Variable selection for high-dimensional models: partial faithful distributions, strong associations and the PC-algorithm

Peter Bühlmann and Markus Kalisch
ETH Zürich

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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. In particular, we present the concept of partially faithful distributions and discuss their role for inferring associations between the response and the covariates. For partially faithful distributions, a simplified version of the PC-algorithm (Spirtes et al., 2000) which is computationally feasible even with thousands of covariates yields consistency for high-dimensional variable selection under clearly weaker conditions than penalty-based approaches; in fact, we prove that the PC-algorithm is consistent for very ill-posed design. If partial faithfulness does not hold, we show that the PC-algorithm still consistently identifies some strong associations which are related to notions of causality. We also provide an efficient implementation of our (simplified) PC-algorithm in the `R`-package `pcalg` and demonstrate the method on simulated and real data.

1 Introduction

The variable selection problem for high-dimensional models has recently gained a lot of attraction. A particular stream of research has focused on estimators and algorithms whose computation is feasible and provably correct (Meinshausen and Bühlmann, 2006; Zou, 2006; Zhao and Yu, 2006; Bunea et al., 2007; Candes and Tao, 2007; Meinshausen and Yu, 2006; van de Geer, 2007; Zhang and Huang, 2007; Huang et al., 2006; Wasserman and Roeder, 2007). As such, these methods distinguish themselves very clearly from heuristic optimization of an objective function or stochastic simulation or search, e.g. MCMC, which are often not really exploiting a high-dimensional search space. Prominent examples of computationally feasible and provably correct (w.r.t. computation) methods are penalty-based approaches, including the Lasso (Tibshirani, 1996), the adaptive Lasso (Zou, 2006) or the Dantzig selector (Candes and Tao, 2007).

We propose here a method for linear models which is "diametrically opposed" to penalty-based schemes. Three reasons for another approach include the following: (i) it can be worthwhile to infer stronger concepts of associations than what is obtained from the usual regression coefficients, in particular when focusing on causal relations; (ii) from a theoretical perspective, we prove that in the framework of so-called partially faithful

distributions, our method leads to consistent model selection for almost arbitrary designs and hence for much more general situations than what has been shown for the Dantzig selector or the Lasso or the adaptive Lasso; (iii) 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 have been selected by say two very different methods. We will address all these reasons, without prioritizing one over the other.

Our method is a simplification of the PC-algorithm (Spirtes et al., 2000) which has been proposed for estimating directed acyclic graphs; the simplification arises because selecting variables in a linear model is easier than assigning a directed association in a graphical model. We prove consistency for variable selection in high-dimensional linear models where the number of covariates can greatly exceed the sample size. For the ordinary problem of inferring the non-zero regression coefficients, we introduce and assume the framework of partially faithful distributions. Partial faithfulness is novel and weaker than the faithfulness condition from graphical models (Spirtes et al., 2000, cf.), and we prove here that partial faithfulness arises naturally in the context of (high-dimensional) linear models. Assuming such partial faithfulness in a linear model, which is arguably only a mild requirement, our simplified PC-algorithm is asymptotically consistent under almost arbitrarily ill-posed designs; essentially, we only need that the variables are identifiable in the population case and there are no conditions on the coherence or minimal sparse eigenvalues of the design. Furthermore, causal relations and stronger notions of associations than what is represented by the regression coefficients can be important. In particular, when faithfulness fails to hold, these concepts distinguish themselves very clearly from the regression-type associations. We also prove that for non-faithful distributions, the PC-algorithm is consistent for inferring some strong associations between the response variable and the covariates.

Moreover, the PC-algorithm is computationally feasible in high-dimensional problems: its computational complexity is crudely bounded by a polynomial in p, the dimension of the covariate space, and we illustrate that our implementation in `R` (CRAN, 1997 ff.) has about the same magnitude for computing time as the LARS-algorithm (Efron et al., 2004). Our approach can also be adapted for preliminary reduction of the dimension of the covariate space: we call it "correlation screening" and the method bears some relations to "sure independence screening" (Fan and Lv, 2007).

Finally, we compare our PC-algorithm with the Lasso and the elastic net (Zou and Hastie, 2005), and we demonstrate on some real data the usefulness of having "diametrically opposed" methods for analyzing a high-dimensional data-set on riboflavin production from bacillus subtilis.

2 Gaussian linear model and partial faithfulness

We are considering here a class of probability distributions for linear models which satisfies a so-called partial faithfulness condition. Such a condition will be crucial for identifying the effective variables (in the sense of regression) with the PC-algorithm whose computational complexity is bounded by a polynomial in the number of covariates.

Consider the Gaussian linear model

$$
\begin{aligned}
&Y_i = \sum_{j=1}^{p} \beta_j X_i^{(j)} + \varepsilon_i, \ (i = 1, \ldots, n), \\
&X_1, \ldots, X_n \text{ i.i.d. } \sim \mathcal{N}_p(\mu_X, \Sigma_X), \\
&\varepsilon_1, \ldots, \varepsilon_n \text{ i.i.d. } \sim \mathcal{N}_1(0, \sigma^2) \text{ and independent of } \{X_1, \ldots, X_n\}.
\end{aligned} \tag{1}
$$

First, we assume:

(A1) Σ_X is strictly positive definite.

Note that (A1) implies identifiability of the regression parameters since $\beta = \Sigma_X^{-1}\gamma$, where $\beta = (\beta_1, \ldots, \beta_p)^T$ and $\gamma = (\mathrm{Cov}(Y, X^{(1)}) \ldots, \mathrm{Cov}(Y, X^{(p)}))^T$. Moreover, the following mild assumption is crucial for what follows. It is a condition on the structure of β_j $(j = 1, \ldots, p)$: to do so, we will use the framework where the non-zero coefficients are fixed realizations from a probability distribution.

(A2) Denote the active set by $\mathcal{A} \subseteq \{1, \ldots p\}$ and by $\mathcal{A}^C$ its complement. The regression coefficients satisfy:

$$
\begin{aligned}
&\beta_j = 0 \text{ for } j \in \mathcal{A}^C, \\
&\{\beta_j;\ j \in \mathcal{A}\} \sim f(b)db,
\end{aligned}
$$

where $f(\cdot)$ denotes a density in (a subset of) $\mathbb{R}^{\mathrm{peff}}$, peff $= |\mathcal{A}|$, of an absolutely continuous distribution with respect to Lebesgue measure.

Assumption (A2) says that the regression coefficients are either equal to zero or (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 Gaussian linear model (1).

Definition 1. *(partial faithfulness)*
The Gaussian linear model (1) satisfies the ***weak partial faithfulness*** *assumption if and only if*

$$
\mathit{Parcor}(Y, X^{(j)} | X^{(S)}) = 0 \implies \beta_j = 0,
$$

for $j \in \{1, \ldots, p\}$ and $\mathcal{S} \subseteq \{1, \ldots, p\} \setminus j$; and it satisfies the ***strong partial faithfulness*** *assumption if and only if*

$$
\begin{aligned}
\mathit{Parcor}(Y, X^{(j)} | X^{(S)}) = 0 \implies \quad & \mathit{Parcor}(Y, X^{(j)} | X^{(S')}) = 0 \\
& \text{for all } \mathcal{S}' \text{ with } \{1, \ldots, p\} \setminus j \supseteq \mathcal{S}' \supseteq \mathcal{S},
\end{aligned}
$$

for $j \in \{1, \ldots, p\}$ and $\mathcal{S} \subseteq \{1, \ldots, p\} \setminus j$.

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

A proof is given in the Appendix. Theorem 1 says that failure of partial faithfulness will have probability zero (i.e. Lebesgue measure zero). Our result is in the spirit of a result by Spirtes et al. (2000, Th. 3.2), saying that non-faithful Gaussian distributions for a directed acyclic graph have Lebesgue measure zero. To appreciate such results, consider the setting of our Theorem 1: the regression coefficients having values zero can arise in an arbitrary order (and they do concentrate on the value 0) and only the non-zero coefficients are required to arise from an absolutely continuous probability distribution where concentration on some particular value does not happen.

The concept of faithful distributions is often used in the graphical modeling literature. There, conditional dependencies of a probability distribution P can be inferred from a graph thanks to some Markov condition. In general, the distribution P may include other conditional independence relations than those entailed by or derived from the Markov condition. If that is not the case, i.e. if all conditional dependencies can be read off the graph, the distribution is called faithful, see Spirtes et al. (2000). In the case of a Gaussian graphical model where the corresponding distribution P is multivariate Gaussian, faithfulness implies the property in Definition 1 among all the variables: since we focus only on partial correlations between the response Y and any other covariate $X^{(j)}$ (but not the partial correlation between say $X^{(j)}$ and $X^{(k)}$ $(j \neq k)$), we use in Definition 1 the terminology of partial faithfulness. A consequence of partial faithfulness is as follows.

Proposition 1. *Consider the Gaussian linear model (1) satisfying the weak partial faithfulness condition. Then,*

$$\textit{Parcor}(Y, X^{(j)}|X^{(\mathcal{S})}) \neq 0 \textit{ for all } \mathcal{S} \subseteq \{1, \ldots, p\} \setminus j \Longleftrightarrow \beta_j \neq 0,$$

for $j \in \{1, \ldots, p\}$.

A proof is given in the Appendix. Proposition 1 shows that an effective variable, which is an element of the active set $\mathcal{A} = \{j; \beta_j \neq 0\}$ has a stronger interpretation in the sense that all corresponding partial correlations are different from zero when conditioning on any subset $\mathcal{S} \subseteq \{1, \ldots, p\} \setminus j$. In many applications, this is a desirable property, and a stronger concept for association which is linked more closely to some notion of causality (Spirtes et al., 2000); more details are given in Section 4.

2.1 Correlation screening using weak partial faithfulness

If partial faithfulness holds, see Definition 1, we can exploit some immediate consequences for construction of algorithms for variable selection. Weak partial faithfulness says:

$$\text{Parcor}(Y, X^{(j)}|X^{(\mathcal{S})}) = 0 \Longrightarrow \beta_j = 0.$$

The easiest relation, in particular when it comes to estimation, is with $\mathcal{S} = \emptyset$:

$$\text{Cor}(Y, X^{(j)}) = 0 \Longrightarrow \beta_j = 0. \tag{2}$$

We can do screening according to marginal correlations and build a first set of candidate active variables

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

We call this the step$_1$ active set or the correlation screening active set. We know by (2) that variables with corresponding correlations being equal to zero will be non-active, i.e. they can be dropped from the model. In other words, the true underlying active set $\mathcal{A} = \{j;\ \beta_j \neq 0\}$ satisfies

$$\mathcal{A} \subseteq \mathcal{A}^{[1]}. \tag{3}$$

Such covariance screening may reduce the dimensionality of the problem already by a substantial or even huge amount, and due to (3), we can use other variable selection methods on the reduced set of variables $\mathcal{A}^{[1]}$.

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

$$\text{Parcor}(Y, X^{(j)}|X^{(k)}) = 0 \text{ for some } k \neq j \Longrightarrow \beta_j = 0. \tag{4}$$

That is, for checking whether the jth covariate remains in the model, we would additionally screen with all partial correlations of order one. As we will see in Section 3, it will be sufficient to use only conditioning variables $X^{(k)}$ which are elements of $\mathcal{A}^{[1]}$. Screening with partial correlations of order one using (4) leads to a smaller active set

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

This new step$_2$ active set $\mathcal{A}^{[2]}$ may have reduced the dimensionality of the original problem a lot. We can then continue screening using higher-order partial correlations, as will be described in Section 3.1, and we end up with a nested sequence of step$_m$ active sets

$$\mathcal{A}^{[1]} \supseteq \mathcal{A}^{[2]} \supseteq \ldots \supseteq \mathcal{A}^{[m]} \supseteq \ldots \supseteq \mathcal{A}. \tag{5}$$

A step$_m$ active set $\mathcal{A}^{[m]}$ can be used as dimensionality reduction and any favored variable selection method could then be used for the reduced linear model with covariates corresponding to indices in $\mathcal{A}^{[m]}$. Alternatively, we can use the sequence in (5) without applying additional variable selection methods. This will be described in Section 3.

3 Estimation using the PC-algorithm

A simplified version of the PC-algorithm (Spirtes et al., 2000) can be used to compute the sequence of step$_m$ active sets in (5).

3.1 The population version of the PC-algorithm

We assume that perfect knowledge about partial correlations is available.

The value of m which is reached by the algorithm is defined as follows:

$$m_{\text{reach}} = \min\{m;\ \mathcal{A}^{[m+1]} = \mathcal{A}^{[m]}\} \tag{6}$$

Proposition 2. *For the Gaussian linear model (1) satisfying (A1) and weak partial faithfulness, the population PC$_{\text{pop}}$-algorithm identifies the true underlying active set, i.e.* $\mathcal{A}^{[m_{\text{reach}}]} = \mathcal{A} = \{1 \leq j \leq p;\ \beta_j \neq 0\}$.

A proof is given in the Appendix. Note that weak partial faithfulness is implied by assumption (A2). Correctness of the population PC$_{\text{pop}}$-algorithm for directed acyclic graphs has been given by Spirtes et al. (2000, Th. 5.1).

Algorithm 1 The $\mathrm{PC}_{\mathrm{pop}}$-algorithm

1: Start with the step_0 active set $\mathcal{A}^{[0]} = \{1, \ldots, p\}$.
2: Set $m = 1$. Do correlation screening, see (2), and build the step_1 active set $\mathcal{A}^{[1]} = \{1 \le j \le p;\ \mathrm{Cor}(Y, X^{(j)}) \neq 0\}$
3: **repeat**
4: $m = m + 1$. Construct the step_m active set:

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

5: **until** the step_m active sets do not change anymore.

3.2 Sample version of the PC-algorithm

For finite samples, we need to estimate partial correlations. The sample partial correlation $\hat{\rho}_{Y,j|\mathcal{S}} = \widehat{\mathrm{Parcor}}(Y, X^{(j)}|X^{(\mathcal{S})})$ and $\hat{\rho}_{i,j|\mathcal{S}} = \widehat{\mathrm{Parcor}}(X^{(i)}, X^{(j)}|X^{(\mathcal{S})})$ can be calculated recursively by using the following identity: for some $k \in \mathcal{S}$,

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

For testing whether a partial correlation is zero or not, we apply Fisher's Z-transform

$$Z(Y, j|\mathcal{S}) = \frac{1}{2}\log\left(\frac{1+\hat{\rho}_{Y,j|\mathcal{S}}}{1-\hat{\rho}_{Y,j|\mathcal{S}}}\right). \tag{7}$$

Classical decision theory yields then the following rule when using the 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 cdf of $\mathcal{N}(0, 1)$.

The sample version of the PC-algorithm is almost identical to the population version in Section 3.1.

The PC-algorithm

Run the $\mathrm{PC}_{\mathrm{pop}}$-algorithm as described in Section 3.1 but replace in steps 2 and 4 of Algorithm 1 the statements about $\mathrm{Parcor}(Y, X^{(j)}|X^{(\mathcal{S})}) \neq 0$ (including $\mathcal{S} = \emptyset$) by

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

The only tuning parameter of the PC-algorithm is α, the significance level for testing partial correlations. The analogue to the reached value of m in (6) is denoted by $\hat{m}_{reach}$.

The computational complexity of the PC-algorithm is difficult to evaluate exactly, but the worst case is bounded by

$$O(np^{\hat{m}_{\mathrm{reach}}}) \text{ which is with high probability bounded by } O(np^{\mathrm{peff}}), \tag{8}$$

where $\mathrm{peff} = |\mathcal{A}|$, cf. Kalisch and Bühlmann (2007). Thus, the PC-algorithm is polynomial in p. In fact, the bound in (8) is often very loose and we can easily use the algorithm for problems where $p \approx 100 - 5'000$, as demonstrated in Section 6.

4 Failure of partial faithfulness and measures of association

By Theorem 1, failure of partial faithfulness happens for very specific parameter constellations in the linear model (1), i.e. the non-zero coefficients do not arise from a continuous probability distribution. We give two examples.

Example 1. *Consider a Gaussian linear model*

$$\begin{aligned} Y &= X^{(1)} - X^{(2)} + \varepsilon, \\ X^{(2)} &= X^{(1)} + \gamma, \end{aligned}$$

where $X^{(1)}$, γ, ε *are i.i.d.* $\sim \mathcal{N}(0, \sigma^2)$. *This is a linear model as in (1) with a specific parameter constellation for the regression parameters. It can be easily calculated that*

$$Cor(Y, X^{(1)}) = 0, \;\; Parcor(Y, X^{(1)} | X^{(2)}) \neq 0,$$

and hence, weak partial faithfulness fails to hold. We may understand this also by writing the model in a different form by simply substituting $X^{(2)} = X^{(1)} + \gamma$*:*

$$Y = -\gamma + \varepsilon.$$

Example 2. *Consider a Gaussian moving average model from time series:*

$$X_t = \theta_1 \varepsilon_{t-1} + \varepsilon_t, \;\; t \in \mathbb{Z},$$

where $\{\varepsilon_t;\ t \in \mathbb{Z}\}$ *is a sequence of i.i.d. variables* $\varepsilon_t \sim \mathcal{N}(0, \sigma^2)$, *and* $|\theta_1| < 1$ *a parameter. In terms of (auto-)regression, the model can be written as*

$$X_t = \sum_{j=1}^{\infty} (-\theta_1)^j X_{t-j} + \varepsilon_t, \;\; t \in \mathbb{Z}$$

and hence, using $Y = X_t$, *this is a linear model with* $p = \infty$. *We focus only on three variables* $\{Y = X_t, X_{t-1}, X_{t-2}\}$ *corresponding to one response and two covariates. It is well known that*

$$Cor(Y, X_{t-2}) = Cor(X_t, X_{t-2}) = 0, \quad Parcor(Y, X_{t-2} | X_{t-1}) = Parcor(X_t, X_{t-2} | X_{t-1}) \neq 0,$$

(Brockwell and Davis, 1991, cf.). Thus, this is another example where weak partial faithfulness does not hold.

The PC-algorithm would fail in both examples: it would drop the variable $X^{(1)}$ in Example 1 or X_{t-2} in Example 2 from the active set because the corresponding correlation is zero. The reason for failure though is - from a certain perspective - not undesirable. In fact, as described below in the continuation of Examples 1 and 2, there is no causal relation between the variables Y and $X^{(1)}$ (Example 1) or Y and X_{t-2} (Example 2), in the sense of the intervention framework with the do(·)-operator from Pearl (2000). Therefore, in a causal sense, the PC-algorithm would correctly declare no relation.

The following definitions of associations between the response Y and some of the covariates $X^{(j)}$ are useful:

$$\mathcal{A} = \{j;\ \text{Parcor}(Y, X^{(j)}|X^{(\{1,\ldots,p\}\setminus j)}) \neq 0\} = \{j;\ \beta_j \neq 0\},$$
$$\mathcal{A}_{strong} = \{j;\ \text{Parcor}(Y, X^{(j)}|X^{(\mathcal{S})}) \neq 0 \text{ for all } \mathcal{S} \subseteq \{1,\ldots,p\} \setminus j\},$$
$$\mathcal{A}_{strong-endo} = \max\{\mathcal{B} \subseteq \{1,\ldots,p\};\ \text{Parcor}(Y, X^{(j)}|X^{(\mathcal{S})}) \neq 0 \text{ for all } j \in \mathcal{B} \text{ and all } \mathcal{S} \subseteq \mathcal{B} \setminus j\}.$$

The set $\mathcal{A}$ is the usual active set from regression containing the covariates having regression coefficients different from zero; the set $\mathcal{A}_{strong}$ contains associations with a stronger notion, requiring that partial correlations remain non-zero when conditioning on any subset of covariates; and finally, the set $\mathcal{A}_{strong-endo}$ requires that partial correlations remain zero when conditioning on any subset of "endogenous" covariates which are associated with the response Y. Because there are fewer conditioning sets involved in $\mathcal{A}$ or $\mathcal{A}_{strong-endo}$ than in $\mathcal{A}_{strong}$, the following holds:

$$\mathcal{A}_{strong} \subseteq \mathcal{A}, \qquad \mathcal{A}_{strong} \subseteq \mathcal{A}_{strong-endo}. \tag{9}$$

Furthermore,

$$\text{for weakly partial faithful distributions: } \mathcal{A}_{strong} = \mathcal{A}_{strong-endo} = \mathcal{A}. \tag{10}$$

The equality $\mathcal{A} = \mathcal{A}_{strong}$ follows from Proposition 1, and the equality $\mathcal{A}_{strong-endo} = \mathcal{A}$ follows exactly as in the proof of Proposition 1. For non-faithful distributions, the equalities in (10) fail.

In general (for non-faithful distributions), the notions of associations in $\mathcal{A}_{strong}$ and $\mathcal{A}_{strong-endo}$ are more of a causal nature than in $\mathcal{A}$. In fact, $\mathcal{A}_{strong-endo}$ is in the two Examples a strong enough measure for causality.

Example 1 (continued)
For the linear model in Example 1, it is easy to see that $\mathcal{A}_{strong} = \mathcal{A}_{strong-endo} = \{2\}$. That is, only the second covariate $X^{(2)}$ is strongly associated with Y. In addition, if assuming a directed acyclic graph as in Figure 1 for generating the model, $\mathcal{A}_{strong} = \mathcal{A}_{strong-endo}$ coincides with the set of causal variables in the sense of the do$(\cdot)$ operator from Pearl (2000). That is, for the distribution of Y with and without intervention, $P(Y|\text{do}(X^{(1)} = u)) = P(Y)$ for all values u while $P(Y|\text{do}(X^{(2)} = u)) \neq P(Y)$ for some value u.

Example 2 (continued)
For the moving average model in Example 2, it is again straightforward to derive that $\mathcal{A}_{strong} = \mathcal{A}_{strong-endo} = \{t-1\}$. That is, only the first lagged variable X_{t-1} is strongly associated with $Y = X_t$. And as for Example 1, by using the directed acyclic graph as in Figure 1 for generating the model, $\mathcal{A}_{strong} = \mathcal{A}_{strong-endo}$ coincides with the set of causal variables in the sense of the do$(\cdot)$ operator from Pearl (2000). That is, for the distribution of $Y = X_t$ with and without intervention, $P(Y|\text{do}(X_{t-2} = u)) = P(Y)$ for all values u while $P(Y|\text{do}(X_{t-1} = u)) \neq P(Y)$ for some value u.

The following holds in the context of potentially non-faithful distributions.

Proposition 3. *Consider the Gaussian linear model (1) satisfying (A1). Then, the population PC_{pop}-algorithm identifies $\mathcal{A}_{strong-endo}$, i.e. $A^{[m_{\text{reach}}]} = \mathcal{A}_{strong-endo}$.*

(a) Example 1 (b) Example 2

Figure 1: Directed acyclic graphs corresponding to Examples 1 and 2.

The proof of Proposition 3 is straightforward since the definition of $\mathcal{A}_{strong-endo}$ coincides with the concept of the PC_{pop}-algorithm which looks for the largest set such that all partial correlations, when conditioning on variables from that set, are non-zero. We summarize that even when partial faithfulness fails, the PC-algorithm is appropriate for inferring strong-endogenous associations or "causal" structures.

5 Asymptotic consistency in high dimensions

We will show that the PC-algorithm from Section 3.2 is asymptotically consistent for variable selection, even if p is much larger than n but assuming that the true underlying linear model is sparse.

5.1 Consistency with faithful distributions

We consider the Gaussian linear model in (1). To capture high-dimensional behavior, we will let the dimension grow as a function of sample size: thus, $p = p_n$ and also the distribution of

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

changes with n which includes that the regression coefficient vectors $\beta = \beta_n$ are depending on n. Our assumptions are as follows.

(B1) The distribution P_n satisfies the weak partial faithfulness condition (see Definition 1) and assumption (A1) for all n.

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

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

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

$$\inf\{|\rho_n(Y, j|\mathcal{S})|;\ 1 \le j \le p_n,\ \mathcal{S} \subseteq \{1, \ldots, p_n\} \setminus j \text{ with } \rho_n(Y, j|\mathcal{S}) \ne 0\} \ge c_n,$$
$$c_n^{-1} = O(n^d) \text{ for some } 0 < d < b/2,$$
$$\sup_{n,j,\mathcal{S} \subseteq \{1,\ldots,p_n\} \setminus j} |\rho_n(Y, j|\mathcal{S})| \le M < 1,$$

where $0 < b \le 1$ is as in (A3).

Assumption (B1) is a mild assumption: the inclusion of (A1) is very weak and partial faithfulness follows from assuming (A2) in Section 2. Assumption (B2) allows for an arbitrary polynomial growth of dimension as a function of sample size, that is, high-dimensionality while (B3) is a sparseness assumption in terms of the number of effective variables. Assumption (B4) is a regularity condition, saying that the non-zero partial correlations have to be of larger order than $1/\sqrt{n}$. Without such a condition, one gets into the domain of super-efficiency, e.g. the behavior of the Hodges-Lehmann estimator. Assumptions (B3) and (B4) are rather minimal: note that with $b = 1$ in (B3), for example fixed $\text{peff}_n = \text{peff} < \infty$, the partial correlations can decay as $n^{-1/2+\varepsilon}$ for any $0 < \varepsilon \leq 1/2$. If the dimension p is fixed (with fixed distribution P in the Gaussian linear model), (B2) and (B3) hold and (B1) and the second part of (B4) remain as the only conditions.

Denote the active set by $\mathcal{A}_n = \{1 \leq j \leq p_n : \ \beta_{j,n} \neq 0\}$ and by $\widehat{\mathcal{A}}_n(\alpha)$ the estimate from the PC-algorithm in Section 3.2 with significance level α.

Theorem 2. *Consider the Gaussian linear model (1) and assume (B1)-(B4). Then, there exists $\alpha_n \to 0$ $(n \to \infty)$, see below, such that the PC-algorithm satisfies:*

$$\begin{aligned} & \mathbb{P}[\widehat{\mathcal{A}}_n(\alpha) = \mathcal{A}_n] \\ = \ & 1 - O(\exp(-Cn^{1-2d})) \to 1 \ (n \to \infty) \textit{ for some } 0 < C < \infty, \end{aligned}$$

where $d > 0$ is as in (B4).

A proof is given in the Appendix. It should be noted that for distributions which satisfy the weak partial faithfulness condition, as required by assumption (B1), the strong and the usual measures of association agree, i.e. $\mathcal{A}_{strong,n} = \mathcal{A}_{strong-endo,n} = \mathcal{A}_n$ and hence, the PC-algorithm consistently infers the strong associations. A choice for the value of the significance level, leading to consistency, is $\alpha_n = 2(1 - \Phi(n^{1/2}c_n/2))$ which depends on the unknown lower bound of partial correlations in (B4).

5.1.1 Comparison of conditions

It is interesting to compare our conditions with results on ℓ^1-penalized estimation and versions thereof for variable selection. Note that we compare conditions for methods which are feasible to compute for high-dimensional problems.

For the Lasso, Meinshausen and Bühlmann (2006) prove 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 "≤" relation). Zou (2006) and Zhao and Yu (2006) give a different, equivalent condition which is termed in the latter work the "irrepresentable" condition. We point out that the neighborhood stability or irrepresentable condition can quite easily fail to hold which, due to the "almost" necessity of the condition, implies inconsistency of the Lasso for variable selection.

In fact, inconsistency of the Lasso typically occurs because of over-estimation, i.e. the Lasso selects too many variables. This has been made more precise with asymptotic results on the ℓ^1- or ℓ^2-norm

$$\|\hat{\beta} - \beta\|_q \ (q = 1, 2), \tag{11}$$

see Bunea et al. (2007); Zhang and Huang (2007); van de Geer (2007); Meinshausen and Yu (2006). Also Candes and Tao (2007) prove, under restrictive conditions on the design, an ℓ^2-norm result for the Dantzig selector which is another penalized least squares estimation algorithm. If the ℓ^q-norm in (11) goes to zero, it then must hold (under some conditions for the size of the non-zero coefficients) that $\widehat{\mathcal{A}} = \{j;\ \hat{\beta}_j \neq 0\} \supseteq \mathcal{A}$. Furthermore, an additional stage of thresholding or using the more sophisticated adaptive Lasso (Zou, 2006) yield consistency of such two-stage procedures (Meinshausen and Yu, 2006; Huang et al., 2006). All of these works assume some conditions on either the minimal eigenvalues of the empirical covariance of the design, the coherence of the fixed design or the population correlations of the random design: these quantities measure the "ill-posedness" or the "degree of linear dependence" of the high-dimensional design matrix. Some of these conditions are substantially weaker than the neighborhood stability or the irrepresentable condition mentioned above.
Our conditions here, if one is willing to assume (A2), are again substantially weaker as we require only (A1) regarding the regularity of the (random) design matrix (assumption (B4) is mainly for the magnitude of partial correlations rather than correlations among columns of the design matrix): we do not need any conditions on coherence or eigenvalues of Gram-submatrices.

5.2 Consistency with non-faithful distributions

We have discussed in Proposition 3 that the PC_{pop}-algorithm identifies the set $\mathcal{A}_{strong-endo}$ from (10) which represents a more "causal" notion of association than the usual active set $\mathcal{A}$. The asymptotic arguments in the non-faithful case are very similar to the analysis before. We assume:

(C1) The distribution P_n satisfies assumption (A1) for all n.

(C2) as assumption (B2).

(C3) The cardinality of set $\mathcal{A}_{strong-endo;n}$ satisfies: $|\mathcal{A}_{strong-endo;n}| = O(n^{1-b})$ for some $0 < b \leq 1$.

(C4) as assumption (B4).

Theorem 3. *Consider the Gaussian linear model (1) and assume (C1)-(C4). Then, there exists $\alpha_n \to 0$ $(n \to \infty)$, see below, such that the PC-algorithm satisfies:*

$$\begin{aligned} & \mathbb{P}[\widehat{\mathcal{A}}_n(\alpha) = \mathcal{A}_{strong-endo;n}] \\ = \ & 1 - O(\exp(-Cn^{1-2d})) \to 1 \ (n \to \infty) \textit{ for some } 0 < C < \infty, \end{aligned}$$

where $d > 0$ is as in (C4).

Theorem 3 follows from Proposition 3 and analogous to the proof of Theorem 2. A possible choice of the tuning parameter is $\alpha = \alpha_n = 2(1 - \Phi(n^{1/2}c_n/2))$.

5.3 Consistency for correlation screening

For correlation screening, see formula (3), we do not require any sparsity. Related to our approach of correlation screening is the "Sure independence screening" by Fan and Lv (2007), but our reasoning, assumptions and mathematical derivations via weak partial faithfulness are very different. We assume:

(D1) as assumption (C1).

(D2) as assumption (B2).

(D3) as assumption (B4) but for marginal correlations $\mathrm{Cor}(Y, X^{(j)}) = \rho_n(Y, j)$ only.

As pointed out already, it is interesting to note that we do not make any assumption on sparsity.

Denote by $\widehat{\mathcal{A}}_n^{[1]}(\alpha)$ the correlation screening active set estimated from data using significance level α (i.e. the second step in the sample version of the PC-algorithm) and by $\mathcal{A}_{strong-endo;n}$, $\mathcal{A}_{strong;n}$ the set of variables from the stronger notions of associations as described in Section 4.

Theorem 4. *Consider the Gaussian linear model (1) and assume (D1)-(D3). Then, there exists $\alpha_n \to 0$ $(n \to \infty)$, see below, such that:*

$$\begin{aligned} & \mathbb{P}[\widehat{\mathcal{A}}_n^{[1]}(\alpha) \supseteq \mathcal{A}_{strong-endo,n}] \\ = \; & 1 - O(\exp(-Cn^{1-2d})) \to 1 \; (n \to \infty) \textit{ for some } 0 < C < \infty, \end{aligned}$$

where $d > 0$ is as in (D3).

A proof is given in the Appendix. We point out that $\mathcal{A}_{strong-endo;n} \supseteq \mathcal{A}_{strong;n}$, see formula (9). Moreover, for weakly partial faithful distributions, i.e. assuming (B1) instead of (D1), Theorem 4 says that $\mathbb{P}[\widehat{\mathcal{A}}_n^{[1]}(\alpha) \supseteq \mathcal{A}_n] \to 1$ $(n \to \infty)$. A possible choice of α 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 hence, $\widehat{\mathcal{A}}^{[1]}$ could still be large, e.g. almost as large as the full set $\{1 \leq j \leq p\}$, and no effective dimensionality reduction would happen.

6 Numerical results

We analyze the variable selection properties using simulated and some high-dimensional real data: we consider the classical association target only, namely the active set $\mathcal{A} = \{j;\ \beta_j \neq 0\}$. This enables a fair comparison of our PC-method with various versions of ℓ^1-penalized approaches. In addition to reporting on goodness of fit measures for estimating associations, we give an overview of the runtime of the different methods.

6.1 ROC analysis

We evaluate here the performance of the methods using ROC curves which measure the capacities for variable selection, independently from the issue to select good tuning parameters. We compare our simplified version of the PC-algorithm (PC, our own 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 `enet` to construct the ROC curve. In the ROC plots to be followed, horizontal and vertical bars indicate 95%-confidence intervals for the false positive rate (FPR) and the true positive rate (TPR), respectively; definitions of FPR and TPR are given in Section 6.2. In our PC-algorithm, the proposed default value for the tuning parameter is $\alpha = 0.05$: its performance is indicated by the intersection of a vertical line and the ROC curve.

We simulate data according to the Gaussian linear model (1) having p covariates with $\mu_X = 0$ and covariance matrix $\mathrm{Cov}(X^{(i)}, X^{(j)}) = \Sigma_{X;i,j} = \rho^{|i-j|}$. The errors are generated as in model (1). 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_js are sampled independently from a standard normal distribution and the indices of the nonzero β_js are evenly spaced between 1 and p. We consider a low- and a high-dimensional setting as follows:

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

6.1.1 Low Dimensional Case

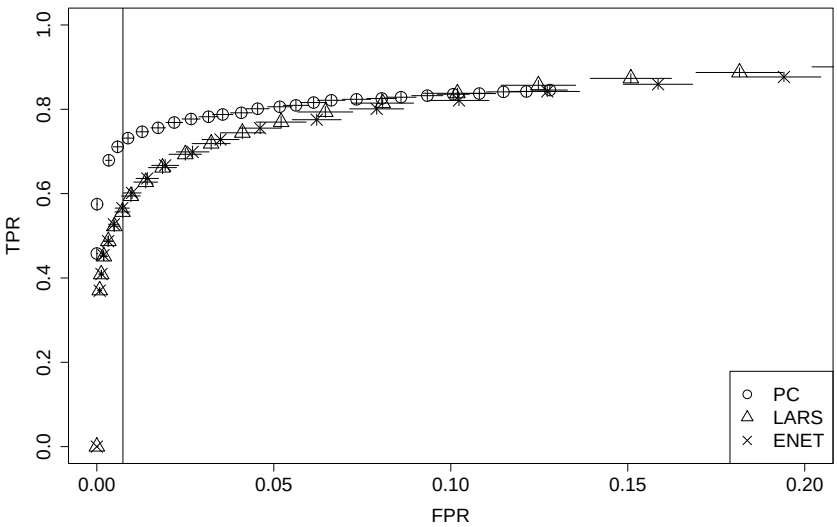

Figure 2: Low dimensional: $p = 19$, $\rho = 0$. Vertical line indicates performance of PC using the default $\alpha = 0.05$.

Results for the low-dimensional case are reported in Figures 2 to 4 which show a clear pattern. For small false positive rates (FPR), our PC method is clearly dominating LARS and ENET. If the correlation among the covariates increases, the performance of ENET

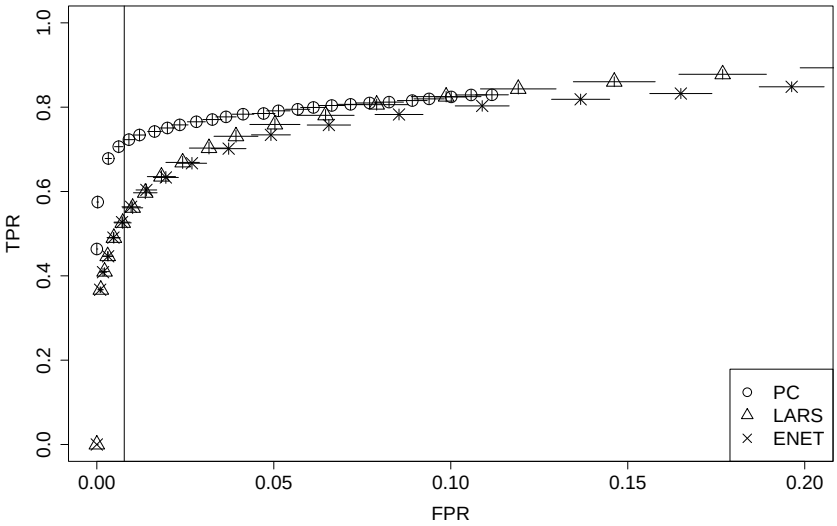

Figure 3: Low dimensional: $p = 19$, $\rho = 0.3$. Vertical line indicates performance of PC using the default $\alpha = 0.05$.

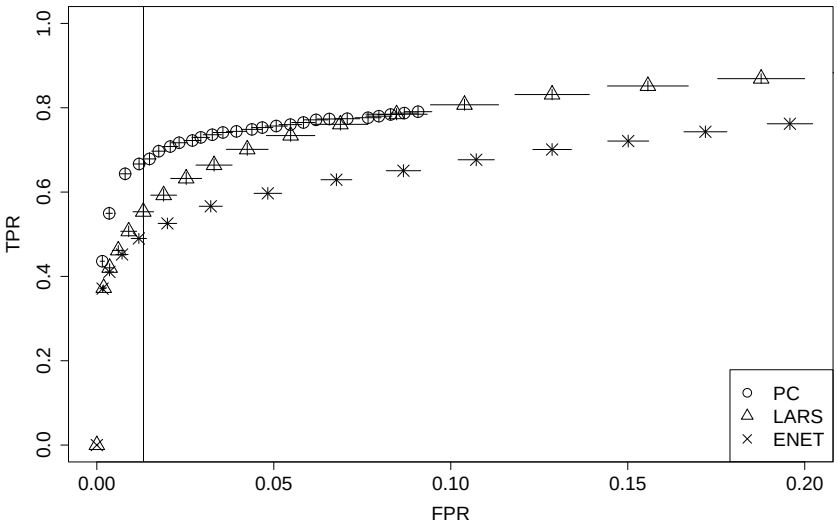

Figure 4: Low dimensional: $p = 19$, $\rho = 0.6$. Vertical line indicates performance of PC using the default $\alpha = 0.05$.

gets worse, whereas the performances of PC and LARS don't vary much. When focusing on values of FPR arising from the default value for α in our method, PC 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.

6.1.2 High Dimensional Case

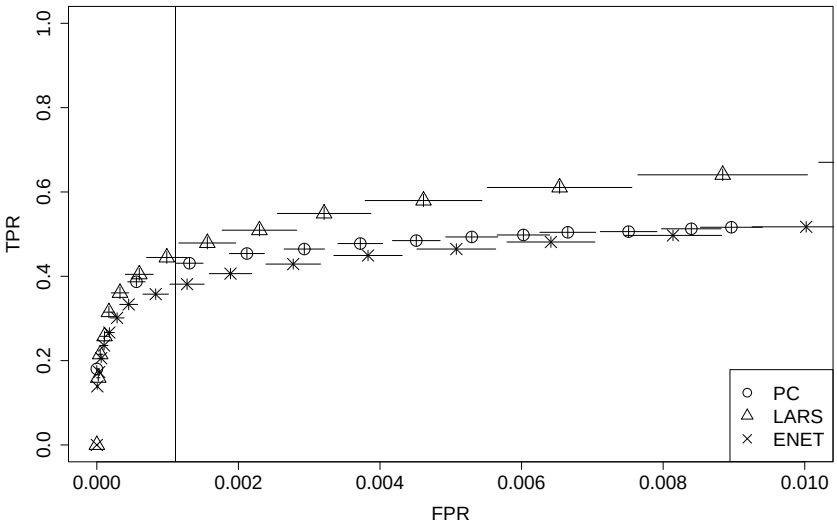

Figure 5: High dimensional: $p = 499$, $\rho = 0$. Vertical line indicates performance of PC using the default $\alpha = 0.05$.

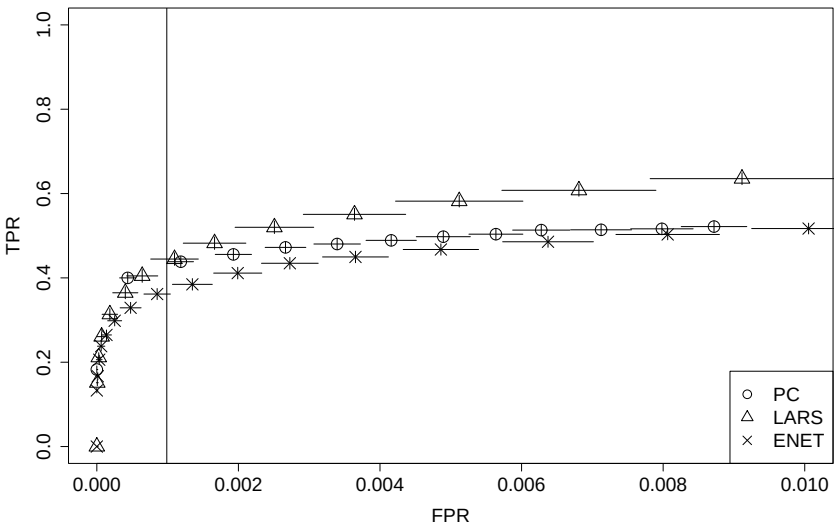

Figure 6: High dimensional: $p = 499$,$\rho = 0.3$. Vertical line indicates performance of PC using the default $\alpha = 0.05$.

For the high-dimensional case, the resulting ROC curves are given in Figures 5 to 7. For small false positive rates (FPR), the difference between the methods is not very big. LARS seems to perform best, while ENET is worst and PC is somewhere in between. For

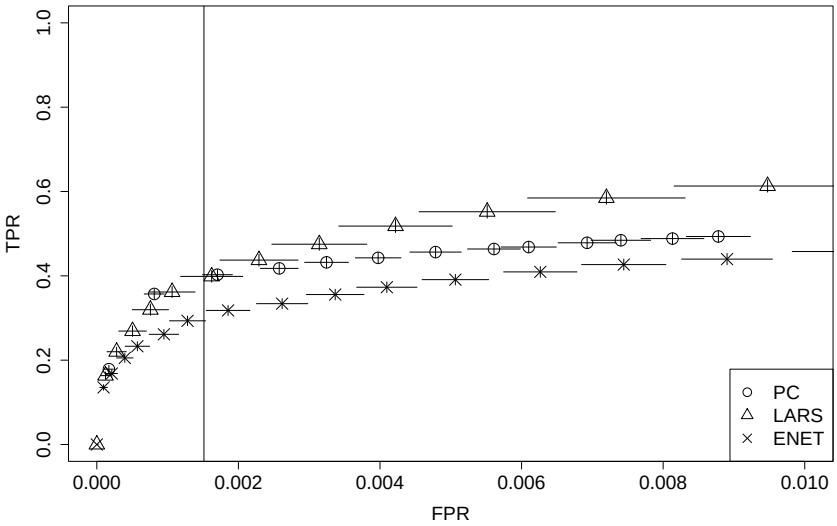

Figure 7: High dimensional: $p = 499$,$\rho = 0.6$. Vertical line indicates performance of PC using the default $\alpha = 0.05$.

larger FPR, this effect gets stronger. Up to the FPR which arises by the default value of $\alpha = 0.05$, PC is never significantly outperformed by either LARS or ENET.

6.1.3 Runtime

All calculations were done on a Dual Core Processor with 2.6 GHz and 32 GB RAM running on Linux and using R 2.5.1. The processor times were averaged in the low and high-dimensional example over 1000 and 300 replications, respectively. The average processor times and standard errors are given in Table 1.

p	ρ	$ave(t_{PC})$ [s]	$ave(t_{LARS})$ [s]	$ave(t_{ENET})$ [s]
19	0	0.004 (4e-5)	0.016 (3e-5)	0.024 (3e-5)
19	0.3	0.004 (4e-5)	0.016 (3e-5)	0.024 (3e-5)
19	0.6	0.005 (5e-5)	0.016 (3e-5)	0.024 (3e-5)
499	0	0.164 (0.003)	0.795 (0.006)	13.23 (0.03)
499	0.3	0.163 (0.002)	0.838 (0.007)	13.41 (0.03)
499	0.6	0.160 (0.002)	0.902 (0.006)	12.91 (0.02)

Table 1: Average runtime in seconds over 1000 and 300 repetitions for $p = 19$ and $p = 499$, respectively. The runtimes for PC were measured using the default of $\alpha = 0.05$ while LARS and ENET compute a whole path of solutions.

We should avoid the conclusion that PC is faster than LARS or ENET since the runtimes for PC were measured using the default of $\alpha = 0.05$ only whereas LARS and ENET compute a whole path of solutions. The purpose of Table 1 is to show that PC is certainly feasible for high-dimensional problems. In addition, when using PC on say 10

different (small) values of α, the computation is about of the same order of magnitude than LARS or ENET for the whole solution path.

6.2 Prediction Optimal Tuned Methods

We compare here different methods when using prediction optimal tuning. It is known that the prediction-optimal tuned Lasso overestimates the true model (Meinshausen and Bühlmann, 2006). The adaptive Lasso Zou (2006) and the relaxed Lasso Meinshausen (2007) correct Lasso's overestimation behavior. Furthermore, we use our simplified version of the PC-algorithm for variable selection and use then the Lasso or the adaptive Lasso to estimate coefficients for the sub-model selected by the PC-method. For simplicity, we do not show results for the elastic net (which was found to be worse in terms of ROC-curves than adaptive relaxed Lasso).

We are considering the following performance measures:

$$\begin{aligned}
&\|\hat{\beta}-\beta\|_2^2 = \sum_{j=1}^{p}(\hat{\beta}_j-\beta_j)^2 \quad \text{(MSE Coeff)},\\
&\mathbb{E}_X[(X^T(\hat{\beta}-\beta))^2] = (\hat{\beta}-\beta)^T\Sigma(\hat{\beta}-\beta)),\ \Sigma = \mathrm{Cov}(X) \quad \text{(MSE Pred)},\\
&\sum_{j=1}^{p} I(\hat{\beta}_j \neq 0)I(\beta_j \neq 0)/\sum_{j=1}^{p} I(\beta_j \neq 0) \quad \text{(true positive rate (TPR))},\\
&\sum_{j=1}^{p} I(\hat{\beta}_j \neq 0)I(\beta_j = 0)/\sum_{j=1}^{p} I(\beta_j = 0) \quad \text{(false positive rate (FPR))}.
\end{aligned} \tag{12}$$

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 with penalty $\lambda\sum_{j=1}^{p}|\beta_j|/|\hat{\beta}_{init,j}|$ 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 simplified version of the PC-algorithm with the Lasso for estimating coefficients is straightforward to do using the `pcalg`- and `lars`-packages from `R`: optimal tuning is with respect to the α-parameter for the PC-algorithm and the penalty parameter for Lasso. For the simplified version of the PC-algorithm with the adaptive Lasso, we first compute the weights w_j as follows: $w_j = 0$ if the variables has not been selected; and if the variable has been selected, w_j = minimum value of the test statistic $\sqrt{n-3-|\mathcal{S}|}Z(Y,j|\mathcal{S})$ (see Section 3.2) over all iterations of the PC-algorithm. Then, we compute the adaptive Lasso with penalty $\lambda\sum_{j=1}^{p} w_j^{-1}|\beta_j|$, i.e. the weights for the adaptive step are from the PC-algorithm.

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

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

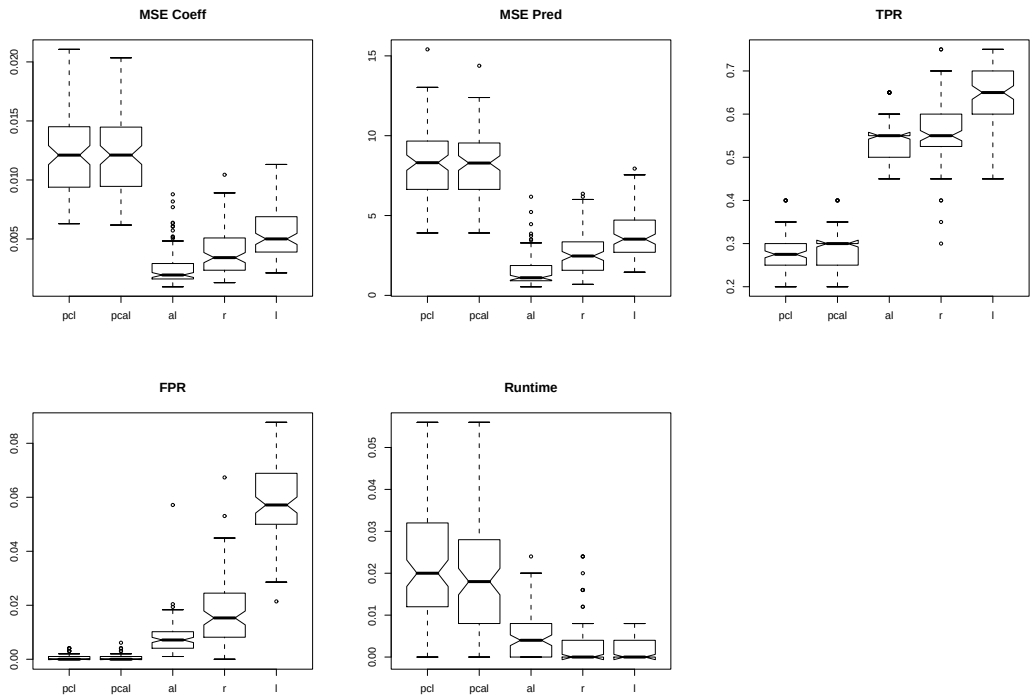

Figure 8: Prediction optimal tuned methods. Boxplots of performance measures as described in (12) and runtimes, based on 100 simulated model realizations. The PC-algorithm with Lasso coefficient estimation (PCl), the PC-algorithm with adaptive Lasso (PCal), Adaptive Lasso (al), Relaxed Lasso (r) and Lasso (l).

with 100 replicates.

Figure 8 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-based methods have clearly lowest false positive rates (FPR) while paying a price in terms of power, the true positive rate (TPR), and in terms of mean squared errors (MSE and prediction MSE).

In quite 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 (covariates) can be experimentally validated and hence, methods with a low false positive rate are preferred, in the hope that most of the top-selected genes are relevant. This type of application is briefly sketched in the next section.

6.3 Real Data: Riboflavin Production from Bacillus Subtilis

We consider a high-dimensional real dataset about riboflavin production in Bacillus Subtilis, provided by DSM Nutritional Products. There is a continuous response variable Y which measures the production rate of riboflavin, and there are $p = 4088$ covariates corresponding to the expression levels of genes. One of the major goals is to genetically modify

Bacillus Subtilis in order to increase its production rate for riboflavin. An important step to achieve this goal is to find some 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, LARS and ENET as for simulated data. We run PC 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. We show the results from a genetically homogeneous group of $n = 72$ individuals.

Table 2 indicates that LARS and ENET are more similar variable selection methods than PC and any of those two. Thus, the PC-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. We remark that we still find a remarkable overlap of the few selected

α for PC	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 2: Variable selection for real dataset on riboflavin production from Bacillus Subtilis. Number of selected variables (selected var.); number of variables which were selected from both PC and LARS (PC-LARS), from both PC and ENET (PC-ENET) and from both LARS and ENET (LARS-ENET).

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

7 Conclusions

The (simplified version of the) PC-algorithm is a very valuable method for inferring associations in a high-dimensional (but sparse) linear model where the number of covariates can greatly exceed the sample size. For weakly partial faithful distributions, and under mild assumptions allowing for very ill-posed designs, we prove consistency for inferring the covariates with corresponding regression coefficients being non-zero (Theorem 2). Furthermore, we show that partial faithful distributions arise quite naturally (Theorem 1). In addition, even if the weak assumption about faithfulness fails to hold, we prove that the PC-algorithm is consistent for some stronger notions of associations (Theorem 3) and we describe in Section 4 some connections to the concept of causality.

We also provide an efficient implementation of our (simplified) PC-algorithm in the `R`-package `pcalg`. The method is computationally feasible for high-dimensional problems with thousands of covariates, and we illustrate some results on simulated and real data in comparison to the Lasso and the Elastic Net.

8 Appendix

Proof of Theorem 1:
Consider first the case for weak partial faithfulness. Then, Theorem 1 reads:

$$Cov(Y, X^{(j)}|X^{(\mathcal{S})}) = 0 \text{ for some } \mathcal{S} \subseteq \{1, \ldots, p\} \setminus \{j\} \Longrightarrow \beta_j = 0. \tag{13}$$

For proving (13), we use the contra-position and assume that $\beta_j \neq 0$.

Then:

$$\mathrm{Cov}(Y, X^{(j)}|X^{(\mathcal{S})}) = \sum_{r \in \mathcal{A} \cap \mathcal{S}^C} \beta_r \Sigma_{X|\mathcal{S};r,j} = \beta_j \mathrm{Var}(X^{(j)}|X^{(\mathcal{S})}) + \sum_{r \in \mathcal{A} \cap \mathcal{S}^C, r \neq j} \beta_r \Sigma_{X|\mathcal{S};r,j},$$

where $\mathcal{A} = \{1 \leq r \leq p;\ \beta_r \neq 0\}$ and $\Sigma_{X|\mathcal{S}} = \mathrm{Cov}(X|X^{(S)})$ (which has degenerate entries for indices in $\mathcal{S}$). In the Gaussian case, conditional covariances are almost surely constant (and equal the partial covariances), cf. Anderson (1984, Th. 2.5.1). Thus, the first quantity on the right-hand side equals some deterministic real-valued number $a_j \neq 0$ almost surely. Therefore, the only way that the covariance $\mathrm{Cov}(Y, X^{(j)}|X^{(\mathcal{S})})$ would equal zero would be:

$$\sum_{r \in \mathcal{A} \cap \mathcal{S}^C, r \neq j} \beta_r \Sigma_{X|\mathcal{S};r,j} + a_j = 0 \text{ a.s..} \tag{14}$$

But this cannot happen, because (14) describes a hyperplane for $\{\beta_r;\ r \in \mathcal{A} \cap \mathcal{S}^C, r \neq j\}$ whose probability is zero since the β_r's are from an absolutely continuous distribution with respect to Lebesgue measure; i.e. the set of β_r's for which (14) holds has Lebesgue measure zero. This proves (13).

For proving the statement about strong partial faithfulness, consider the model

$$Y = \sum_{r \in \mathcal{S}' \cup j} \gamma_r X^{(r)} + \eta, \tag{15}$$

where η is independent of $\{X^{(r)}; r \in \mathcal{S}' \cup j\}$. The proof is now analogous to (13) but working with the model (15) where $\mathrm{Parcor}(Y, X^{(j)}|X^{(\mathcal{S}')}) = 0$ is equivalent to $\gamma_j = 0$. In addition, the non-zero regression coefficients are again realizations of a distribution which is absolutely continuous with respect to Lebesgue measure. This completes the proof. □

Proof of Proposition 1:
The implication "$\Longrightarrow$" obviously holds by considering the set $\mathcal{S} = \{1, \ldots, p\} \setminus j$.
For the other implication "$\Longleftarrow$" we use contra-position. Assume that $\mathrm{Parcor}(Y, X^{(j)}|X^{(\mathcal{S})}) = 0$ for some $\mathcal{S} \subseteq \{1, \ldots, p\} \setminus j$, and we want to show that $\beta_j = 0$. But this follows by definition of weak partial faithfulness. □

Proof of Proposition 2:
By definition and weak partial faithfulness, $\mathcal{A} \subseteq \mathcal{A}^{[m_{\text{reach}}]}$. Thus, it remains to show that $\mathcal{A}^{[m_{\text{reach}}]} \subseteq \mathcal{A}$.

Consider $j \in \mathcal{A}^{[m_{\text{reach}}]}$. The value of m_{reach} is such that $\mathrm{Parcor}(Y, X^{(j)}|X^{(\mathcal{S})}) \neq 0$ for all $\mathcal{S} \subseteq \mathcal{A}^{[m_{reach}]} \setminus j \supseteq \mathcal{A} \setminus j$. In particular,

$$\mathrm{Parcor}(Y, X^{(j)}|X^{(\mathcal{A})} \setminus j) \neq 0. \tag{16}$$

Suppose that $\beta_j = 0$. Then, by definition of the linear model and the active set $\mathcal{A}$,

$$\mathrm{Cov}(Y, X^{(j)} | X^{(\mathcal{A})} \setminus j) = 0$$

which is a contradiction to (16). Hence, it must hold that $\beta_j \neq 0$ and therefore $\mathcal{A}^{[m_{\mathrm{reach}}]} \subseteq \mathcal{A}$. □

Proof of Theorem 2:
The arguments are the same as for proving Theorem 1 in Kalisch and Bühlmann (2007). We note here that for weakly partial faithful distributions, the active set $\mathcal{A}_n = \mathcal{A}_{strong;n}$ coincides with the strong associations (see formula (10)), and the latter coincides with the skeleton of a directed acyclic graph (see Kalisch and Bühlmann (2007, formula (1))). □

Proof of Theorem 4:
Denote by $Z_n(Y, j)$ the quantity as in (7) with $\mathcal{S} = \emptyset$ and by $z_n(Y, j)$ its population analogue. i.e. the Z-transformed 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} whose probability can be bounded as

$$\sup_j \mathbb{P}[E_j^{II}] \leq O(n) \exp(-C_1 n c_n^2),$$

for some $0 < C_1 < \infty$, see Kalisch and Bühlmann (2007, formula (17)) (no sparsity assumption is used for this derivation). Thus, the probability of an error occurring in the correlation screening procedure is bounded by

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

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

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