Covariate Selection Based on an Assumption-free Approach to Linear Regression with Exact Probabilities

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Abstract

In this paper we give a completely new approach to the problem of covariate selection in linear regression. A covariate or a set of covariates is included only if it is better in the sense of least squares than the same number of Gaussian covariates consisting of i.i.d. $N(0, 1)$ random variables. The Gaussian P-value is defined as the probability that the Gaussian covariates are better. It is given in terms of the Beta distribution, it is exact and it holds for all data. The covariate selection procedures based on this require only a cut-off value $\alpha$ for the Gaussian P-value: the default value in this paper is $\alpha = 0.01$. The resulting procedures are very simple, very fast, do not overfit and require only least squares. In particular there is no regularization parameter, no data splitting, no use of simulations, no shrinkage and no post selection inference is required. The paper includes the results of simulations, applications to real data sets and theorems on the asymptotic behaviour under the standard linear model. Here the stepwise procedure performs overwhelmingly better than any other procedure we are aware of. An R-package gausscov is available.

Keywords. Linear regression, covariate selection, Gaussian covariates, exact probabilities, model free

1 Introduction

Wasserman (2011) states that for him ‘the most pressing foundational problem’ is how to reconcile ‘the need to make methods assumption free and the need to make methods work in high dimensions’. In Huber (2011) we read ‘Pay attention to computational complexity; keep it below $O(n^{3/2})$, or forget about the algorithm’. This paper can be seen as an attempt to fulfill both demands for linear regression.

We point out that Wasserman’s requirement that the methods be ‘assumption free’ has far reaching consequences. All model based concepts such as true parameter values, null hypotheses, errors of the first and second kind, the standard definition of P-values, confidence regions and false discovery rate and post selection inference must be abandoned and replaced by assumption free concepts. We do this in the context of linear regression. The resulting covariate selection procedures are very simple, very fast and in all simulations and applications to real data sets we
have considered they are overwhelming superior to all other selection procedures of which we are aware.

Most statistical problems can be interpreted as ones of distinguishing a signal, here a relevant covariate, from noise. In this paper this is accomplished in a direct manner by comparing each covariate $x_i$ with Gaussian i.i.d. noise generated by the statistician. The comparison is based on the Gaussian P-value $P_G(x_i)$ which is defined as the probability that Gaussian noise is better than the covariate as measured by the reduction in the sum of squared residuals.

More precisely consider a dependent variable $y$ of size $n$ and $q$ covariates $x_i, i = 1, \ldots, q$. Regress $y$ on a subset $S$ of size $k < n - 1$ with sum of squared residuals by $\text{rss}_k$. Now include a Gaussian covariate $Z_1$ consisting of $n$ i.i.d. $N(0,1)$ random variables and regress $y$ on $S \cup Z_1$ with sum of squared residuals $\text{RSS}$. Then it follows from Theorem 1 below

$$\frac{\text{RSS}}{\text{rss}_k} \sim \text{Beta}\left(\frac{n-k-1}{2}, 1/2\right)$$

where $\text{Beta}(a,b)$ denotes a Beta random variable with parameters $(a,b)$. The whole of this paper derives from (1) and a slightly more general result when $y$ is regressed on $S \cup \{Z_1, \ldots, Z_k\}$ Indeed in a sense (1) is the paper. The result is rather surprising for two reasons. Firstly, it is assumption free as it depends only on $\text{rss}_k$ and, secondly, the distribution can be stated exactly. In particular (1) remains valid no matter how the subset $S$ was chosen removing the necessity of post selection inference.

We can use (1) to define a P-value. Take the subset $S$ and a covariate $x_i \in S$, replace $x_i$ by a Gaussian covariate $Z_i$ and regress $y$ on $(S \setminus \{x_i\}) \cup \{Z_i\}$ to give a sum of squared residuals $\text{RSS}_i$. The Gaussian P-value of $x_i$ is defined by

$$P_G(x_i) = P(\text{RSS}_i \leq \text{rss}_k) = \text{Beta}\left(\frac{n-k}{2}, 1/2\right)\left(\frac{\text{rss}_k}{\text{rss}_k - \text{rss}_{-i}}\right)$$

where $\text{RSS}_{-i}$ is the sum of squared residuals based on $S \setminus \{x_i\}$ and $\text{Beta}(a,b)$ denotes the distribution function of the Beta distribution with parameters $(a,b)$. It has the interpretation as the probability that $Z_i$ is better than $x_i$. This P-value inherits the properties of (1): it can be calculated exactly without the need for simulations, data splitting or the determination of some regularization parameter and it is assumption free and thus remains valid no matter how the subset $S$ was selected.

A further surprise, Theorem 2, is the equality $P_G(x_i) = P_F(x_i)$ where $P_F$ is the usual P-value based on the F-distribution. In spite of this equality the two P-values are entirely different. The randomness in the case of $P_G$ is inserted by the statistician who replaces $x_i$ by a Gaussian covariate $Z_i$. The randomness in the case of $P_F$ comes from the error term $\varepsilon$ in the standard model

$$y = \sum_{x_j \in S} \beta_j x_j + \sigma \varepsilon.$$
with \( \varepsilon \) Gaussian noise. The Gaussian P-value \( P_G(x_i) \) is always valid, the F P-value \( P_F(x_i) \) is only valid under the model (3). The P-value \( P_G(x_i) \) can be calculated by simulation. Simply replace \( x_i \) by \( Z_i \), run the simulations and calculate the relative frequency with which \( Z_i \) is better than \( x_i \). The P-value \( P_F(x_i) \) cannot be simulated as this would require knowledge of the true model (3) as well as the true values of the \( \beta_j \) and \( \sigma \).

Below we introduce \( \alpha \)-free regions and \( \alpha \)-free intervals based on (1) and its multi-dimensional version. They are identical with \( (1 - \alpha) \)-confidence regions and \( (1 - \alpha) \)-confidence intervals but are universally valid whereas confidence regions and intervals are only valid under the model (3).

The P-value (2) is for each covariate \( x_i \) in the given subset \( S \): it is not used for choosing \( S \). A decision to select a covariate \( x_i \) or not will be based on its selection Gaussian P-value defined as follows. All covariates not yet chosen including \( x_i \) itself are replaced by i.i.d. Gaussian covariates \( Z \). The P-value of \( x_i \) is the probability that the best of the Gaussian covariates is better than \( x_i \). We give two selection procedures. The first considers all subsets of the covariates and is only possible if \( q \) is not too large. The second is a step-wise procedure where the candidate for selection is the best of the remaining covariates \( x_b \). The relevant covariate is selected if its Gaussian P-value is less than a cut-off value \( \alpha \) the default value of which used in this paper is \( \alpha = 0.01 \). The Gaussian P-values for the all subset procedure and for the step-wise procedure are (4) and (5) below respectively

\[
P_G(x_i) = \text{Beta}_{1,q-k+1}(\text{Beta}_{(n-k)/2,1/2}(\text{rss}_k/\text{rss}_{-i}))
\]

\[
P_G(x_b) = \text{Beta}_{1,q-k}(\text{Beta}_{(n-k-1)/2,1/2}(\text{rss}_b/\text{rss}_k)).
\]

In (4) a subset \( S \) of \( k \) covariates is under consideration and \( x_i \in S \). The sum of squared residuals based on \( S \) is \( \text{rss}_k \) and on \( S \setminus \{x_i\} \) is \( \text{rss}_{-i} \). Subsets \( S \) are selected for which all Gaussian P-values of \( x_i \in S \) are less than \( \alpha \). In (5) a set \( S \) has been selected and \( \text{rss}_k \) is as before. The best of the remaining covariates is \( x_b \) and \( \text{rss}_b \) denotes the sum of squared residuals based on \( S \cup \{x_b\} \). The covariate \( x_b \) is selected if its Gaussian P-value is less than \( \alpha \) otherwise the procedure terminates. The Gaussian P-value (5) can be much larger than the corresponding F P-values. If \( k = 1 \) and \( q = 203490 \), an example considered below, then the Gaussian P-value 0.01 of (5) corresponds to a standard F P-value of 4.94e-08

The step-wise version is very fast. If \( k \) covariates are chosen it requires about \( 5nq(k+1) \) multiplications which is a factor of \( \sqrt{nq} \) smaller than the complexity given by Huber.

Finally we point out that Gaussian white noise is the only noise for which all this holds, it is a universal irrelevant covariate.

An R package gausscov is available.
The remainder of this paper is organized as follows. In Section 2 we derive state Theorems 1 and 2 from which follow (1) and (2) and show that \( P_G = P_F \) in more generality. In Section 3 we define the two selection procedures, the all subsets and the stepwise procedures and derive the selection Gaussian P-values (4) and (5). \( \alpha \)-free regions and intervals are defined in Section 4. Section 5 considers the problem of false positives and false negatives. The problem of relevant groups rather than individual covariates is considered in Section 6. The dependency graphs and lagged covariates are discussed in Section 7.1. Extensions to \( M \)-regression and non-linear regression and are described in Section 8. Some asymptotic results on the behaviour of the stepwise procedure are given in Section 9. Simulation results and applications to real data sets are presented in Section 10. These are also done for lasso using the R packages \textit{glmnet} (Friedman et al. (2021)) and \textit{glasso} (Friedman et al. (2019)) to provide a comparison. Proofs of theoretical results and technical details are deferred to appendices.

2 Exact probabilities for the model-free approach

2.1 Gaussian covariates

Consider a subset \( S \) of covariates of size \( k \) and a subset \( S_0 \subset S \) of size \( k_0 \). Regress the dependent variable \( y \) on the \( x_i \in S_0 \) to give sum of squared residuals of \( \text{rss}_0 \). Now replace the covariates \( x_i \in S \setminus S_0 \) by \( k - k_0 \) independent Gaussian covariates \( Z_i = N_n(0, I) \), \( i = k_0 + 1, \ldots, k \) and regress \( y \) on the covariates \( x_i \in S_0, Z_{k_0+1}, \ldots, Z_k \) with resulting in a sum \( \text{RSS} \) of squared residuals. We have

**Theorem 1.**

\[
\frac{\text{RSS}}{\text{rss}_0} \sim B((n - k)/2, (k - k_0)/2). 
\]

Theorem 1 is exact and assumption free. It is the basis of the whole paper, in a sense it is the paper as as all else follows from it in what can only be described as a trivial manner. The only exceptions are the Theorems 3, 4 and 5 on the asymptotic behaviour of the stepwise procedure whose proofs are not trivial.

The assumption free approach for the combined relevance of the covariates \( x_i \in S \setminus S_0 \) is as follows. Regress \( y \) on all covariates \( x_i \in S \) with sum of squared residuals \( \text{rss} \). The Gaussian P-value is defined by

\[
P_G = P(\text{RSS} \leq \text{rss}).
\]

It the probability that the Gaussian covariates \( Z_{k_0+1}, \ldots, Z_k \) are better than the \( x_i \in S \setminus S_0 \).

Assumption A:
The standard model (3) holds with $\beta_j = 0$ for all $x_j \notin \mathcal{S}$.

Under this assumption the P-value using the standard F test to test the null hypothesis $H_0$:

$$\beta_i = 0 \text{ for all } x_i \in \mathcal{S} \setminus \mathcal{S}_0$$

is

$$P_F = 1 - F_{k-k_0, n-k} \left( \frac{\text{rss}_0 - \text{rss}}{(k-k_0)} \right)$$

where rss$_0$ denotes the sum of squared residuals for the regression based on all $x_i \in \mathcal{S}_0$.

**Theorem 2.** The P-value (6) satisfies

$$P_G = B_{(n-k)/2, (k-k_0)/2} \left( \frac{\text{rss}}{\text{rss}_0} \right)$$

Furthermore if Assumption A holds then

$$P_F = P_G$$

The proof is given in the Appendix. The case $k_0 = k - 1$ follows from (1) which is (25). The general case with $k_0 < k$ follows from (26).

3 Selecting covariates

3.1 All subsets

The $P_G$-value of (4) is derived as follows. Given a subset $\mathcal{S}$ of size $k$ and a covariate $x_i \in \mathcal{S}$ all the remaining covariates and $x_i$ itself are replaced by $q - k + 1$ i.i.d. Gaussian covariates $Z_j, j = 1, \ldots, q - k + 1$. The sum of squared residuals based on $\mathcal{S}$ is denoted by rss$_k$. The covariate $x_i$ is replaced by each of the covariates $Z_j$ in turn to gives sums of squares residuals $\text{RSS}_j, j = 1, \ldots, q - k + 1$. The best of the $\text{RSS}_j$ is better than $x_i$ if

$$\min_{j=1, \ldots, q-k+1} \text{RSS}_j \leq \text{rss}_k$$

Thus the Gaussian P-value of $x_i$ is given by

$$P_G(x_i) = P \left( \min_{j=1, \ldots, q-k+1} \text{RSS}_j \leq \text{rss}_k \right) = 1 - P \left( \min_{j=1, \ldots, q-k+1} \text{RSS}_j > \text{rss}_k \right)$$

$$= 1 - P(\text{RSS}_j > \text{rss}_k)^{q-k+1} = 1 - \left( 1 - B_{(n-k)/2, (k-k_0)/2} \left( \frac{\text{rss}_k}{\text{rss} - \text{rss}_k} \right) \right)^{q-k+1}$$

(by Theorem 2)

$$= B_{1, q-k+1} \left( B_{(n-k)/2, (k-k_0)/2} \left( \frac{\text{rss}_k}{\text{rss} - \text{rss}_k} \right) \right)$$

which is (4).

All subsets are retained for which each covariate in the subset has a Gaussian P-value (7) at most $\alpha$. In a second step all subsets which are subsets of some other retained subset are discarded. The remaining subsets are maximal in the sense that it is not possible to include another covariate whilst still maintaining the upper bound $\alpha$ for all covariates in the subset. Finally if desired the retained subsets may be ordered by the sums of the squared residuals.
3.2 The Gaussian stepwise procedure

Suppose a subset \( S \) of \( k \) covariates has already been selected with sum of squared residuals \( \text{rss}_k \). There remain \( q - k \) covariates. The candidate for selection is that covariate \( x_b \) with the smallest sum of squared residuals \( \text{rss}_b \) when \( y \) is regressed on \( S \cup \{ x_b \} \). Its Gaussian P-value is given by

\[
P_G(x_b) = \text{Beta}_{1,q-k}(\text{Beta}_{(n-k-1)/2,1/2}(\text{rss}_b/\text{rss}_k))
\]

by the same argument which lead to (7). If this is less than the cut-off value \( \alpha \) then \( x_b \) is selected and the procedure continues. Otherwise the procedure terminates.

Instead of considering just one covariate for selection the first \( km \) can be selected for a specified number \( km \). If \( km \) is not too large for example \( km = 20 \) then all subsets of these \( km \) covariates can be considered as in Section 3.1. If there is no subset all of whose Gaussian P-values are less than the cut-off value \( \alpha \) the procedure terminates without specifying a subset. Otherwise that subset with the largest reduction in the sum of squared residuals is returned.

No stepwise procedure is guaranteed to work but Theorems 3, 4 and 5 in Section 9 give sufficient condition when considering data generated under the standard linear model with a known correct set of covariates. For large \( n \) the probability of not selecting the correct subset is bounded above by \( \alpha \). This supports the interpretation of \( \alpha \) as the probability of selecting a false positive.

3.3 The repeated Gaussian stepwise procedure

A selected subset \( S \) of covariates represents a linear approximation to the dependent variable \( y \). There will in general be more than one such approximation. Further ones may be obtained by removing the set \( S \) of covariates and repeating the one-step method of the previous section using the remaining covariates. This is continued until there are no covariates left with a Gaussian P-value less than \( \alpha \). An example is the leukemia data of Section 10.2.1 where the method results in 115 linear approximations involving 281 covariates.

3.4 Constructing models

The Gaussian covariate selection procedures produce linear approximations and not models. However given such an approximation it is possible to construct a model making use only of the selected covariates. We do this for the leukemia and sunspot data in Sections 10.2.1 and 10.2.4 respectively.
\section{\(\alpha\)-free regions and intervals}

The Gaussian P-value \(P_G\) of Theorem 2 is valid for any \(k\) and \(k_0\) irrespective of how the \(k\) covariates were selected. We now show how confidence regions and intervals may be re-interpreted so that they are also valid after selection.

Suppose the standard linear model (3) holds for a subset \(S\) of size \(k\) of covariates with true vector of coefficients \(\beta(\text{true})\). Then a \(1 - \alpha\) confidence region \(C(1 - \alpha)\) for \(\beta(\text{true})\) is given by

\[
C(1 - \alpha) = \left\{ \beta : \|x(\beta - \beta(\text{ls}))\|^2 \leq \|y - x\beta(\text{ls})\|^2 \frac{kF^{-1}(1 - \alpha, k, n - k)}{n - k} \right\}. \tag{8}
\]

This can be rewritten as

\[
C(1 - \alpha) = \left\{ \beta : \|y - x\beta\|^2 \leq \|y - x\beta(\text{ls})\|^2 / \text{Beta}^{-1}(\alpha, (n - k)/2, k/2) \right\}. \tag{9}
\]

In other words \(C(1 - \alpha)\) denotes those \(\beta\) for which the sum of the squared residuals is no larger by a specified quantity than the minimum sum of squared residuals based on \(\beta(\text{ls})\). We use this interpretation in the assumption free case.

\subsection{\(\alpha\)-free regions}

Suppose \(k\) covariates have been chosen. Then for a given \(\beta\) the sum of squared residuals \(\|y - x\beta\|^2\) may be reduced by regressing \(y - x\beta\) on \(k\) i.i.d. Gaussian covariates. If \(\text{RSS}\) is the sum of the squared residuals then it follows from Theorem 1 that

\[
\frac{\text{RSS}}{\|y - x\beta\|^2} \sim \text{Beta}((n - k)/2, k/2).
\]

This implies

\[
P(\text{RSS} \leq \text{Beta}^{-1}(\alpha, (n - k)/2, k/2) \|y - x\beta\|^2) = \alpha
\]

for any given \(\alpha\). This reduction in the sum of squared residuals is free, it comes at no cost and requires no knowledge of the data. For this reason we call a sum of squared residuals of at most \(\text{Beta}^{-1}(\alpha, (n - k)/2, k/2) \|y - x\beta\|^2\) \(\alpha\)-free. The region \(C(1 - \alpha)\) of (9) now has the following assumption free interpretation: it is the set of coefficients \(\beta\) whose \(\alpha\)-free residuals have with probability at least \(\alpha\) a smaller sum of squares than the least squares residuals.

This can be done for confidence intervals as follows. Take the \(k\)th covariate \(x_k\) with least squares coefficient \(\beta_k(\text{ls})\). Regress \(y - (\beta_k(\text{ls}) + \lambda)x_k\) on the remaining \(k - 1\) covariates. Then the sum of the squared residuals is

\[
\|y - x\beta(\text{ls})\|^2 + \lambda^2\|x_k - \text{Proj}_{k-1}(x_k)\|^2 = \|y - x\beta(\text{ls})\|^2 + \lambda^2\sigma_k^2.
\]
where \( \text{Proj}_{k-1} \) denotes the projection onto the subspace spanned by the remaining \( k-1 \) covariates and \( \sigma_k^2 = (x'x)_{kk}^{-1} \). Now regress \( y - (\beta_k(\text{ls}) + \lambda)x_k \) on the remaining \( k-1 \) covariates and a Gaussian covariate \( Z_k \) to give a sum of squared residuals \( RSS_k \). From (1) we have for a given \( \alpha \)

\[
P(\text{RSS}_k \leq \text{Beta}^{-1}(\alpha, (n - k)/2, 1/2) (\|y - x\beta(\text{ls})\|^2 + \lambda^2 \sigma_k^2)) = \alpha \tag{10}
\]

so that \( P(\text{RSS}_k \leq \|y - x\beta(\text{ls})\|^2) \geq \alpha \) if

\[
\lambda^2 \leq \frac{\|y - x\beta(\text{ls})\|^2}{\sigma_k^2} \left( \frac{1}{\text{Beta}^{-1}(\alpha, (n - k)/2, 1/2)} - 1 \right)
\]

which corresponds to the standard \( 1 - \alpha \) confidence interval based on the t-distribution.

5 False positives and false negatives

5.1 False positives

We regard a Gaussian covariate to be a universal irrelevant covariate and its acceptance to be a universal false positive. It is a false positive in precise form so to speak and it is this precision which enables the exact calculation of P-values and the derivation of the selection procedures. Such procedures would be worthless if their use was limited to such Gaussian covariates. As an example take a Gaussian covariate \( Z \) but make \( y \) dependent on \( Z \) by including the term \( 10^{-100}Z \) in the regression. Is now the selection of \( Z \) a false positive? How large must the coefficient be before it is not a false positive? Such problems can be investigated by simulation, mathematical probes (Theorems 3, 4 and 5) and real data sets. In Tukey’s language these are multiple challenges; ‘C is for Challenges’ in Tukey (1993). Such challenges are considered in Section 10.

5.2 False negatives

A false negative is a covariate which is relevant but is not selected. This can happen in multiple ways, a non-linearity in the relationship between the dependent variable and one or more covariates, the stepwise procedure failing because the first Gaussian P-value exceeds the cut-off value, an inability to consider all subsets when \( q \) is large. This latter problem can be mitigated to some extent as described in Sections 3.2 and 3.3. A claim about false negatives is more difficult to make than one about false positives as it involves a statement about a relevant covariate existing although its existence cannot be established.
6 Relevant groups

It can happen that a group of covariates is relevant although the effect of the individual covariates is not sufficiently strong for this to be detected. The group lasso was proposed in Yuan and Lin (2006) to try and identify such groups (see also Section 4 of Dezeure et al. (2015)). We consider here the case that the Gaussian P-values exceed the cut-off value $\alpha$ but the P-value of the $R^2$ statistic is small in a sense to be made clear indicating that the covariates taken as a whole do have a relevant effect. So far we have only come across this problem in the simulations in Sections 10.1.1 and 10.1.2. The reason seems to be that in these simulations all the covariates are Gaussian and all the $\beta_i$ are the same.

As an example we take the simulations discussed in Section 10.1.1. The parameters are $(n, q) = (1000, 1000)$ and 60 of the covariates have a non-zero coefficient value, namely $\beta = 4.5/\sqrt{1000}$. We use the stepwise Gaussian method to choose 60 covariates. In one such simulation default version of the Gaussian method 54 of these had non-zero coefficients but the P-values of only nine covariates were below the cut-off values of which eight had a non-zero coefficient. The sum of the squared residuals was 888.65 based on all 60. We now regress the dependent variable $Y_{1000}$ on 1000 covariates generated in the same manner but with all coefficients zero. Of these the first 60 were chosen using the Gaussian stepwise procedure with $km = 60$ as in Section 3.2 and the dependent variable regressed on these 60. Over 500 such simulations the smallest sum of squared residuals was 1099 giving a P-value so to speak of 0. Repeating this with $\beta = 1/\sqrt{1000}$ gave a P-value of 0.2 indicating that this value of $\beta$ is about the limit of detectability.

We propose the following. The default stepwise method compares the best of the remaining covariates with the best of the same number of i.i.d. $N_n(0, I)$ which is the first order statistic. We weaken this by comparing the best of the remaining covariates with the $\nu$th best of the random Gaussian covariates. If a subset of size $k$ has already been selected the Gaussian P-value of the next best covariate $x_b$ is defined as

$$P_G(x_b) = B_{\nu, q-k+1-\nu}(B_{n-k-1}/2, 1/2 (r_{SS_b}/r_{SS_k}))$$

where we use the same notation as for (4). Again, this probability is exact. One could instead just specify another cut-off probability instead of the default value $\alpha = 0.01$ but is not easily interpretable which is why we prefer specifying $\nu$.

The larger $\nu$ the more likely it is that false positives will be selected. To estimate the number of false positives we regress $y \in \mathbb{R}^n$, any $y$ as it is model-free, on $q$ i.i.d. $N_n(0, I)$ Gaussian covariates for a given $\nu$. Any selected covariate is a false positive. Simulations can be performed
using fsimords which is part of the gausscov R-package. As an example we put \((n, q, \alpha, \nu) = (1000, 1000, 0.01, c(1, 5, 10))\) which is used in Section \ref{sec:10.1.1}. The result of 10000 simulations is given in Table \ref{table:1}. The means for \(\nu = 5\) and \(\nu = 10\) are 1.89 and 4.73 and the standard deviations 1.61 and 3.06 respectively. Thus increasing \(\nu\) from 1 to 5 will on average lead to about two false positives. If the increase in the number of covariates selected is much greater than this it may be deemed reasonable to use \(\nu = 5\). Examples of this are given in the simulations in Sections \ref{sec:10.1.1} and \ref{sec:10.1.2}.

### 7 Graphs and lagged covariates

One major advantage of the assumption free nature of the covariate selection procedures is that they can be applied without change to situations which are modelled in very different ways. We give two examples, the construction of graphs and the use of lagged covariates.

#### 7.1 Graphs

Given the model

\[
X = (X_1, \ldots, X_k) \sim \mathcal{N}(\mu, \Sigma)
\]

with \(k < n\) the graphical independence structure of the distribution can be obtained from the location of zeros in the inverse matrix \(\Sigma^{-1}\) (Whittaker \cite{1990}). The structure can also be obtained by regressing each \(X_i\) on the remaining \(X_j\). This approach can be extended to the case \(k > n\) using covariate selection methods as is shown in Meinshausen and Buhlmann \cite{2006} where lasso was used as a covariate selection method. There is a version of lasso, glasso, for the estimation of Gaussian graphical models \cite{2019}.

A graph can be constructed as follows. Each covariate \(x_i\) is regressed on the remaining covariates using the stepwise Gaussian covariate method. The covariate \(x_i\) is then joined to the selected covariates \(x_\ell, \ell \in S_i\) to give the edges \((i, \ell)\). In the default version the cut-off values \(\alpha\) is set to \(\alpha/q\) where \(q\) is the number of covariates. As the Gaussian procedure is assumption free care

\begin{tabular}{cccccccccccc}
\(\nu\) & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & \(\geq 11\) \\
1 & 0.99 & 0.01 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.00 \\
5 & 0.21 & 0.26 & 0.22 & 0.15 & 0.08 & 0.05 & 0.02 & 0.01 & 0.00 & 0.00 & 0.00 & 0.00 \\
10 & 0.05 & 0.10 & 0.12 & 0.13 & 0.12 & 0.12 & 0.10 & 0.10 & 0.08 & 0.06 & 0.05 & 0.06 \\
\end{tabular}

Table 1: Histogram of false positives \((n, q, \alpha) = (1000, 1000, 0.01)\) with \(\nu = 1, 5\) and 10 based on 10000 simulations using fsimords.
needs to be taken when interpreting the graph. The repeated stepwise procedure of Section 3.3 can also be used. Typically it gives much larger graphs. Examples are given in Section 10.

7.2 Lagged covariates

Most data sets are such that the covariates are not highly correlated. An exception are lagged covariates which can be highly correlated. Modelling and analysing a data set using models based on lagged data is not simple involving as it does the determination of the coefficients and the order of the lags involved. Furthermore it seems only to be possible to do such an analysis if the order is small. The Gaussian stepwise selection procedure avoids these problems and can include other lagged covariates. We give two examples in Section 10.2.7 the sunspot data and some American Business Cycle data.

8 Beyond least squares

We briefly consider extension to robust ($M$-)regression and non-linear regression.

8.1 $M$-regression

Let $\rho$ by a symmetric, positive and twice differentiable convex function with $\rho(0) = 0$. The default function will be the Huber’s $\rho$-function with a tuning constant $c$ (Huber and Ronchetti (2009), page 69) defined by

$$
\rho_c(u) = \begin{cases} 
\frac{u^2}{2}, & |u| \leq c, \\
\frac{c^2}{2} - \frac{c^2}{2}, & |u| > c.
\end{cases} 
$$

(13)

The default value of $c$ will be $c = 1$.

For a given subset $S$ of covariates of size $k$ the sum of squared residuals is replaced by

$$
s_0(\rho, \sigma) = \min_{\beta(S)} \frac{1}{n} \sum_{i=1}^{n} \rho \left( \frac{y_i - \sum_{j \in S} x_{ij} \beta_j(S)}{\sigma} \right). 
$$

(14)

which can be calculated using the algorithm described in 7.8.2 of Huber and Ronchetti (2009). The minimizing $\beta_j(S)$ will be denoted by $\beta_j(S, lr)$.

For some $x_\nu \not\in S$ put

$$
s_\nu(\rho, \sigma) = \min_{\beta(S \cup \{x_\nu\})} \frac{1}{n} \sum_{j=1}^{n} \rho \left( \frac{y_j - \sum_{j \in S \cup \{x_\nu\}} x_{ij} \beta_j(S \cup \{x_\nu\})}{\sigma} \right). 
$$

(15)
Replace all the covariates not in \( S \) by standard Gaussian white noise, include the \( \ell \)th such random covariate denoted by \( Z_\ell \) and put
\[
S_\ell(\rho, \sigma) = \min_{\beta(S), b} \frac{1}{n} \sum_{i=1}^{n} \rho \left( \frac{y_i - \sum_{j \in S} x_{ij} \beta_j(S) - b Z_\ell}{\sigma} \right).
\] (16)

A Taylor expansion gives
\[
S_\ell(\rho, \sigma) \approx \frac{1}{2} \sum_{i=1}^{n} \rho^{(1)} \left( \frac{r_i}{\sigma} \right) Z_i^2
\approx s_0(\rho, \sigma) - \frac{1}{2} \sum_{i=1}^{n} \rho^{(2)} \left( \frac{r_i}{\sigma} \right)^2 \chi^2
\] (17)
with \( r_i = y_i - \sum_{j \in S} x_{ij} \beta_j(S, l) \). This leads to the asymptotic \( P \)-value for \( x_\nu \)
\[
1 - \text{Chisq} \left( \frac{2s_0(\rho^{(2)}, \sigma)}{s_0(\rho^{(1)}, \sigma)} (s_0(\rho, \sigma) - s_\nu(\rho, \sigma)) \right)^{q-k}.
\] (18)

corresponding to the exact Gaussian \( P \)-value (5) for the stepwise procedure. The \( P \)-value corresponding to the exact Gaussian \( P \)-value (4) for the all subsets procedure is obtained by replacing \( k \) by \( k - 1 \). Here
\[
s_0(\rho^{(1)}, \sigma) = \frac{1}{n} \sum_{i=1}^{n} \rho^{(1)} \left( \frac{r_i}{\sigma} \right)^2, \quad s_0(\rho^{(2)}, \sigma) = \frac{1}{n} \sum_{i=1}^{n} \rho^{(2)} \left( \frac{r_i}{\sigma} \right)^2.
\]

It remains to specify the choice of scale \( \sigma \). The initial value of \( \sigma \) is the median absolute deviation of \( y \) multiplied by the Fisher consistency factor \( 1.4826 \). After the next covariate has been included the new scale \( \sigma_1 \) is taken to be
\[
\sigma_1^2 = \frac{1}{(n - k - 1)} c_f \sum_{i=1}^{n} \rho^{(1)} (r_1(i)/\sigma_0)^2
\] (19)
where the \( r_1(i) \) are the residuals based on the \( k + 1 \) covariates and \( c_f \) is the Fisher consistency factor given by
\[
c_f = E(\rho^{(1)}(Z)^2)
\]
where \( Z \) is \( N(0, 1) \) (see Huber and Ronchetti (2009)). Other choices are possible.

8.2 Non-linear approximation

For a given subset \( S \) of covariates of size \( k \) the dependent variable \( y \) is now approximated by \( g(\mathbf{x}(S)\beta(S)) \) where \( g \) is a smooth function. Write
\[
ss_0 = \min_{\beta(S)} \frac{1}{n} \sum_{i=1}^{n} (y_i - g(\mathbf{x}(S)^\top \beta(S)))^2.
\] (20)
and denote the minimizing \( \beta(S) \) by \( \beta(S, ls) \). Now include one additional covariate \( x_\nu \) with \( x_\nu \notin S \) and denote the mean sum of squared residuals by \( ss_\nu \). As before all covariates not in \( S \) are replaced by standard Gaussian white noise. Include the \( \ell \)th random covariate denoted by \( Z_\ell \) and put

\[
SS_\ell = \min_{\beta(S), b} \frac{1}{n} \sum_{i=1}^{n} (y_i - g(x_i(S)^\top \beta(S) + bZ_\ell))^2.
\]

Arguing as above for robust regression results in

\[
SS_1 \approx ss_0 - \frac{\sum_{i=1}^{n} r_i(S)^2 g^{(1)}(x_i(S)^\top \beta(S, ls))^2}{\sum_{i=1}^{n} g^{(1)}(x_i(S)^\top \beta(S, ls))^2} - \chi^2_1
\]

where

\[
r_i(S) = y_i - g(x_i(S)^\top \beta(S, ls)).
\]

The asymptotic \( P \)-value for the covariate \( x_\nu \) corresponding to the asymptotic \( P \)-value (18) for \( M \)-regression is

\[
1 - \text{Chisq} \left( \frac{(ss_0 - ss_\nu) \sum_{i=1}^{n} g^{(1)}(x_i(S)^\top \beta(S, ls))^2}{\sum_{i=1}^{n} r_i(S)^2 g^{(1)}(x_i(S)^\top \beta(S, ls))^2}, 1 \right)^{q-k}.
\]

In the case of logistic regression with \( g(u) = \exp(u)/(1 + \exp(u)) \) we have

\[
\frac{\sum_{i=1}^{n} r_i(S)^2 g^{(1)}(x_i(S)^\top \beta(S, ls))^2}{\sum_{i=1}^{n} g^{(1)}(x_i(S)^\top \beta(S, ls))^2} = \frac{\sum_{i=1}^{n} (y_i - p_i(0))^2 p_i(0)^2 (1 - p_i(0))^2}{\sum_{i=1}^{n} p_i(0)^2 (1 - p_i(0))^2}
\]

where

\[
p_i(0) = \frac{\exp(x_i(S)^\top \beta(S, ls))}{1 + \exp(x_i(S)^\top \beta(S, ls))}.
\]

This corrects a mistake in Chapter 11.6.1.2 of [Davies 2014] where

\[
\frac{\sum_{i=1}^{n} p_i^2 (1 - p_i)^3}{\sum_{i=1}^{n} p_i^2 (1 - p_i)^2}
\]

occurs repeatedly instead of

\[
\frac{\sum_{i=1}^{n} (y_i - p_i)^2 p_i^2 (1 - p_i)^2}{\sum_{i=1}^{n} p_i^2 (1 - p_i)^2}.
\]

9 Bounds and asymptotics

We provide some theoretical results about the stepwise choice of covariates in the model-based framework, in Tukey’s sense a ‘challenge’. Throughout this section we assume that

\[
y = \mu + \sigma Z
\]
with unknown parameters \( \mu \in \mathbb{R}^n, \sigma > 0 \) and random noise \( Z \sim N_n (0, I) \). Moreover, we assume without loss of generality that \( \| x_i \| = 1, i = 1, \ldots, q \). The set of chosen covariates is denoted by \( \hat{S} \).

We consider firstly the case of no signal, \( \mu = 0 \). In this situation the correct decision is \( \hat{S} = \emptyset \).

**Theorem 3.** If \( \mu = 0 \) then

\[
    P(\hat{S} \neq \emptyset) \leq -\log(1 - \alpha).
\]

Furthermore if \( q \to \infty \) and \( n/\log(q)^2 \to \infty \) then for fixed \( \alpha \in (0, 1) \),

\[
    P(\hat{S} \neq \emptyset) \leq \alpha + o(1)
\]

as uniformly in \((x_i), i = 1, \ldots, q\). In the special case of orthonormal regressors \( x_i \),

\[
    P(\hat{S} \neq \emptyset) \to \alpha
\]

\( q \to \infty \).

If \( \mu \neq 0 \) we suppose that \( \mu = \sum_{x_i \in S_s} \beta_i x_i \) where \( S_s \) is a subset of size \( k_s < n \) and the \( x_i \in S_s \) are linearly independent. For any subset \( S \) we denote the linear subspace of \( \mathbb{R}^n \) spanned by the \( x_i \in S \) by \( V_S \) and the orthogonal complement of this subspace by \( V_S^\perp \). The orthogonal projection onto \( V_S^\perp \) is denoted by \( Q_S \) and for any \( x_i \notin S \) we write

\[
    x_{S, i} := \| Q_S x_i \|^{-1} Q_S x_i
\]

(with \( 0^{-1} 0 := 0 \)).

With the above notation we have

**Theorem 4** (Consistency of stepwise choice, general design). Suppose that

\[
    \mu \in V_{S_s}
\]

and that the two following assumptions hold:

(A.1) \( \min(n, q)/k_s \to \infty \) and \( \log(q)^2/n \to 0 \), and

(A.2) for some fixed \( \tau > 2 \),

\[
    \min_{x_j \in S_s, S \subseteq S_s \setminus \{x_j\}, x_i \notin S_s} \frac{|x_{S, j}^\top \mu| - |x_{S, i}^\top \mu|}{\sqrt{n} \sigma^2 + \| \mu \|^2} \geq \frac{\sqrt{\tau} \log q + 2 \sqrt{k_s}}{\sqrt{n}}.
\]

Then the stepwise procedure yields a random set \( \hat{S} \) such that

\[
    P(S_s \subset \hat{S}) \to 1 \quad \text{and} \quad P(S_s \subset \hat{S}) \leq \alpha + o(1),
\]

\( q \to \infty \).
If the $x_i \in S_*$ are orthonormal the result can be simplified.

**Theorem 5** (Consistency of stepwise choice, orthogonal design). Suppose

$$\mu = \sum_{i \in S_*} \beta_i x_i$$

where the $x_i$ are orthonormal and that the two following conditions hold

(A.1') $q/k_* \to \infty$, and

(A.2') for some fixed $\tau > 2$,

$$\min_{i \in S_*} \frac{|\beta_i|}{\sqrt{n\sigma^2 + \sum_{i \in S_*} \beta_i^2}} \geq \frac{\sqrt{\tau \log q + 2 \log k_*}}{\sqrt{n}}.$$  

Then stepwise procedure yields a random set $\hat{S}$ such that

$$P(S_* \subset \hat{S}) \to 1 \quad \text{and} \quad P(S_* \not\subset \hat{S}) \leq \alpha + o(1).$$

It is of interest to compare Theorem 5 with Theorem 1 of Lockhart et al. (2014) for lasso regression. There they prove (in our notation) that the first $m_*$ covariates entering the lasso path are, with probability tending to 1, those in $S_*$. Our condition (A.2’) is replaced by the weaker

$$\min_{x_i \in S_*} |\beta_i| - \sigma \sqrt{2 \log(q)} \to \infty.$$  

However their result is restricted to $q < n$, they use the given $\sigma$, not an estimate, and there is no termination rule. See their Remark 1 on page 420 and their Section 6.

**10 Simulations and real data**

All the following were done using R version 4.0.2 (2020-06-22) and the package `gausscov` with the default value 0.01 for $\alpha$. There is one exception: in Section 10.1.1 we use several values of $nu$ chosen as described in Section 5.2. For lasso we use the default version of `cv.glmnet` (Friedman et al. (2021)) which chooses the regularization parameter $\lambda$ using 10-fold cross-validation. In Section 10.1.2 we use `glasso` (Friedman et al. (2019)) and choose the regularization parameter $\rho$ so that the number of false positives and false negatives are about equal.

In the following the intercept is denoted by 0.

**10.1 Simulations**

**10.1.1 Tutorial 1**

The knockoff procedure is explained in Candes et al. (2018). The tutorial in question is Tutorial 1 of
which gives a simulation using knockoff. The dimensions are \((n, q) = (1000, 1000)\). The 1000
covariates are Gaussian and dependent with a Toeplitz covariance matrix \(\Sigma\) given by \(\Sigma_{i,j} = \rho^{|i-j|}\)
with \(\rho = 0.25\). Of the covariates \(\rho = 60\) are chosen at random and denoted by \(X_i, i = 1, \ldots, 60\).
The dependent variable \(Y\) is given by
\[
Y = \sum_{i=1}^{60} \beta_i X_i + N_{1000}(0, I)
\]
with all the \(\beta_i = \text{amplitude}/\sqrt{n}\) with \(\text{amplitude} = 4.5\). These are the particular values chosen
for the first simulation discussed below. There is a second tutorial with a binary dependent vari-
able. The results are similar and not given here but are available in Davies (2018) with however
\(\alpha = 0.05\).

| method  | fp   | fn | time |
|---------|------|----|------|
| lasso   | 68.7 | 1.5| 12.6 |
| knockoff| 6.8 | 10.4| 74.1|
| \(\nu = 1\) | 0.0 | 53.1| 0.05|
| \(\nu = 5\) | 2.5 | 14.5| 0.19|
| \(\nu = 10\) | 5.6 | 7.5 | 0.23|

Table 2: Comparison of lasso, knockoff and Gaussian covariates based on 10 simulations with
\((n, q, p, \text{amplitude}, \rho) = (1000, 1000, 60, 4.5, 0.25)\).

The number of false positives is denoted by ‘fp’ and false negatives by ‘fn’. The total number
of covariates selected is given by 60-fn+fp. The time for each simulation is given in seconds. The
first line for lasso shows that on average it selects about 130 covariates each selection requiring
about 12 seconds. Almost all the relevant covariates are chosen but also on average about 70 false
ones. Knockoff selects on average about 60 covariates of which about 7 are false positives. It
requires about 74 seconds for each selection. The Gaussian covariate method with default value
\(\alpha = 0.01\) selects on average just 7 covariates. None of these are false positives. Putting \(\nu = 5\)
results in \(60 - 14.5 + 2.5 \approx 48\) covariates being selected. To judge how many of these are false
positives we run \(fsimords\) as described in Section 5.2. The result is given in Table 1 suggesting
that only about two of these are false positives and consequently about four are false negatives.
These numbers agree with the Table 2. Running \(fsimords\) with \(\nu = 10\) suggests at most five are
false positives and consequently about four are false negatives which agrees with the values in
Table 2. Thus in terms of minimizing the number of false decisions \(\nu = 10\) would seem to be the
best choice. We emphasize here that the choice \(\nu = 10\) results from running \(fsimords\) and not by
choosing the best value on running Tutorial 1.
Table 3: Comparison of lasso, knockoff and Gaussian covariates based on 25 simulations with \((n, q, p, \text{amplitude}, \rho) = (1000, 1000, 5, 45, 0.25)\).

| method    | fp  | fn  | time |
|-----------|-----|-----|------|
| lasso     | 0.5 | 0.00| 2.27 |
| knockoff  | 0.00| 5.00| 74.7 |
| \(\nu = 1\) | 0.0 | 0.00| 0.04 |
| \(\nu = 5\) | 0.7 | 0.00| 0.06 |
| \(\nu = 10\) | 3.7 | 0.00| 0.05 |

Knockoff and the choice \(\nu = 10\) give about the same results in terms of the sum \(fp + fn\). The big difference is the running times. Whereas knockoff requires over two minutes for each simulation the Gaussian covariate method requires less than 0.5 seconds.

Table 3 is interesting. As before we put \((n, q) = (1000, 1000)\) but only five of the covariates are chosen a with very large \(\beta_i = 45/\sqrt{1000}\). Lasso and the three versions of the Gaussian covariate method have no false negatives. Knockoff has five false negatives no false positives every time meaning that it selected nothing.

10.1.2 Random graphs

This is based on [Meinshausen and Bühlmann (2006)] with \((n, q) = (n, p) = (1000, 600)\) where \(n = 1000\) is the dimension of each covariate and \(p = 600\) the number of covariates. On the last line of page 13 the expression \(\varphi(d/\sqrt{p})\) with \(\varphi\) the density of the standard normal distribution and \(d\) the Euclidean distance is clearly false. It has been replaced by \(\varphi(23.5d)\) which gives about 1800 nodes compared with the 1747 of [Meinshausen and Bühlmann (2006)]. The Meinshausen-Bühlmann method with \(\alpha = 0.05\) and non-directed edges resulted in 1109 edges of which two were false positives giving 640 false negatives.

One simulation of the modified (as described above) Meinshausen-Bühlmann random graph method produced 1823 edges. The Gaussian method described in Section 7.1 yielded 1590 edges of which two were false positive and 235 were false negatives. The time required was about 9 seconds.

Putting \(\nu = 2\) resulted 1821 edges, that is 231 more edges than with \(\nu = 1\). To judge this 10,000 simulations with \(\nu = 2\) were performed as in Section 5.2 with \((n, q, \alpha) = (1000, 600, 0.01/600)\). The mean number of false positives per covariate was 0.01 suggesting a Poisson distribution with mean 6 for the number of false positives. Thus of the 231 additional edges one can expect that between one and 12 are false positives. The actual number was nine with 11 false negatives.
approx. | covariate | coef. | Gauss P-value | st. P-value
---|---|---|---|---
1 | 1182 | 0.20 | 1.49e-15 | 4.17e-19
1 | 1219 | -0.18 | 4.12e-04 | 1.16e-07
1 | 2888 | 0.28 | 3.58e-03 | 1.01e-06
1 | 0 | 1.00 | 7.65e-21 | 7.65e-21
2 | 979 | 0.14 | 9.37e-05 | 2.62e-08
2 | 1652 | 0.21 | 7.24e-05 | 2.03e-08
2 | 0 | 0.39 | 1.73e-19 | 1.73e-19

Table 4: The first two linear approximations for the leukemia data.

One application of glasso with $\rho = 0.236$ to the same graph resulted in 1823 edges of which 316 were false positives and 313 false negatives. The value of $\rho$ was chosen to make these two numbers roughly equal. The time required was about 14 seconds.

10.2 Real data

10.2.1 Leukemia data

The dimensions of the leukemia data (Golub et al. (1999)) are $(n, q + 1) = (72, 3572)$. The data are available from

http://stat.ethz.ch/~dettling/bagboost.html

For more information about the data see [Dettling and Bühlmann (2002)].

The repeated Gaussian covariate procedure gave 115 linear approximations and involving 281 covariates. The time required was 0.65 seconds. The first two linear approximations are given in Table 4. The first column gives the number of the linear approximation, the second the covariates included in this approximation, the third the linear regression coefficients, the fourth the Gaussian P-values as defined by (2) and the fifth the standard P-values.

If we now apply the strategy of Section 3.2 setting the number of covariates to ten, $km = 10$, and choosing the best subset the repeated stepwise procedure results in 137 linear approximations involving 387 covariates. The time required was 2.8 seconds. The first two linear approximations is given in Table 5.

Five applications of lasso resulted in between 11 and 24 covariates. The time required for each was about 0.4 seconds.

10.2.2 Constructing models: the leukemia data

Data such as the leukemia data are usually analysed using the logit model. This can be done by taking the covariates selected for the linear approximations using the Gaussian stepwise proce-
| approx. | covariate | coef. | Gauss P-value | st. P-value |
|---------|-----------|-------|---------------|-------------|
| 1       | 183       | -0.24 | 1.46e-04      | 4.11e-08    |
| 1       | 1182      | 0.12  | 2.72e-07      | 7.63e-11    |
| 1       | 1219      | -0.17 | 3.23e-07      | 9.05e-11    |
| 1       | 2558      | -0.14 | 7.98e-03      | 2.25e-06    |
| 1       | 2888      | 0.24  | 4.90e-05      | 1.37e-08    |
| 1       | 3038      | 0.12  | 4.47e-03      | 1.26e-06    |
| 1       | 0         | 1.20  | 9.89e-21      | 9.89e-21    |
| 2       | 657       | -0.31 | 5.21e-07      | 1.46e-10    |
| 2       | 979       | 0.18  | 2.63e-15      | 7.39e-19    |
| 2       | 2260      | -0.20 | 4.43e-04      | 1.24e-07    |
| 2       | 0         | 0.58  | 2.90e-22      | 2.90e-22    |

Table 5: The first two linear approximations for the leukemia data with $km = 10$ and choosing the best subset.

dure and running a logistic regression using these covariates. If this is done for the 137 linear approximations mentioned above 32 of them give a perfect fit.

10.2.3 Interactions

We now consider the Boston Housing data with the covariates consisting of all 203490 interactions of order at most 8. The result of the Gaussian stepwise procedure with $km = 20$ and the subset option as described in Section 3.2 are given in Table 6. The time required was about 90 seconds. The sum of squared residuals is 4711. Each covariate can be decomposed into its constituent parts using decomp of the R package gausscov. The covariate 7782 is boston[, 6] boston[, 12].

Five applications of lasso resulted in 56, 4, 13, 8 and 47 covariates chosen. On average each application took about 150 seconds. The sum of squared residuals for the first selection of 56 covariates was 4706 which is only slightly less than the 4711 based on the 12 covariates of Table 6.

10.2.4 Non-parametric regression

The Gaussian stepwise can be applied to non-parametric regression with covariates of the form $x_\ell = (f_\ell(u_i))_{i=1}^n$ with given basis functions $f_\ell, \ell = 1, \ldots, q$. What the method cannot do in this context is to take shape or other restrictions into account as for example in Davies and Kovac (2001); Kovac (2007); Dümbgen and Kovac (2009). It is however well adapted to finding periodicities in the dependent variable by taking the basis functions to be of the form $f_\ell = \sin(\pi\ell(1 : n)/n), \cos(\pi\ell(1 : n)/n), \ell = 1, \ldots, m$.

We consider the monthly average number of sunspots from 1749 to 2020 giving in all $n =$
### Table 6: Boston housing data: interactions of order \( \leq 8 \) in order of selection by the Gaussian stepwise procedure with \( km = 20 \) and the best subset option of Section 3.2.

| number | coef.  | Gauss P-value | st. P-value |
|--------|--------|---------------|-------------|
| 7782   | 2.50e-05 | 6.91e-140     | 3.39e-145   |
| 191925 | -9.23e-05 | 7.92e-05     | 3.89e-10    |
| 121517 | -1.34e-03 | 2.15e-05     | 1.06e-10    |
| 91842  | -2.10e-03 | 6.24e-04     | 3.07e-09    |
| 31989  | 3.16e-07  | 6.82e-06     | 3.35e-11    |
| 197587 | -1.00e-11 | 8.11e-20     | 3.98e-25    |
| 93     | 1.26e-03  | 3.62e-18     | 1.78e-23    |
| 25719  | -1.95e-10 | 2.33e-26     | 1.14e-31    |
| 197378 | 2.19e-09  | 7.55e-07     | 3.71e-12    |
| 6422   | 3.66e-11  | 4.71e-15     | 2.32e-20    |
| 6487   | -4.25e-07 | 1.47e-03     | 7.22e-09    |
| 197079 | -5.40e-09 | 6.77e-03     | 3.34e-08    |
| 0      | 1.47e+01  | 2.30e-99     | 2.30e-99    |

3253 observations. The data are available from

**Source:** WDC-SILSO, Royal Observatory of Belgium, Brussels

We take \( m = 1626 \) as above giving 3252 covariates. The stepwise Gaussian procedure returns 54 covariates in two seconds with a maximum Gaussian P-value of 0.0085. For this data set lasso fails completely returning between 727 and 787 covariates, each selection taking about 16 seconds.

### 10.2.5 Constructing a model: the sunspot data

Let \( s \) denote the number of sunspots, \( f_1 \) the function returned by the stepwise procedure and \( tr_j, j = 1, \ldots, 3252 \) the trigonometric functions. The residuals are \( r_1 = s - \log(1 + \exp(f_1)) \) where the transformation is made to force the function to be non-negative. The residuals are reasonably described by an autoregressive process of order 1 with coefficient 0.4. We write

\[
d(t) = s(t) - 0.4s(t - 1), t = 2, \ldots, 3253
\]

which removes the autocorrelation. We now apply the stepwise procedure to \( d \) with the covariates \( tr_j(t), t = 2, \ldots, 3253, j = 1, \ldots, 3252 \) and denote the resulting function by \( f_2 \). This eliminates the high frequency trigonometric functions caused by the autocorrelations. We define a new approximating function by

\[
f_3(t) = \sum_{j=0}^{6} 0.4^j f_2(t - j)
\]
Figure 1: From top to bottom (i) the original data, (ii) the function $f_3$, and (iii) simulated data.

with residuals $r_3 = s - \log(1 + \exp(f_3))$. The size of the residuals depends on $\log(1 + \exp(f_3))$ and a simple linear regression shows that

$$z = r_3 / (1.28(9.4 + 0.125 \log(1 + \exp(f_3))))$$

can be well approximated by an autoregressive Gaussian process of order one with parameter 0.5. This leads to the model

$$S(t) = f_3(t) + 1.28(9.4 + 0.125 \log(1 + \exp(f_3)))Z(t)$$

where $Z(t) \sim N(0, 1)$ is a Gaussian autoregressive process of order one with parameter 0.5.

From top to bottom panels of Figure[1] show (i) the original data, (ii) the function $f_3$ and (iii) a simulated data set.
Table 7: Sunspot data using autoregressive regression allowing for lags of up to 150.

| lag | coef. | Gauss P-value | st. P-value |
|-----|-------|---------------|-------------|
| 1   | 0.541 | 5.56e-178     | 3.92e-180   |
| 4   | 0.130 | 5.46e-12      | 3.85e-14    |
| 111 | 0.05  | 9.00e-09      | 6.33e-11    |
| 2   | 0.124 | 4.22e-09      | 2.97e-11    |
| 9   | 0.113 | 1.97e-11      | 1.39e-13    |
| 27  | -0.080| 3.83e-18      | 2.7e-20     |
| 6   | 0.077 | 6.26e-04      | 4.41e-06    |
| 0   | 3.673 | 1.09e-04      | 1.09e-04    |

10.2.6 Dependency graphs

The graph for the covariates of the leukemia data resulted in 1577 directed edges in six seconds. The number of edges was 1294. The repeated Gaussian method gives 11655 edges in about 25 seconds. It was not possible to compare this with glasso as there seems to be no default method of choosing the regularization parameter $\rho$.

10.2.7 Lagged covariates

The result for the Gaussian stepwise procedure applied to the sunspot data and allowing for lags of up to 150 is given in Table 7. The sum of squared residuals was 1852357. Including one further lag of 18 reduces this to 1843950.

Lasso results in either 16 or 18 lags with sums of squared residuals of 1861044 and 1850958 respectively.

The American Business Cycle data we considered are the USA quarterly data 1919-1941,1947-1983 available from

http://data.nber.org/data/abc/

We merged the two time intervals and used the values given in 1972$. The dependent variable was taken to be the Gross national Product (GNP72). The following further indices (see the above data source for an explanation) were included each with lags of 1:16 giving 352 covariates in all:

CPRATE, CORPYIELD, M1, M2, BASE, CSTOCK, WRICE67, PRODUR72, NONRES72, IRES72, DBUSI72, CDUR72, CNDUR72, XPT72, MPT72, GOVPUR72, NCSPDE72, NCSBS72, NCSCON72,CCSPDE72,CCSBS72

We are not economists so whether this makes sense or not we leave to the reader. The result of the Gaussian stepwise procedure is given in Table 8 with sum of squared residuals 18765.
| Gauss P-value | st.P-value | covariate                        |
|--------------|-----------|----------------------------------|
| 1.21e-315    | 3.45e-318 | Gross National Product, lag 1    |
| 6.85e-15     | 1.97e-17  | Commercial Paper Rate, lag 2     |
| 1.71e-04     | 4.8e-07   | Change Business Inventories, lag 4|
| 4.66e-01     | 4.66e-01  | intercept                        |

Table 8: The USA Gross National Product data using the first 16 lags of the 22 indices listed above.

| Gauss P-value | st.P-value | covariate                        |
|--------------|-----------|----------------------------------|
| 8.93e-140    | 2.56e-142 | Gross National Product, lag1     |
| 1.00e+00     | 3.17e-01  | Index of all Common Stocks, lag 1|
| 7.18e-01     | 3.61e-03  | Non-Residential Structures, lag 1|
| 1.00e+00     | 2.42e-01  | Imports, lag 15                  |
| 4.59e-02     | 4.59e-02  | intercept                        |

Table 9: The USA Gross National Product data using the first 16 lags of the 22 indices listed above using lasso.

Five applications of lasso resulted each time in the covariates lasso 1, 97, 161 and 271. The results are given in Table 9 with sum of squared residuals 24980.

11 Appendix: Technical details and proofs

11.1 Details and Proofs for Section 2

In what follows, we utilize some basic facts about multivariate Gaussian distributions, see for example [Mardia et al. (1979)]

**Special distributions.** Let \( b_1, \ldots, b_p \) be an orthonormal basis of a linear subspace \( V \) of \( \mathbb{R}^n \), and let \( Z \sim N_p(0, I) \). Then \( \tilde{Z} := \sum_{i=1}^p Z_i b_i \) has a standard Gaussian distribution on \( V \) with \( \|Z\| = \|\tilde{Z}\| \).

The chi-squared distribution with \( p \) degrees of freedom coincides with Gamma\( (p/2, 2) \), where Gamma\( (a, c) \) stands for the gamma distribution with shape parameter \( a > 0 \) and scale parameter \( c > 0 \). The statements of the next Lemma are well known.

**Lemma 6.** Let \( a, b, c > 0 \), and let \( Y_a \) and \( Y_b \) be independent random variables with distributions Gamma\( (a, c) \) and Gamma\( (b, c) \), respectively. Then \( Y_a + Y_b \) and \( U := Y_a/(Y_a + Y_b) \) are stochastically independent with \( Y_a + Y_b \sim \text{Gamma}(a + b, c) \) and \( U \sim \text{Beta}_{a,b} \).

With \( Y_a, Y_b \) and \( U \) as in the previous lemma, \( F := (Y_a/a)/(Y_b/b) \sim F_{2a,2b} \). Note also that
\[ U = (a/b) F/((a/b)F + 1) \] and \( 1 - U \sim \text{Beta}_{a,b}. \) In particular, for \( x > 0, \)
\[ 1 - F_{2a,2b}(x) = P(F \geq x) = P\left(U \geq \frac{(a/b)x}{(a/b)x + 1}\right) = P\left(1 - U \leq \frac{1}{(a/b)x + 1}\right) = \text{Beta}_{a,b}\left(\frac{1}{(a/b)x + 1}\right). \]

With \( a = (q - q_0)/2, b = (n - q)/2 \) and \( x = (b/a)(\text{RSS}_0 - \text{RSS})/\text{RSS}, \) we obtain the equation
\[ 1 - F_{q - q_0,n - q}\left(\frac{\text{RSS}_0 - \text{RSS}}{\text{RSS}}/(n - q)\right) = \text{Beta}(n - q)/2,(q - q_0)/2\left(\frac{\text{RSS}}{\text{RSS}_0}\right), \]
i.e. equality two of the P-values of Theorem 2.

Lemma 6 implies useful facts about products of beta random variables.

**Lemma 7.** (i) For \( a,b,c > 0, \) let \( U \sim \text{Beta}(a,b) \) and \( V \sim \text{Beta}(a + b,c) \) be stochastically independent. Then \( UV \sim \text{Beta}(a,b + c). \)

(ii) For \( a,\delta > 0 \) and \( k \in \mathbb{N}, \) let \( U_1, \ldots, U_k \) be stochastically independent random variables such that \( U_j \sim \text{Beta}(a + (j - 1)\delta,\delta). \) Then \( \prod_{j=1}^k U_j \sim \text{Beta}(a,k\delta). \)

**Proof of Lemma 7.** For proving part (i), we start with independent random variables \( G_a \sim \text{Gamma}(a,1), G_b \sim \text{Gamma}(b,1) \) and \( G_c \sim \text{Gamma}(c,1). \) By Lemma 6,
\[ U := \frac{G_a}{G_a + G_b} \sim \text{Beta}(a,b), \quad G_a + G_b \sim \text{Gamma}(a + b,1) \quad \text{and} \quad G_c \]
are independent. A second application of Lemma 6 implies that the random variables \( U \) and
\[ V := \frac{G_a + G_b}{G_a + G_b + G_c} \sim \text{Beta}(a + b,c) \]
are also independent so that
\[ UV = \frac{G_a}{G_a + G_b + G_c} \sim \text{Beta}(a,b + c), \]
because \( G_a \) and \( G_b + G_c \sim \text{Gamma}(b + c,1) \) are independent.

Part (ii) follows from part (i) via induction.

**Proof of Theorems 1 and 2** We consider firstly the case \( q_0 = q - 1, \) put
\[ \mathbb{V}_0^\perp = \{ \mathbf{w} \in \mathbb{R}^n : \mathbf{w}^\top \mathbf{x} = 0 \text{ for all } \mathbf{x} \in \mathbb{V}_0 \} \]
where \( \mathbb{V}_0 \) is the linear space spanned by the covariates \( \mathbf{x}_i, i \in \mathcal{M}_0. \)

Let \( \mathbf{b}_i, i = 1, \ldots, n \) be an orthonormal basis of \( \mathbb{R}^n \) such that
\[ \mathbb{V}_0 = \text{span}(\mathbf{b}_1, \ldots, \mathbf{b}_{q_0}) \quad \text{and} \quad \mathbf{b}_{q_0+1} = (\mathbf{y} - P_{\mathcal{M}_0}(\mathbf{y}))/\text{(SS}_0)^{-1/2} \]

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where \( P_{M_0} \) is the projection onto the subspace \( \mathbb{V}_0 \). We now replace \( x_\nu \) by a Gaussian covariate \( Z_\nu \) consisting of \( n \) i.i.d. \( N(0,1) \) random variables. By the rotational symmetry of the standard Gaussian distribution on \( \mathbb{R}^n \), \( Z_j := b_j^T Z_\nu \) defines stochastically independent standard Gaussian random variables \( Z_1, \ldots, Z_n \). The orthogonal projection of \( Z_\nu \) onto \( \mathbb{V}_0^\perp \) is given by

\[
\tilde{Z}_\nu := \sum_{j=q_0+1}^{n} Z_j b_j.
\]

In particular

\[
\text{span}(b_1, \ldots, b_{q_0}, Z) = \text{span}(b_1, \ldots, b_{q_0}, \tilde{Z})
\]

and as

\[
P_{M_1}(y) = P_{M_0}(y) - (ss_0)^{1/2} \frac{\tilde{Z}_\nu^T b_{q_0+1}}{||\tilde{Z}_\nu||^2} \tilde{Z}_\nu
\]

it follows that

\[
SS_1 = ss_0 - ss_0 \frac{(\tilde{Z}_\nu^T b_{q_0+1})^2}{||\tilde{Z}_\nu||^2}
\]

and hence

\[
\frac{SS_1}{ss_0} = 1 - \frac{(\tilde{Z}_\nu^T b_{q_0+1})^2}{||\tilde{Z}_\nu||^2} = \frac{\sum_{j=q_0+2}^{n} Z_j^2}{\sum_{j=q_0+1}^{n} Z_j^2} \sim \text{Beta}((n - q_0 - 1)/2, 1/2). \tag{25}
\]

In the general case with \( q - q_0 = k > 1 \) the above argument may be applied inductively to show that

\[
\frac{SS_1}{ss_0} = \prod_{\ell=1}^{k} U_\ell
\]

in distribution where the \( U_1, \ldots, U_k \) are stochastically independent with

\[
U_\ell \sim \text{Beta}((n - q_0 - \ell)/2, 1/2)
\]

We now use the standard result that if \( U \sim \text{Beta}(a, b) \) and \( V \sim \text{Beta}(a + b, c) \) and \( U \) and \( V \) are independent then \( UV \sim \text{Beta}(a, b + c) \). From this it follows that

\[
\frac{SS_1}{ss_0} \sim \text{Beta}((n - q)/2, (q - q_0)/2) \tag{26}
\]

which proves Theorem 1 and the first part of Theorem 2.

To prove the second part we note that if \( \chi^2_{\nu_1} \) and \( \chi^2_{\nu_2} \) are independent chi-squared random variables with \( \nu_1 \) and \( \nu_2 \) degrees of freedom respectively then

\[
\frac{\chi^2_{\nu_1}/\nu_1}{\chi^2_{\nu_2}/\nu_2} \sim F(\nu_1, \nu_2)
\]

and

\[
\frac{\chi^2_{\nu_1}}{\chi^2_{\nu_1} + \chi^2_{\nu_2}} \sim \text{Beta}(\nu_1/2, \nu_2/2).
\]

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From this it follows that for all \( x > 0 \)
\[
F_{\nu_1, \nu_2}(x) = \text{Beta}_{\nu_1/2, \nu_2/2}((\nu_1/\nu_2)x/((\nu_1/\nu_2)x + 1))
\]
and hence the second equality of the theorem.

### 11.2 Details and Proofs for Section 9

An important ingredient are bounds for the quantile functions of beta and gamma distributions.

**Lemma 8.** Let \( G \) be the distribution function of \( \Gamma(1/2, 2) = \chi^2_1 \). Then,
\[
\text{Beta}^{-1}_{1/2, (n-1)/2} \left\{ \begin{array}{ll}
\geq G^{-1}/(n - 1 + G^{-1}) & \text{if } n \geq 2, \\
\leq (n - 2)^{-1}G^{-1} & \text{if } n \geq 3.
\end{array} \right.
\]
Moreover, for \( \delta \in (0, 1) \),
\[
G^{-1}(1 - \delta) = 2 \log(1/\delta) - \log \log(1/\delta) - \log \pi + o(1) \text{ as } \delta \to 0.
\]

For the second part see for example Chapter 2 of [de Haan and Ferreira (2006)](https://doi.org/10.1007/978-3-0348-7817-0). It has various implications for the maximum of squared standard Gaussian random variables:

**Lemma 9.** Let \( Z \in \mathbb{R}^q \) be a random vector with components \( Z_i \sim N(0, 1) \). Then
\[
P\left( \max_{1 \leq i \leq q} Z_i^2 \leq 2 \log q \right) \to 1
\]
as \( q \to \infty \). If \( Z \sim N_q(0, I) \), then
\[
\max_{1 \leq i \leq q} Z_i^2 = 2 \log q - \log \log q - \log \pi + 2X_q
\]
with a random variable \( X_q \) such that \( \lim_{q \to \infty} P(X_q \leq x) = \exp(-e^{-x}) \) for any \( x \in \mathbb{R} \).

Lemma 8 also leads to a particular approximation of beta quantiles:

**Lemma 10.** For integers \( n, q \geq 2 \) and fixed \( \alpha \in (0, 1) \),
\[
n\text{Beta}^{-1}_{1/2, (n-1)/2}((1 - \alpha)^{1/2}) = 2 \log q - \log \log q - \log \pi - 2 \log(-\log(1 - \alpha)) + o(1)
\]
as \( q \to \infty \) and \( n/\log(q)^2 \to \infty \).

**Proof of Lemma 8.** Recall that \( B := \text{Beta}_{1/2, (n-1)/2} \) is the distribution function of \( Z_1^2/(Z_1^2 + S^2) \) with \( S^2 = \sum_{i=2}^n Z_i^2 \) and \( Z \sim N_n(0, I) \). Then Jensen’s inequality implies that for \( 0 < x < 1 \),
\[
B(x) = \mathbb{E}\left( P\left( Z_1^2 \leq \frac{S^2}{1-x} \bigg| S^2 \right) \right) = \mathbb{E}\left( G\left( \frac{S^2}{1-x} \right) \right) \leq G\left( \frac{(n-1)x}{1-x} \right),
\]

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because \( E(S^2) = n - 1 \) and \( G \) is concave. Consequently, for \( 0 < u < 1 \), \( B^{-1}(u) \) is not smaller than the solution \( x \) of \((n - 1)x/(1 - x) = G^{-1}(u)\), which is \( G^{-1}(u)/(n - 1 + G^{-1}(u))\).

On the other hand, if \( n \geq 3 \), then it it follows from independence of \( X := Z_1^2/\|Z\|^2 \) and \( T := \|Z\|^2 \) with \( E(T^{-1}) = (n - 2)^{-1} \) that
\[
G(y) = P(TX \leq y) = E(B(T^{-1}y)) \leq B((n - 2)^{-1}y)
\]
by Jensen’s inequality and concavity of \( B \). Consequently, \( B \geq G((n - 2)^{-1}) \), and this implies that \( B^{-1} \geq (n - 2)^{-1}G^{-1} \).

For the reader’s convenience, a proof of the second part is provided as well. Since \( G'(x) = (2\pi x)^{-1/2}e^{-x^2/2} \), partial integration and elementary bounds yield the inequalities
\[
2^{1/2}(\pi x)^{-1/2}e^{-x^2/2}(1 - 2x^{-1}) \leq 1 - G(x) \leq 2^{1/2}(\pi x)^{-1/2}e^{-x^2/2}.\]
If we fix an arbitrary real number \( z \) and set \( x := 2\log(1/\delta) - \log \log(1/\delta) - \log\pi + z \), then \( x = 2\log(1/\delta)(1 + o(1)) \to \infty \) and
\[
2\log(1 - G(x)) = 2\log(\delta) - z + o(1)
\]
as \( \delta \downarrow 0 \). This implies the asserted expansion for \( G^{-1}(1 - \delta) \) as \( \delta \downarrow 0 \). \( \square \)

**Proof of Lemma** \(^{[10]} \). Note first that \((1 - \alpha)^{1/q} = \exp(\log(1 - \alpha)/q)\) may be written as \( 1 - \delta \) with \( \delta := q^{-1}\alpha(1 + O(q^{-1})) \) and \( \tilde{\alpha} := -\log(1 - \alpha) \). Since \( \log(1/\delta) = \log q - \log \tilde{\alpha} + o(1) \) and \( \log \log(1/\delta) = \log(\log q + O(1)) = \log \log q + o(1) \), it follows from the second part of Lemma \(^{[8]} \) that
\[
G^{-1}((1 - \alpha)^{1/q}) = 2\log q - \log \log q - \log\pi - 2\log\tilde{\alpha} + o(1) = O(\log q)
\]
as \( q \to \infty \). Then the first part of that lemma implies that
\[
\text{Beta}^{-1}_{1/2,(n-1)/2}((1 - \alpha)^{1/q}) = (n + O(\log q))^{-1}G^{-1}((1 - \alpha)^{1/q})
\]
\[
= n^{-1}(1 + O(n^{-1}\log q))G^{-1}((1 - \alpha)^{1/q})
\]
\[
= n^{-1}(2\log q - \log \log q - \log\pi - 2\log\tilde{\alpha} + o(1))
\]
as \( q \to \infty \) and \( n/\log(q)^2 \to 0 \). \( \square \)

**Proof of Theorem** \(^{[3]} \). Note first that \((x^\top y)^2/\|y\|^2 = (x^\top Z)^2/\|Z\|^2 \) has distribution function \( B = \text{Beta}_{1/2,(n-1)/2} \). Hence, with \( x_{n,q} := B^{-1}((1 - \alpha)^{1/q}) \),
\[
P\left(\max_{x^\top y \geq x_{n,q}} \frac{(x^\top y)^2}{\|y\|^2} \geq x_{n,q}\right) \leq q\left(1 - (1 - \alpha)^{1/q}\right) \leq -\log(1 - \alpha),
\]
27
because \((1 - \alpha)^{1/q} = \exp(q^{-1}\log(1 - \alpha)) \geq 1 + q^{-1}\log(1 - \alpha)\). Note also that \(\|Z\|^2\) has expectation \(n\) and variance \(2n\), whence for arbitrary \(c > 0\),

\[
P(\|Z\|^2 \leq n - cn^{1/2}), P(\|Z\|^2 \geq n + cn^{1/2}) \leq \frac{2}{2 + c^2}
\]

by the Tchebyshev-Cantelli inequality. Consequently,

\[
P\left(\max_{x_{\nu}} \frac{(x_{\nu}^\top y)^2}{\|y\|^2} \geq x_{n,q}\right) \leq P\left(\max_{x_{\nu}} (x_{\nu}^\top Z)^2 \geq (1 - cn^{-1/2})nx_{n,q}\right) + \frac{2}{2 + c^2}
\]

and

\[
P\left(\max_{x_{\nu}} \frac{(x_{\nu}^\top y)^2}{\|y\|^2} \geq x_{n,q}\right) \geq P\left(\max_{x_{\nu}} (x_{\nu}^\top Z)^2 \geq (1 + c^{-1/2})nx_{n,q}\right) - \frac{2}{2 + c^2}.
\]

But it follow from the Gaussian inequality (cf. Sidák (1967) or Royen (2014)) that for any number \(x\),

\[
P\left(\max_{x_{\nu}} (x_{\nu}^\top Z)^2 \geq x\right) \leq P\left(\max_{\nu} Z_{\nu}^2 \geq 2 \log q - \log \log q - \log \pi - 2 \log \tilde{\alpha} + o(1)\right)
\]

with independent random variables \(Z_{\nu} \sim N(0, 1), \nu = 1, \ldots, q\) with equality in case of orthonormal regressors \(x_{\nu}\). Now the claims follow from the fact that for any fixed \(c > 0\) and \(\tilde{\alpha} := -\log(1 - \alpha)\),

\[
(1 \pm cn^{-1/2})n_{x_{n,q}} = (1 \pm cn^{-1/2})(2 \log q - \log \log q - \log \pi - 2 \log \tilde{\alpha} + o(1))
\]

\[
= 2 \log q - \log \log q - \log \pi - 2 \log \tilde{\alpha} + o(1)
\]

by Lemma 10, and

\[
P\left(\max_{\nu} Z_{\nu}^2 \geq 2 \log q - \log \log q - \log \pi - 2 \log \tilde{\alpha} + o(1)\right) \to 1 - \exp(-\exp(\log \tilde{\alpha})) = \alpha
\]

by Lemma 9.

**Proof of Theorems 4 and 5.** Note first that in case of orthonormal regressors, \(q \leq n\), and Condition (A.1’) implies Condition (A.1). Without loss of generality we assume that \(\sigma = 1\).

At first we verify that \(\hat{\mathcal{S}} \supset \mathcal{S}_*\) with asymptotic probability one. Having started stepwise selection with \(\mathcal{S} = \emptyset\), suppose we have chosen a set \(\mathcal{S} \subset \mathcal{S}_*\) of \(k\) covariates. The question is whether an additional regressor \(x_{\nu}\) with \(x_{\nu} \in \mathcal{S}_* \setminus \mathcal{S}\) will be added to \(\mathcal{S}\), regardless of the choice of \(\mathcal{S}\). This is certainly the case if

\[
\min_{\mathcal{S} \subseteq \mathcal{S}_*} \left(\max_{x_{\nu} \in \mathcal{S}_* \setminus \mathcal{S}} |x_{S,\nu}^\top y| - \max_{x_{s} \notin \mathcal{S}_*} |x_{S,s}^\top y| \right) > 0
\]

(27)

and

\[
\min_{\mathcal{S} \subseteq \mathcal{S}_*} \left(\max_{x_{\nu} \in \mathcal{S}_* \setminus \mathcal{S}} \frac{|x_{S,\nu}^\top y|}{\|Q_S y\|} - \kappa_{n-k,q-k} \right) > 0
\]

(28)
with asymptotic probability one, where \( \kappa_{n',q'} := \sqrt{B_{1/2,(n'-1)/2}} \left( (1 - \alpha)^{1/q'} \right) \). Inequality (27) can be replaced by the stronger but simpler inequality

\[
\min_{x_\nu \in S, S \subseteq S_* \setminus \{x_\nu\}, x_s \notin S_*} (|x_{S,\nu}^\top y| - |x_{S,s}^\top y|) > 0. 
\] (29)

Moreover, according to Lemma 10,

\[
\max_{0 \leq k \leq k_*} \kappa_{n-k,q-k} = \sqrt{(2 + o(1)) \log q \over n},
\]

and \( \|Q_S y\| \leq \|y\| \). But \( \|y\|^2 \) has a non-central chi-squared distribution with \( n \) degrees of freedom and non-centrality parameter \( \|\mu\|^2 \). In particular, it has expectation \( n + \|\mu\|^2 \) and variance \( 2n + 4\|\mu\|^2 \), and this implies that

\[
\|y\| = \sqrt{n + \|\mu\|^2 + O_p(1)} = \sqrt{n + \|\mu\|^2(1 + o_p(1))}. 
\] (30)

Hence we may replace (28) with

\[
\min_{x_\nu \in S, S \subseteq S_* \setminus \{x_\nu\}} \frac{|x_{S,\nu}^\top y|}{\sqrt{n + \|\mu\|^2}} > \sqrt{\tau' \log q \over n} 
\] (31)

for some \( \tau' > 2 \).

Let us verify (29) and (31) for orthonormal regressors \( x_\nu \) and \( \mu = \sum x_\nu \in S_* \beta_\nu x_\nu \). Here \( x_{S,\nu} = x_\nu \) and \( S \subset S_* \setminus \{x_\nu\} \), whence the left hand side of (29) equals

\[
\min_{x_\nu \in S_*} |\beta_\nu| - \max_{x_\nu \in S_*} |x_\nu^\top Z| - \max_{x_s \notin S_*} |x_s^\top Z| \geq \min_{x_\nu \in S_*} |\beta_\nu| - \sqrt{2 \log k_*} - \sqrt{2 \log q} - O_p(1) \\
\geq \sqrt{\tau \log q - 2 \log q - O_p(1)} \to_p \infty,
\]

where the second last inequality follows from Lemma 9 and the last inequality is a consequence of Condition (A.2'). This proves (29). Similarly one can show that the left hand side of (31) is equal to

\[
\min_{x_\nu \in S_*} \frac{|x_\nu^\top y|}{\sqrt{n + \|\mu\|^2}} \geq \min_{x_\nu \in S_*} \frac{|\beta_\nu| - |x_\nu^\top Z|}{\sqrt{n + \|\mu\|^2}} \\
\geq \min_{x_\nu \in S_*} \frac{|\beta_\nu| - \sqrt{2 \log k_*} - O_p(1)}{\sqrt{n + \|\mu\|^2}} \\
\geq \sqrt{\tau \log q - O_p(1)} \over \sqrt{n} = \sqrt{(\tau + o_p(1)) \log q \over n},
\]

and the latter quantity is greater than \( \sqrt{\tau' \log(q) / n} \) with asymptotic probability one, provided that \( 2 < \tau' < \tau \).
Now we verify (29) and (31) in the general case. On the one hand, since all vectors \( x_{S,v} \) with \( x_v \in S \) and \( S \subset S_v \setminus \{ x_v \} \) belong to the unit ball of \( V_{S_v} \),

\[
\min_{x_v \in S_v, S \subset S_v \setminus \{ x_v \}} |x_{S,v}^\top y| \geq \min_{x_v \in S_v, S \subset S_v \setminus \{ x_v \}} |x_{S,v}^\top \mu| - \| \hat{Z}_S \| \\
\geq \min_{x_v \in S_v, S \subset S_v \setminus \{ x_v \}} |x_{S,v}^\top \mu| - \sqrt{k_s} - O_p(1),
\]

because \( \| \hat{Z}_S \|^2 \) has a chi-squared distribution with \( m_s \) degrees of freedom, see also the arguments for (30). On the other hand, for any \( S \subset S_v \) and \( x_s \notin S_v \), it follows from \( V_{S_v} \supset V_{S_v} \) that the vector \( Q_S x_s \) is the sum of \( Q_S x_s \in V_{S_v} ^\perp \) and \( (Q_S - Q_{S_v}) x_s \in (V_{S_v} ^\perp) ^\perp = V_{S_v} \). Consequently,

\[
x_{S,s} = \lambda_{S,s} v_s + \hat{\lambda}_{S,s} \hat{v}_{S,s}
\]

with

\[
\lambda_{S,s} := \| Q_S x_s \| / \| Q_S x_s \|^2 + \| (Q_S - Q_{S_v}) x_s \|^2 \in [0, 1],
\]

\[
v_s := \| Q_S x_s \|^{-1} Q_S x_s \in V_{S_v} ^\perp,
\]

\[
\hat{\lambda}_{S,s} := \sqrt{1 - \lambda_{S,s}^2} \in [0, 1],
\]

\[
\hat{v}_{S,s} := \| (Q_S - Q_{S_v}) x_s \|^{-1} (Q_S - Q_{S_v}) x_s \in V_{S_v}.
\]

This implies that

\[
\max_{S \subset S_v, x_s \notin S_v} |x_{S,s}^\top y| \leq \max_{S \subset S_v, x_s \notin S_v} |x_{S,v}^\top \mu| + \| \hat{Z}_S \| + \max_{s \in N \setminus S_v} \| v_s Z \| \\
\leq \max_{S \subset S_v, x_s \notin S_v} |x_{S,v}^\top \mu| + \sqrt{k_s} + \sqrt{2 \log q} - O_p(1).
\]

These inequalities and assumption (A.2) imply that the left hand side of (29) is not smaller than

\[
\min_{x_v \in S_v, S \subset S_v \setminus \{ x_v \}, x_s \notin S_v} \left( |x_{S,v}^\top \mu| - |x_{S,v}^\top \mu| \right) - 2\sqrt{k_s} - \sqrt{2 \log q} - O_p(1) \\
\geq \sqrt{\tau \log q} - \sqrt{2 \log q} - O_p(1) \rightarrow_p \infty.
\]

Hence (29) is satisfied with asymptotic probability one. Moreover, a second application of (A.2) shows that the left hand side of (31) is not smaller than

\[
\min_{x_v \in S_v, S \subset S_v \setminus \{ x_v \}} \frac{|x_{S,v}^\top \mu| - \| \hat{Z}_S \|}{\sqrt{n + \| \mu \|^2}} \geq \min_{x_v \in S_v, S \subset S_v \setminus \{ x_v \}} \frac{\sqrt{\tau \log q} + \sqrt{k_s} - O_p(1)}{\sqrt{n}} \\
\geq \sqrt{\frac{(\tau + o_p(1)) \log q}{n}},
\]

and the latter quantity is greater than \( \sqrt{\tau' \log(q)/n} \) with asymptotic probability one, provided that \( 2 < \tau' < \tau \).
So far we have shown that with asymptotic probability one, the stepwise selection will lead to the candidate $S = S^*$ for $\hat{S}$. But at that stage, $x_{S^*,v}^\top y = x_{S^*,v}^\top Z = x_{S^*,v}^\top Q_{S^*} Z$ for all $x_v \notin S^*$, so

$$P(S^*_v \subset \hat{S}) \leq o(1) + P\left( \max_{x_v \notin S^*} \frac{(x_{S^*,v}^\top Q_{S^*} Z)^2}{\|Q_{S^*} Z\|^2} \geq \kappa_{n-k, q-k}, \right) \leq \alpha + o(1)$$

by a simple adaptation of Theorem 3.

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