(i, j | S) = \rho(X^{(i)}, X^{(j)} | X(S))\) satisfy:

\[
(i) \sup_{n, j, S \subseteq \{j\} C, |S| \leq m_n} |\rho_n(Y, j | S)| \leq M < 1, \quad (ii) \sup_{n, i \neq j, S \subseteq \{i, j\} C, |S| \leq m_n} |\rho_n(i, j | S)| \leq M < 1.
\]

We will later see in Lemma 3 that we need \(m_n \leq p_{\text{eff}} n\) only, and hence, assumptions (D4\(_{m_n}\)) and (D5\(_{m_n}\)) coincide with (D4) and (D5), respectively.

We have, for \(m_n < n - 4\) and \(0 < \gamma < 2\),

\[
\sup_{S \subseteq K_{m_n}^n, j=1,\ldots,p_n} \Pr\{|\hat{\rho}_n(Y, j | S) - \rho_n(Y, j | S)| > \gamma\} \leq C_1 n \exp(n - m_n - 4) \log \left(\frac{4 - \gamma^2}{4 + \gamma^2}\right).
\]
where \(0 < C_1 < \infty\) depends on \(M\) in (D5\(_{m_n}\)) only. This bound appears in Kalisch & Bühlmann (2007, Corollary 1): for proving it, we require the Gaussian assumption for the distribution and (D5\(_{m_n}\)). It is now straightforward to derive an exponential inequality for the estimated \(Z\)-transformed partial correlations. We define \(Z_n(Y, j \mid S) = g(\hat{\rho}_n(Y, j \mid S))\) and \(z_n(Y, j \mid S) = g(\rho_n(Y, j \mid S))\), where \(g(\rho) = \frac{1}{2} \log\left((1 + \rho)/(1 - \rho)\right)\).

**Lemma 1.** Suppose that the Gaussian assumption from (D1) and condition (D5\(_{m_n}\)) hold. Define \(L = 1/\{1 - (1 + M)^2/4\}\), with \(M\) as in assumption (D5\(_{m_n}\)). Then, for \(m_n < n - 4\) and \(0 < \gamma < 2L\),

\[
\sup_{S \in K \_m, j = 1, \ldots, p_n} \Pr\{\left| Z_n(Y, j \mid S) - z_n(Y, j \mid S) \right| > \gamma \leq O(n) \left( \exp\left( (n - 4 - m_n) \log\left( \frac{4 - (\gamma/L)^2}{4 + (\gamma/L)^2} \right) \right) + \exp\{-C_2(n - m_n)\} \right)
\]

for some constant \(C_2 > 0\).

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

We now consider a version of the PC-simple algorithm that stops after a fixed number of \(m\) iterations. If \(m \geq \hat{m}_{\text{reach}}\), where \(\hat{m}_{\text{reach}}\) is the estimation analogue of (9), we set \(\hat{A}[m] = \hat{A}[\hat{m}_{\text{reach}}]\). We denote this version by PC-simple(\(m\)) and the resulting estimate by \(\hat{A}(\alpha, m)\).

**Lemma 2.** Assume (D1)-(D3), (D4\(_{m_n}\)) and (D5\(_{m_n}\)). Then, for \(m_n\) satisfying \(m_n \geq m_{\text{reach}}, n\) and \(m_n = O(n^{-1/6})\) with \(b\) as in (D3), there exists a sequence \(\alpha_n \rightarrow 0\) such that

\[
\Pr\{\hat{A}_n(\alpha_n, m_n) = A_n\} = 1 - O\{\exp(-C n^{-1/2})\} \rightarrow 1 (n \rightarrow \infty)\text{ for some } C > 0.
\]

A concrete choice of \(\alpha_n\) is \(\alpha_n = 2\{1 - \Phi(n^{1/2} c_n/2)\}\), where \(c_n\) is the lower bound from (D4\(_{m_n}\)), which is typically unknown.

**Proof.** Obviously, the population version of the PC-simple(m\(_n\)) algorithm is correct for \(m_n \geq m_{\text{reach}}, n\); 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 \(S \in K^{m_n}\) for which an error event \(E_{j|S}\) occurs, where \(E_{j|S}\) denotes the event that an error occurred when testing \(\rho_n(Y, j \mid S) = 0\). Thus,

\[
\Pr\{\text{an error occurs in the PC-simple(m\(_n\)-algorithm)} \leq \Pr\left( \bigcup_{S \in K^{m_n}, j = 1, \ldots, p_n} E_{j|S} \right) \leq O(p^{m_n+1}) \sup_{S \in K^{m_n}, j} \Pr(E_{j|S}),
\]

using that the cardinality of the index set \(\{S \in K^{m_n}, j = 1, \ldots, p_n\}\) in the union is bounded by \(O(p^{m_n+1})\). Now

\[
E_{j|S} = E_{j|S}^I \cup E_{j|S}^{II},
\]

where

\[
\text{type I error } E_{j|S}^I: (n - |S| - 3)^{1/2}|Z_n(Y, j \mid S)| > \Phi^{-1}(1 - \alpha/2) \text{ and } z_n(Y, j \mid S) = 0,
\]

\[
\text{type II error } E_{j|S}^{II}: (n - |S| - 3)^{1/2}|Z_n(Y, j \mid S)| \leq \Phi^{-1}(1 - \alpha/2) \text{ and } z_n(Y, j \mid S) \neq 0.
\]

Choose \(\alpha = \alpha_n = 2\{1 - \Phi(n^{1/2} c_n/2)\}\), where \(c_n\) is from (D4\(_{m_n}\)). Then,

\[
\sup_{S \in K^{m_n}, j = 1, \ldots, p_n} \Pr(E_{j|S}^I) = \sup_{S \in K^{m_n}, j} \Pr\{\left| Z_n(Y, j \mid S) - z_n(Y, j \mid S) \right| > \{n/(n - |S| - 3)\}^{1/2}c_n/2 \}
\]

\[
\leq O(n) \exp\{-C_3(n - m_n)c_n^2\},
\]

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

\[
\sup_{S \in \mathbb{K}_j^{m, n}} \text{pr}(E_{j|S}^{II}) = \sup_{S \in \mathbb{K}_j^{m, n}} \text{pr}\left[|Z_n(Y, j | S)| \leq \{n/(n - |S| - 3)\}^{1/2}c_n/2\right]
\]

\[
\leq \sup_{S \in \mathbb{K}_j^{m, n}} \text{pr}\left(|Z_n(Y, j | S) - z_n(Y, j | S)| > c_n[1 - \{n/(n - |S| - 3)\}^{1/2}/2]\right),
\]

because \( \inf_{S \in \mathbb{K}_j^{m, n}}\{|z_n(Y, j | S)|; \; z_n(Y, j | S) \neq 0\} \geq c_n \) since \( |g(\rho)| = \frac{1}{2} \log\{(1 + \rho)/(1 - \rho)\} \geq |\rho| \) for all \( \rho \) and using assumption (D4\(_m,n\)). This shows the crucial role of assumption (D4\(_m,n\)) in controlling the type II error. By invoking Lemma 1 we then obtain:

\[
\sup_{S \in \mathbb{K}_j^{m, n}} \text{pr}(E_{j|S}^{II}) \leq O(n) \exp\{-C_4(n - m_n)c_n^2\}
\]  

(A6)

for some \( C_4 > 0 \). Now, by (A3)-(A6) we get

\[
\text{pr}\{\text{an error occurs in the PC-simple}(m_n)\text{-algorithm}\}
\]

\[
\leq O[p_{m_n + 1}n \exp\{-C_5(n - m_n)c_n^2\}] \leq O[n^{a(m_n + 1)}\exp\{-C_5(n - m_n)n^{-2d}\}]
\]

\[
= O\left[\exp\{a(m_n + 1)\log(n) + \log(n) - C_5(n^{1-2d} - m_nn^{-2d})\}\right] = o(1),
\]

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 (D4\(_m,n\)) 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 (9).

**Lemma 3.** Assume (D1)-(D5). Then,

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

for some \( C > 0 \), with \( d \) as in (D4).

**Proof.** Consider the population version of the PC-simple algorithm, with stopping level \( m_{\text{reach}} \) as defined in (9). Note that \( m_{\text{reach}} = m_{\text{reach}, n} = O(n^{1-b}) \) under assumption (D3). The sample PC-simple\(_{\text{m}}\text{-algorithm with stopping level in the range of } m_n \geq m_{\text{reach}} \text{ (} m_n = O(n^{1-b}) \text{), coincides with the population version on a set } A \text{ having probability } \text{pr}\{A\} = 1 - O\{\exp(-Cn^{1-2d})\}, \text{ 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 with \( m_n = \text{peff}_n \) together with Lemma 3, and using that \( m_{\text{reach}, n} \leq \text{peff}_n \), complete the proof of Theorem 4.

**Proof of Theorem 5.** By definition, \( A_n \subseteq A^{[1]} \) for the population version. Denote by \( Z_n(Y, j) \) the quantity as in (10) with \( S = \emptyset \) and by \( z_n(Y, j) \) its population analogue, i.e., the \( Z \)-transformed population correlation. An error occurs when screening the \( j \)-th 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

\[
\sup_{j=1, \ldots, p_n} \text{pr}(E_{j}^{II}) \leq O(n) \exp\{-C_1nc_n^2\},
\]

for some \( C_1 > 0 \), see formula (A6) above. We do not use any sparsity assumption for this derivation, but we do invoke (E1) which requires a lower bound on non-zero marginal correlations. Thus, the probability of an error occurring in the correlation screening procedure is bounded: for some \( C_2 > 0 \),

\[
\text{pr}\{\bigcup_{j=1, \ldots, p_n} E_{j}^{II}\} = O(p_n n) \exp\{-C_1nc_n^2\} = O[\exp\{(1 + a)\log(n) - C_1n^{1-2d}\}]
\]

\[
= O\{\exp(-C_2n^{1-2d})\}.
\]

\( \Box \)
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