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RANKING-BASED VARIABLE SELECTION FOR HIGH-DIMENSIONAL DATA

Rafal Baranowski, Yining Chen and Piotr Fryzlewicz

London School of Economics and Political Science

Abstract: We propose a ranking-based variable selection (RBVS) technique that identifies important variables influencing the response in high-dimensional data. RBVS uses subsampling to identify the covariates that appear nonspuriously at the top of a chosen variable ranking. We study the conditions under which such a set is unique, and show that it can be recovered successfully from the data by our procedure. Unlike many existing high-dimensional variable selection techniques, among all relevant variables, RBVS distinguishes between important and unimportant variables, and aims to recover only the important ones. Moreover, RBVS does not require model restrictions on the relationship between the response and the covariates, and, thus, is widely applicable in both parametric and nonparametric contexts. Lastly, we illustrate the good practical performance of the proposed technique by means of a comparative simulation study. The RBVS algorithm is implemented in **rbvs**, a publicly available R package.

Key words and phrases: Bootstrap, stability selection, subset selection, variable screening.

1. Introduction

Suppose Y is a response, the covariates $X_1, \dots, X_p$ constitute the set of random variables that potentially influence Y, and we observe $\mathbf{Z}_i = (Y_i, X_{i1}, \dots, X_{ip})$, for $i = 1, \dots, n$, independent copies of $\mathbf{Z} = (Y, X_1, \dots, X_p)$. In modern statistical applications, where p could be very large, even in tens or hundreds of thousands, it is often assumed that many variables have no impact on the response. It is then of interest to use the observed data to identify a subset of $X_1, \dots, X_p$ that affects Y. This so-called variable selection or subset selection problem plays an important role in statistical modeling for the following reasons. First, the number of parameters in a model, including all covariates, can exceed the number of observations when $n < p$, which means precise statistical inferences are not possible using traditional methods. Even when $n \geq p$, constructing a model with a small subset of initial covariates can boost the estimation and prediction accuracy. Second, parsimonious models are often more interpretable. Third, identifying the set of important variables can be the main goal of statistical analysis, which precedes further scientific investigations.

Our aim is to identify a subset of $\{X_1, \ldots, X_p\}$ that contributes to Y, under scenarios in which p is potentially much larger than n. To model this phenomenon, we work in a framework in which p diverges with n. Therefore, both p and the distribution of $\mathbf{Z}$ depend on n, and we work with a triangular array, rather than a sequence. To facilitate interpretability, for each j, what the variable X_j represents does not change as p (and n) increases. Our framework includes, for instance, high-dimensional linear and nonlinear regression models. Our proposed ranking-based variable selection (RBVS) can be applied to any technique that allows the ranking of covariates according to their impact on the response. Therefore, we do not impose any particular model structure on the relationship between Y and $X_1, \ldots, X_p$. However, $\hat{\omega}_j = \hat{\omega}_j(\mathbf{Z}_1, \ldots, \mathbf{Z}_n)$, for $j = 1, \ldots, p$, a measure used to assess the importance of covariates (either joint or marginal), may require some assumptions on the model. The main component of the RBVS methodology is the variable ranking, defined as follows.

Definition 1. The variable ranking $\mathbf{R}_n = (R_{n1}, \ldots, R_{np})$ based on $\hat{\omega}_1, \ldots, \hat{\omega}_p$ is a permutation of $\{1, \ldots, p\}$ satisfying $\hat{\omega}_{R_{n1}} > \cdots > \hat{\omega}_{R_{np}}$. Potential ties are broken at random uniformly.

Numerous measures can be used to construct variable rankings. For linear models, the marginal correlation coefficient serves as an example of such a measure, and is the main component of sure independence screening (SIS, Fan and Lv (2008)). Hall and Miller (2009a) consider a generalized correlation coefficient, that can capture (possible) nonlinear dependence between Y and X_j. Along the same lines, Fan, Feng and Song (2011) propose a procedure based on the magnitudes of spline approximations of Y over each X_j, aiming to capture dependencies in nonparametric additive models. Fan and Song (2010) extend SIS to a class of generalized linear models (GLMs), using estimates of the maximum marginal likelihood as the measure of association. Cho and Fryzlewicz (2012) consider variable screening based on a tilted correlation, which accounts for high correlations between the variables, when such are present. Li et al. (2012) use the Kendall rank correlation coefficient, which is applicable when Y is, for example, a monotonic function of the linear combination of $X_1, \ldots, X_p$. In addition, several model-free variable ranking procedures have been advocated in the literature. Li, Zhong and Zhu (2012) propose ranking the covariates according to their distance correlation (Székely and Rizzo (2009)) to the response. Zhu et al. (2011) propose using the covariance between X_j and the cumulative distribution function of Y, conditioning on X_j at point Y, as the quantity estimated for screening purposes. He, Wang and Hong (2013) suggest a ranking procedure that relies on the marginal quantile utility, and Shao and Zhang (2014) introduce a ranking based on the martingale difference correlation. An extensive overview of these and other measures that can be used for variable screening can be found in Liu, Zhong and Li (2015). In this work, we also consider variable rankings based on measures that were not originally developed for this purpose, such as regression coefficients estimated using penalized likelihood minimization procedures such as the Lasso (Tibshirani (1996)), SCAD (Fan and Li (2001)), or MC+ (Zhang (2010)).

Variable rankings are used for the purpose of so-called variable screening (Fan and Lv (2008)). The main idea behind this concept is that important covariates are likely to be ranked ahead of irrelevant ones, which means variable selection can be performed on the set of top-ranked variables. Variable screening procedures have gained in popularity, owing to their simplicity and wide applicability, as well as the computational gains they offer to practitioners. Hall and Miller (2009a) suggest that variable rankings can be used for actual variable selection. They propose constructing bootstrap confidence intervals for the position of each variable in the ranking, and then selecting the covariates for which the right end of the confidence interval is lower than some cutoff, for example, $p/2$. This principle, as its authors admit, may lead to an undesirable high rate of false positives, and the choice of the ideal cutoff might be very difficult in practice, as was the case in our real-data study (see the Supplementary Material). Hall and Miller (2009b) show that various types of bootstrap estimate the distribution of the ranks consistently. However, they do not prove that their procedure is able to recover the set of important variables.

Another approach that involves subsampling is that of Meinshausen and Bühlmann (2010), who propose stability selection (StabSel), a general methodology that aims to improve any variable selection procedure. In the first stage of the StabSel algorithm, a variable selection technique is applied to randomly chosen subsamples of data of size $\lfloor n/2 \rfloor$. Then, the variables most likely to be selected by the initial procedure, that is, their selection probabilities exceed a prespecified threshold, are taken as the final estimate of the set of important variables. An appropriate choice of threshold leads to finite-sample control of the rate of false discoveries of a certain type. Shah and Samworth (2013) propose a variant of StabSel with improved error control.

Our proposed method also incorporates subsampling to boost existing variable selection techniques. Conceptually, it is different from StabSel. Informally, RBVS sorts covariates from the most to the least important, whereas StabSel treats variables as either relevant or irrelevant, and equally important in either of the categories. This has several important consequences. First, RBVS is able to simultaneously identify subsets of covariates that appear to be important, consistently over subsamples. The same is not feasible for StabSel, which analyzes only the marginal distribution of the initial variable selection procedure. The bootstrap ranking approach of Hall and Miller (2009a) relies on marginal confidence intervals, and thus can also be regarded as a “marginal” technique. Second, RBVS does not require that we choose a threshold. The main parameters that RBVS require are those from the incorporated subsampling procedure (naturally, these are also required by the approaches of Hall and Miller (2009a) and Meinshausen and Bühlmann (2010)). Thus, RBVS appears to be more automatic than either StabSel or the approach of Hall and Miller (2009a).

The key idea behind RBVS stems from the following observation: although some subsets of $\{X_1, \ldots, X_p\}$ that contain irrelevant covariates may appear to have a high influence over Y, the probability that they will consistently exhibit this relationship over many subsamples of observations is small. On the other hand, truly important covariates will typically consistently appear to be related to Y, both over the entire sample and over randomly chosen subsamples. This motivates the following procedure. In the first stage, we repeatedly assess the impact of each variable on the response, using randomly chosen subsamples of the data. For each random draw, we sort the covariates in decreasing order according to their impact on Y, obtaining a ranking of variables. In the next step, we identify the sets of variables that appear frequently in the top of the rankings, and record the corresponding frequencies. The final set of variables is selected based on these frequencies.

RBVS is a general and widely applicable approach to variable selection, and can be used with any measure of dependence between X_j and Y, whether marginal or joint, in both parametric and nonparametric contexts. The framework does not require that Y and X_j be scalar; they may, for example, be multivariate or curves or graphs. Furthermore, covariates that are highly, but spuriously related to the response are, intuitively, less likely to exhibit a consistent relationship with Y over the subsamples; thus, our approach is “reluctant” to select irrelevant variables. Finally, the RBVS algorithm is easily parallelizable and adjustable to available computational resources, making it useful in analyses of extremely high-dimensional data sets. Its R implementation is publicly available in the R package **rbvs** (Baranowski, Breheny and Turner (2015)).

The rest of the paper is organized as follows. In Section 2, we define the set of important covariates for the variable rankings and introduce the RBVS algorithm. We then show that RBVS is a consistent statistical procedure. We also propose an iterative extension of RBVS that boosts its performance in the presence of strong dependencies between the covariates. The empirical performance of RBVS is discussed in Section 3. All proofs are deferred to the Appendix. Additional numerical experiments and real-data examples can be found in the online Supplementary Material.

1.1. Motivating examples

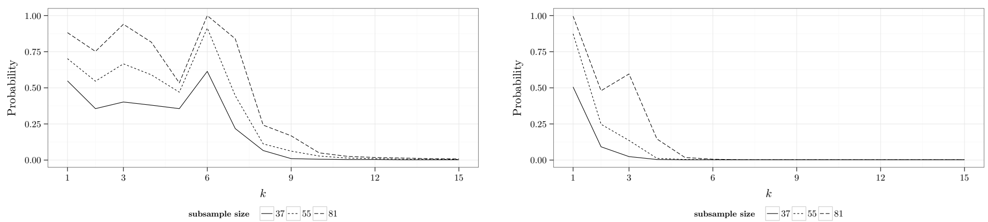
To further motivate our methodology, we discuss the following examples.

Example 1 (riboflavin production with *Bacillus subtils* (Meinshausen and Bühlmann (2010))**.** The data set consists of the response variable (the logarithm of the riboflavin production rate) and transformed expression levels of $p = 4,088$ genes for $n = 111$ observations. The aim is to identify those genes whose mutation leads to a high concentration of riboflavin.

Example 2 (Fan and Lv (2008))**.** Consider a random sample generated from the linear model $Y_i = 5X_{i1}+5X_{i2}+5X_{i3}+\varepsilon_i$, for $i = 1, \ldots, n$, where $(X_{i1}, \ldots, X_{ip}) \sim \mathcal{N}(0, \Sigma)$ and $\varepsilon_i \sim \mathcal{N}(0, 1)$ are independent, and $\Sigma_{jk} = 0.75$ for $j \neq k$, and $\Sigma_{jk} = 1$ otherwise. The number of covariates $p = 4,088$ and the sample size $n = 111$ are the same as in Example 1.

We consider the variable ranking defined in Definition 1, based on the sample marginal correlation coefficient in both examples. This choice is particularly reasonable in Example 2, where at the population level, the Pearson correlation coefficient is largest for X_1, X_2, and X_3, which are the only truly important ones. The linear model has been used previously to analyze the riboflavin data set (Meinshausen and Bühlmann (2010)). Therefore, the sample correlation may be useful in identifying important variables in Example 1 as well.

Figure 1 shows the "paths" generated by Algorithm 1, which we introduce in the next section. In both examples, the paths share common features, namely, that the estimated probability is large for the first few values of k, but then decreases afterwards. Interestingly, in Example 2, the curves reach levels very close to zero shortly after $k = 3$, which is the number of important covariates here. Crucially, the subset corresponding to $k = 3$ contains the first three covariates



(a) Example 1

(b) Example 2

Figure 1. Estimated probabilities corresponding to the k-element sets that appear to be the most highly correlated to the response based on subsamples. On the x-axis, k denotes the number of elements in a set. On the y-axis we have the estimated probability corresponding to the most frequently occurring subset of covariates of size k. The three different lines in each example correspond to a different subsample size used to generate paths (see Section 2).

(X_{i1}, X_{i2}, X_{i3}), which are relevant in this example. This observation suggests that paths such as those presented in Figure 1 may be used to identify how many and which variables are important, and, hence, may be used for variable selection.

2. Methodology of RBVS

In this section, we introduce the RBVS algorithm and its extension. The main purpose of RBVS is to find the set of *top-ranked* variables, which we define formally here.

2.1. Notation

Hereafter, $|\mathcal{A}|$ denotes the number of elements in a set $\mathcal{A}$. For every $k = 0, \ldots, p$ (where p grows with n), we denote $\Omega_{n,k} = \{\mathcal{A} \subset \{1, \ldots, p\} : |\mathcal{A}| = k\}$. In the remainder of the paper, we suppress the dependence of $\Omega_{n,k}$ on p (and thus n) for notational convenience, and simply write $\Omega_{n,k} \equiv \Omega_k$. For any $\mathcal{A} \in \Omega_k$, $k = 1, \ldots, p$, we define the probability of its being ranked at the top by a given ranking method as

$$\pi_n(\mathcal{A}) = \mathbb{P}\left(\{R_{n1}(\mathbf{Z}_1, \ldots, \mathbf{Z}_n), \ldots, R_{n,|\mathcal{A}|}(\mathbf{Z}_1, \ldots, \mathbf{Z}_n)\} = \mathcal{A}\right). \qquad (2.1)$$

For $k = 0$, we set $\pi_n(\mathcal{A}) = \pi_n(\emptyset) = 1$. Furthermore, for any integer m satisfying $1 \le m \le n$, we define

$$\pi_{m,n}(\mathcal{A}) = \mathbb{P}\left(\{R_{n1}(\mathbf{Z}_1,\ldots,\mathbf{Z}_m),\ldots,R_{n,|\mathcal{A}|}(\mathbf{Z}_1,\ldots,\mathbf{Z}_m)\} = \mathcal{A}\right). \tag{2.2}$$

Here, we are interested in the probability of being ranked at the top using partial observations. Note that the random samples in our framework can be viewed as forming a triangular array; thus, a double subscript is used in the definition above.

2.2. Definition of k-top-ranked, locally top-ranked, and top-ranked sets

Given a ranking scheme, we define the set of important variables in the context of variable rankings.

Definition 2. $\mathcal{A} \in \Omega_k$ (with $k \in \{0,\ldots,p-1\}$) is k-top-ranked if $\limsup_{n\to\infty} \pi_n(\mathcal{A}) > 0$.

Definition 3. $\mathcal{A} \in \Omega_k$ is said to be locally top-ranked if it is k-top-ranked and a $k+1$-top-ranked set does not exist; i.e., $\limsup_{n\to\infty} \pi_n(\mathcal{A}) = 0$, for all $\mathcal{A} \in \Omega_{k+1}$.

Definition 4. $\mathcal{A} \in \Omega_k$ is said to be top-ranked if it is locally top-ranked, and there do not exist any other locally top-ranked sets $\mathcal{A}' \in \Omega_{k'}$, for any $k' < k$. It is unique when the existence of another top-ranked set $\mathcal{A}' \in \Omega_k$ implies $\mathcal{A} = \mathcal{A}'$.

Some remarks are in order. First, Definition 2 formalizes the statement that $\mathcal{A}$ appears at the top of the ranking with non-negligible probability. We use limit-supremum in the definitions above, because $\lim_{n\to\infty} \pi_n(\mathcal{A})$ might not exist in general. Furthermore, we consider $\limsup_{n\to\infty} \pi_n(\mathcal{A}) > 0$ in Definition 2, because in some scenarios, it is strictly less than one. In Example 2, for instance, X_1, X_2, and X_3 have an equal impact on Y. Hence, under a reasonable ranking scheme (e.g., via marginal correlations), $\lim_{n\to\infty} \pi_n(\mathcal{A}) = 1/3$, for $k = 1$ and $\mathcal{A} = \{1\}, \{2\}, \{3\}$.

Second, in carefully constructed examples, it can be shown that locally top-ranked sets might exist for different values of k, where k is allowed to grow with n. For instance, suppose that $Y_i = \sum_{j=1}^{\lfloor p/3\rfloor} 2X_{ij} + \sum_{j=\lfloor p/3\rfloor+1}^{\lfloor 2p/3\rfloor} X_{ij} + \varepsilon_i$, where $(X_{i1},\ldots,X_{ip}) \sim \mathcal{N}(0, I_p)$ and $\varepsilon_i \sim \mathcal{N}(0,1)$. Then, using marginal correlations, it is easy to see that both $\{1,\ldots,\lfloor p/3\rfloor\}$ and $\{1,\ldots,\lfloor 2p/3\rfloor\}$ are locally top-ranked. Nevertheless, this issue can be handled by selecting the smallest k in Definiton 4. The appropriateness of this definition is demonstrated in Section 2.3.

Third, although the top-ranked set is unique under our assumptions (see Section 2.3), this does not imply that other k-top-ranked sets are unique as well.

In Example 2 again, we observe that $\{1\}$, $\{2\}$, and $\{3\}$ are 1-top-ranked, and $\{1,2\}$, $\{1,3\}$, and $\{2,3\}$ are 2-top-ranked. However, the top-ranked set is unique and equal to $\{1,2,3\}$.

Finally, note that for any given $\{\mathbf{Z}_i\}_{i=1}^n$, $1 = \sum_{\mathcal{A}\in\Omega_k} \mathbf{1}_{\{R_{n1}(\mathbf{Z}_1,\ldots,\mathbf{Z}_n),\ldots, R_{nk}(\mathbf{Z}_1,\ldots,\mathbf{Z}_n)\}=\mathcal{A}\}}|\{\mathbf{Z}_i\}_{i=1}^n = \sum_{\mathcal{A}\in\Omega_k} \mathbb{P}(\{R_{n1}(\mathbf{Z}_1,\ldots,\mathbf{Z}_n),\ldots,R_{nk}(\mathbf{Z}_1,\ldots,\mathbf{Z}_n)\} = \mathcal{A}\{\mathbf{Z}_i\}_{i=1}^n)$. By taking the expection over $\{\mathbf{Z}_i\}_{i=1}^n$ on both sides, we have that $\sum_{\mathcal{A}\in\Omega_k} \pi_n(\mathcal{A}) = 1$ for every k and n, and hence $\max_{\mathcal{A}\in\Omega_k} \pi_n(\mathcal{A}) \geq 1/\binom{p}{k}$, for every $k = 1,\ldots,p$. In particular, if p were bounded in n, the top-ranked set (as well as the locally top-ranked sets) would not exist. Therefore, we restrict ourselves to the case of p diverging with n (but allowing for both $p \leq n$ and $p > n$). In Section 3, we show that RBVS works well empirically when p is comparable to or much larger than n.

2.3. Top-ranked set for a class of variable rankings

The top-ranked set defined in Definition 4 exists for a wide class of variable rankings, as we show in Proposition 1 below. Let ω_j, for $j = 1,\ldots,p$, be a measure of the contribution of each X_j to the response at the population level. Note that ω_j could depend on the distribution of $\mathbf{Z} = (Y, X_1,\ldots,X_p)$ (and, thus, on n, because p changes with n), and so could, in theory, change with n. However, we suppress this dependence in the notation, for simplicity. Furthermore, let $\hat{\omega}_j = \hat{\omega}_j(\mathbf{Z}_1,\ldots,\mathbf{Z}_n)$ be an estimator of ω_j. We make the following assumptions.

(C1) $\mathbf{Z}_1,\ldots,\mathbf{Z}_n$ are independent. For some $\vartheta > 0$ and any $c_\vartheta > 0$, we have

$$\max_{j=1,\ldots,p} \mathbb{P}\left(|\hat{\omega}_j - \omega_j| \geq c_\vartheta n^{-\vartheta}\right) \leq C_\vartheta \exp\left(-n^\gamma\right),$$

where the constants $C_\vartheta, \gamma > 0$ do not depend on n.

(C2) The index set of important variables is denoted as $\mathcal{S} \subset \{1,\ldots,p\}$. $\mathcal{S}$ does not depend on n or p, and could potentially be an empty set.

(C3) For every $a \notin \mathcal{S}$, there exists $\mathcal{M}_a \subset \{1,\ldots,p\}\backslash\mathcal{S}$, such that $a \in \mathcal{M}_a$, the distribution of $\{\hat{\omega}_j\}_{j\in\mathcal{M}_a}$ is exchangeable, and $|\mathcal{M}_a| \underset{n}{\to} \infty$.

(C4) There exists $\eta \in (0,\vartheta]$, where ϑ is defined in (C1), and $c_\eta > 0$, such that $\min_{j\in\mathcal{S}} \omega_j - \max_{j\notin\mathcal{S}} \omega_j \geq c_\eta n^{-\eta}$ uniformly in n.

(C5) The number of covariates $p \leq C_1 \exp\left(n^{b_1}\right)$, where $0 < b_1 < \gamma$ and γ is defined in (C1).

Condition (C1) is a concentration bound that holds for a wide range of measures. A few examples are listed below. The sample correlation coefficient satisfies (C1) when the data follow a multivariate normal distribution (Kalisch and Bühlmann (2007, Lemma 1)), or when $Y, X_1, \ldots, X_p$ are uniformly bounded (Delaigle and Hall (2012, Thm. 1)), which follows from the Bernstein inequality. Li et al. (2012), in their Theorem 2, demonstrate that Kendall's τ meets (C1) under the marginally symmetric condition and the multi-modal condition. Distance correlation satisfies (C1) under regularity assumptions on the tails of the distributions of X_j and Y (Li, Zhong and Zhu (2012, Thm. 1)). Both the Lasso and the Dantzig selector (Candes and Tao (2007)) estimates of the regression coefficients in the linear model meet (C1), with additional assumptions on the covariates, and on the sparsity of the regression coefficients (Lounici (2008, Thm. 1)).

Condition (C2) implies that $|\mathcal{S}|$ is bounded in n, which, combined with diverging p, implies that the number of important covariates is small. This, together with Conditions (C3) and (C4), can be viewed as a variant of the well-known "sparsity" assumption.

We are interested in scenarios in which a few variables have a large impact on the response, and many variables have a similar impact on the response; in the latter case, the variables can only have zero or a small impact on the response. Here, the first part is characterized by Condition (C3), and the second part is characterized by Condition (C4).

Condition (C3) can be linked to the sparsity assumption, which requires that only a few covariates have a significant impact on the response. In our framework, these are $\{X_j\}_{j \in \mathcal{S}}$. For all remaining covariates, the sparsity may require that their corresponding regression coefficients be zero. On the other hand, in (C3), each X_a, with $a \notin \mathcal{S}$, may contribute to Y. However, heuristically, it is difficult to select a particular X_a, with $a \notin \mathcal{S}$, because many covariates have the same impact on Y. As such, none of these would be included in our framework. We believe that this assumption is likely to be met, at least approximately (in the sense that large groups of covariates exhibit a similar small impact on the response), especially for large dimensions p. In addition, note that Meinshausen and Bühlmann (2010) use the exchangeability assumption on the selection of noise variables. However, it concerns a variable selection procedure, whereas we impose restrictions on the measure $\hat{\omega}_j$. The main difference between their assumption and (C3) is that they require that all covariates be equally likely to be selected, whereas we allow for many groups, within which each variable has the same impact on Y. In the remainder of the paper, we refer to the elements of set $\mathcal{S}$ as "relevant and important" (or just "important") variables, the covariates with zero impact on the response as "irrelevant" variables, and the rest as "relevant but unimportant" variables.

Furthermore, in Condition (C4), we assume that there is a gap between $\min_{j\in\mathcal{S}}\omega_j$ and $\max_{j\notin\mathcal{S}}\omega_j$, which separates the important variables from the remainder (i.e., irrelevant, and relevant but unimportant). This gap is allowed to decrease slowly to zero. Conditions (C1) and (C4) together imply that the ranking based on $\hat{\omega}_j$ satisfies the SIS property (Fan and Lv (2008)).

Finally, Condition (C5) restricts the maximum number of covariates, but allows an ultra high-dimensional setting where the number of covariates grows exponentially with n^{b_1}, for some $b_1 > 0$.

Proposition 1. *Let* $\mathbf{R}_n$ *be a variable ranking based on* $\hat{\omega}_j$*, for* $j = 1,\dots,p$*, given in Definition* 1*. Under conditions* (C1)–(C5)*, the unique top-ranked set defined in Definition* 4 *exists and is equal to* $\mathcal{S}$*.*

Proposition 1 can be applied to establish a link between the top-ranked set and the set of important variables, understood in a classic way. Consider the linear regression model $Y = \sum_{j=1}^{p}\beta_j X_j + \varepsilon$, where β_j is an unknown regression coefficient, X_j is a random predictor, and ε is an error term. In this model, the top-ranked set could coincide with $\{k : \beta_k \neq 0\}$. To see that, we consider the variable ranking based on $\hat{\omega}_j = \widehat{\mathrm{Cor}}(Y, X_j)$, which satisfies (C1) when $(Y, X_1, \dots, X_p)$ is, for example, Gaussian (Kalisch and Bühlmann (2007)). Condition (C3) is met when, for example, $\widehat{\mathrm{Cor}}(Y, X_j) = \rho$, for some $\rho \in (-1, 1)$ and all j such that $\beta_j = 0$, and $p \underset{n}{\to} \infty$. Imposing some restrictions on the correlations between the covariates, we also guarantee that (C4) holds. Finally, provided that $p \underset{n}{\to} \infty$ no faster than indicated in (C5), Proposition 1 implies that $\{k : \beta_k \neq 0\}$ is the unique top-ranked set.

Nevertheless, note that the top-ranked set only contains relevant and important variables with respect to the chosen measure. Relevant but unimportant variables (unimportant via exchangeability, in the sense of (C3), so not necessarily having small impact in the traditional sense) are not included in the top-ranked set. For instance, in the setting of Example 2, but with $Y_i = 5X_{i1} + 5X_{i2} + 5X_{i3} + \sum_{j=\lceil p/2\rceil+1}^{p}\beta X_{ij} + \varepsilon_i$ and $|\beta| < 5$, the top-ranked set via marginal correlations is still $\{1, 2, 3\}$, even though for all $j = 1, 2, 3, \lceil p/2\rceil + 1 \dots, p$, X_j has a nonnegligible impact on Y. For other work on overcoming the issue of small relevant covariates, see Barut, Fan and Verhasselt (2016). In particular, Barut, Fan and Verhasselt (2016) also deal with the issue of marginally uncorrelated covariates, which we address by proposing an iterative approach in Section 2.7. See also our simulation examples in this direction in Section 3.

2.4. Main idea of RBVS

Now, assume the existence and uniqueness of the top-ranked set $\mathcal{S}$. To construct an estimate of $\mathcal{S}$, we introduce the estimators of $\pi_{m,n}(\mathcal{A})$ defined by (2.2) using a variant of the m-out-of-n bootstrap (Bickel, Götze and van Zwet (2012)).

Definition 5. Fix $m \in \{1, \ldots, n\}$ and $B \in \mathbb{N}$, and set $r = \lfloor n/m \rfloor$. For any $b = 1, \ldots, B$, let $I_{b1}, \ldots, I_{br}$ be mutually exclusive subsets of $\{1, \ldots, n\}$ of size m, drawn uniformly from $\{1, \ldots, n\}$, without replacement. Assume that the sets of subsamples are independently drawn for each b. For any $\mathcal{A} \in \Omega_k$, we estimate $\pi_{m,n}(\mathcal{A})$ as the fraction of subsamples in which $\mathcal{A}$ appeared at the top of the ranking; that is,

$$\hat{\pi}_{m,n}(\mathcal{A}) = B^{-1} \sum_{b=1}^{B} r^{-1} \sum_{j=1}^{r} \mathbf{1}_{\left\{\mathcal{A}=\left\{R_{n,1}(\{\mathbf{Z}_i\}_{i \in I_{bj}}),\ldots,R_{n,|\mathcal{A}|}(\{\mathbf{Z}_i\}_{i \in I_{bj}})\right\}\right\}}.$$

In general, $\pi_{m,n}(\mathcal{A})$ can differ from $\pi_n(\mathcal{A})$. However, we show in Section 2.6 that $\pi_{m,n}(\mathcal{A})$ and $\pi_n(\mathcal{A})$ are similar (in term of their magnitudes) for the same subsets, provided that m is not too small. This, combined with some bounds on the estimation accuracy of $\hat{\pi}_{m,n}(\mathcal{A})$, imply that $\hat{\pi}_{m,n}(\mathcal{A})$ can be used to find the k-top-ranked sets from the data. In practice, the number of elements in $\mathcal{S}$ is typically unknown. Thus, we need to consider subsets of any size in our estimation procedure. From our argument above, for n sufficiently large, the top-ranked set $\mathcal{S}$, given its existence and uniqueness, will have to be one of the following sets for a particular $k \in \{0, 1, \ldots, p-1\}$, where

$$\mathcal{A}_{k,m} = \operatorname{argmax}_{\mathcal{A} \in \Omega_k} \pi_{m,n}(\mathcal{A}). \tag{2.3}$$

We define the corresponding sample version of $\mathcal{A}_{k,m}$ as

$$\hat{\mathcal{A}}_{k,m} = \operatorname{argmax}_{\mathcal{A} \in \Omega_k} \hat{\pi}_{m,n}(\mathcal{A}). \tag{2.4}$$

To motivate the use of the resampling scheme, note that some irrelevant covariates (i.e., those with zero impact on the response) can spuriously exhibit a large empirical impact on the response, especially when $p \gg n$. The resampling-based set probability estimation could provide estimates that are more stable, helping to identify variables that appear nonspuriously at the top of the analyzed rankings. Moreover, to understand the importance of the parameter B introduced in Definition 5, note that $\max_{\mathcal{A}\in\Omega_k}\hat{\pi}_{m,n}(\mathcal{A}) \geq (Br)^{-1}$. For moderate sample sizes, r may not be large, while we expect the majority of $\pi_{m,n}(\mathcal{A})$ to be small, smaller even than $1/r$. In this situation, the estimation error of $\max_{\mathcal{A}\in\Omega_k}\hat{\pi}_{m,n}(\mathcal{A})$ with $B=1$ is expected to be high, and the estimate of $\hat{\mathcal{A}}_{k,m}$ could be inaccurate. A moderate value of B aims to bring $\hat{\mathcal{A}}_{k,m}$ closer to its population counterpart $\mathcal{A}_{k,m}$. The theoretical requirements on m and B are given in Section 2.6; our suggestions for the choices of m and B are provided in Section 3.3.

In practice, we do not know the size of the top-ranked set $s=|\mathcal{S}|$; thus, it should be estimated as well. One possibility is to apply the hard thresholding rule and set

$$\hat{s}_\zeta = \min\left\{k:\ \hat{\pi}_{m,n}\left(\hat{\mathcal{A}}_{k+1,m}\right) \leq \zeta\right\},$$

where $\zeta > 0$ is a prespecified threshold. This approach could be justified by the existence of the asymptotic gap between $\pi_{m,n}(\mathcal{A}_{s+1,m})$ and $\pi_{m,n}(\mathcal{A}_{s,m})$. However, the magnitude of this difference is typically unknown, and can be rather small, which makes the choice of ζ difficult. As an alternative, we propose estimating s by

$$\hat{s} = \operatorname{argmin}_{k=0,\dots,k_{\max}-1} \frac{\hat{\pi}^{\tau}_{m,n}(\hat{\mathcal{A}}_{k+1,m})}{\hat{\pi}_{m,n}(\hat{\mathcal{A}}_{k,m})}, \tag{2.5}$$

for some prespecified $\tau \in (0,1]$, and some prespecified large integer $k_{\max}$. The intuition of this choice is explained as follows. Note that

$$\frac{\hat{\pi}^{\tau}_{m,n}(\hat{\mathcal{A}}_{k+1,m})}{\hat{\pi}_{m,n}(\hat{\mathcal{A}}_{k,m})} = \left(\frac{\hat{\pi}_{m,n}(\hat{\mathcal{A}}_{k+1,m})}{\hat{\pi}_{m,n}(\hat{\mathcal{A}}_{k,m})}\right)^{\tau}\left(\frac{1}{\hat{\pi}_{m,n}(\hat{\mathcal{A}}_{k,m})}\right)^{1-\tau}.$$

When $\tau = 1$, we look for k, where $\hat{\pi}_{m,n}(\hat{\mathcal{A}}_{k+1,m})$ decreases in proportion the most drastically. For a general τ, in essence, we look for k that is a trade-off between the latter case and the hard thresholding rule (by not permitting $\hat{\pi}_{m,n}(\hat{\mathcal{A}}_{k,m})$ to be too small). Furthermore, because we assume that $|\mathcal{S}|$ is much smaller than p, it is computationally more efficient to optimize over $\{0,\dots,k_{\max}\}$ rather than $\{0,\dots,p-1\}$ in (2.5). In Section 2.6, we show that this approach leads to consistent estimations of $\mathcal{S}$.

2.5. The RBVS algorithm and its computational cost

The RBVS algorithm consists of four main steps. Its pseudocode is described in Algorithm 1. In Step 1, we draw subsamples from the data using the subsampling scheme introduced in Definition 5. In Step 2, for each subsample drawn, we estimate ω_j based on the subsamples I_{bl}, and sort the sample measures $\left\{\hat{\omega}_j(\{\mathbf{Z}_i\}_{i\in I_{bl}})\right\}_{j=1}^{p}$ in nonincreasing order to find $\mathbf{R}_n(\{\mathbf{Z}_i\}_{i\in I_{bl}})$, as defined in Definition 1. In Step 3, for each $k = 1,\ldots,k_{\max}$, we find $\hat{\mathcal{A}}_{k,m}$, the k-element set that occurs most frequently at the top of $\mathbf{R}_n(\{\mathbf{Z}_i\}_{i\in I_{bl}})$, for all $b = 1,\ldots,B$ and $l = 1,\ldots,r$. In Step 4, probabilities $\hat{\pi}_{m,n}(\hat{\mathcal{A}}_{k,m})$ are used to find $\hat{s}$, the estimate of the size of the top-ranked set; $\hat{\mathcal{S}} = \hat{\mathcal{A}}_{\hat{s},m}$ is returned as the final estimate of $\mathcal{S}$.

Algorithm 1 The RBVS algorithm

Require: Random sample $\mathbf{Z}_i = (Y_i, X_{i1},\ldots,X_{ip})$, $i = 1,\ldots,n$, subsample size m with $1 \le m \le n$, positive integers $k_{\max}$, B, and $\tau \in (0,1]$.
Ensure: The estimate of the set of important variables $\hat{\mathcal{S}}$.
procedure RBVS($\mathbf{Z}_1,\ldots,\mathbf{Z}_n, m, B, k_{\max}, \tau$)
 Step 1 Let $r = \lfloor n/m \rfloor$. For each $b = 1,\ldots,B$, draw uniformly without replacement m-element subsets $I_{b1},\ldots,I_{br} \subset \{1,\ldots,n\}$.
 Step 2 Calculate $\hat{\omega}_j(\{\mathbf{Z}_i\}_{i\in I_{bl}})$ and the corresponding variable ranking $\mathbf{R}_n(\{\mathbf{Z}_i\}_{i\in I_{bl}})$ for all $b = 1,\ldots,B$, $l = 1,\ldots,r$ and $j = 1,\ldots,p$.
 Step 3 For $k = 1,\ldots,k_{\max}$, find $\hat{\mathcal{A}}_{k,m}$ given by (2.4) and compute $\hat{\pi}_{m,n}(\hat{\mathcal{A}}_{k,m})$.
 Step 4 Find $\hat{s} = \operatorname{argmin}_{k=0,\ldots,k_{\max}-1} \hat{\pi}^{\tau}_{m,n}(\hat{\mathcal{A}}_{k+1,m})/\hat{\pi}_{m,n}(\hat{\mathcal{A}}_{k,m})$.
 return $\hat{\mathcal{S}} = \hat{\mathcal{A}}_{\hat{s},m}$.
end procedure

We now investigate the computational complexity of Algorithm 1. Denote by $c(n,p)$ the computational cost of evaluating $\hat{\omega}_j$, for all $j = 1,\ldots,p$, using n observations. First, performing B random partitions of n observations into r subsets (each of size m and dimension p) takes $O(Bn)$ operations. Furthermore, finding all $\hat{\omega}_j$ for all Br different subsets takes $c(m,p)\times Br$ manipulations. Next, evaluating the rankings based on each subset (for the $k_{\max}$ highest only) takes $O(p + k_{\max}\log(k_{\max}))$ operations, using the selection algorithm and the QuickSort partition scheme. Thus, doing so for all Br subsets takes $O\big((p + k_{\max}\log(k_{\max}))Br\big)$ operations. Moreover, Step 3 can be performed in $O(Brk_{\max}^2)$ basic operations (see the Supplementary Material for more information). Finally, the remaining step requires $O(k_{\max})$ operations. Consequently, the total computational complexity of Algorithm 1 is $c(m,p)\times Br + O(\max\{p, k_{\max}^2\}Br)$. For our recommended choices of $k_{\max}$ and m, see Section 3.3.

2.6. Theoretical results

Under the theoretical framework below, we show that Algorithm 1 recovers the top-ranked set given by Definition 4 with probability tending to 1 as $n \to \infty$. We make the following assumptions.

(A1) $\mathbf{Z}_1, \ldots, \mathbf{Z}_n$ are independent. For some $\vartheta > 0$ and any $c_\vartheta > 0$, we have that for any n,

$$\max_{j=1,\ldots,p} \mathbb{P}\left(|\hat{\omega}_j(\mathbf{Z}_1, \ldots, \mathbf{Z}_m) - \omega_j| \geq c_\vartheta m^{-\vartheta}\right) \leq C_\vartheta \exp\left(-m^\gamma\right),$$

where constants $C_\vartheta, \gamma > 0$, and m (as a function of n) are specified in Assumption (A3) below.

(A2) There exist constants $C_1 > 0$ and $0 < b_1 < \gamma$, with γ as in (A1), s.t. $p \leq C_1 \exp\left(n^{b_1}\right)$.

(A3) The subsample size m goes to infinity at rate n^{b_2}, with $0 < b_2 < 1$ and $\gamma b_2 - b_1 > 0$, where γ is defined in (A1) and b_1 is defined in (A2).

(A4) The index set of important variables is denoted as $\mathcal{S} \subset \{1, \ldots, p\}$. $\mathcal{S}$ does not depend on n (or p). Denote $s = |\mathcal{S}|$. For every $a \notin \mathcal{S}$, there exists $\mathcal{M}_a \subset \{1, \ldots, p\} \backslash \mathcal{S}$, such that $a \in \mathcal{M}_a$, the distribution of $\{\hat{\omega}_{j,m}\}_{j \in \mathcal{M}_a}$ is exchangeable, and $\min_{a \notin \mathcal{S}} |\mathcal{M}_a| \geq C_3 n^{b_3}$, with $C_3 > 0$ and $b_3/2 < 1 - b_2 < b_3$, where b_2 is defined in (A3).

(A5) There exists $\eta \in (0, \vartheta]$, where ϑ is defined in (C1), and $c_\eta > 0$, such that $\min_{j \in \mathcal{S}} \omega_j - \max_{j \notin \mathcal{S}} \omega_j \geq c_\eta m^{-\eta}$ uniformly in n. (Here, m, as in (A3), depends solely on n.)

(A6) The number of random draws B is bounded in n.

(A7) The maximum subset size $k_{\max} \in [s, C_4 n^{b_4}]$, with $C_4 > 0$ and b_4 satisfying $b_3 > b_4$, where b_3 is defined in (A4).

Assumptions (A1), (A2), (A4), and (A5) can be viewed as natural extensions or restatements of (C1)–(C5) to the case in which $\hat{\omega}_j$ is evaluated using m out of n observations only. They are formally repeated here for the sake of clarity. Note that the last part of (A4) implies a lower bound on p ($\geq C_3 n^{b_3}$).

Assumption (A3) establishes the required size of the subsample, m, and implies that both $n/m \underset{n}{\to} \infty$ and $m \underset{n}{\to} \infty$. Such conditions are common in the literature on bootstrap resampling and U-statistics; see, for instance, Bickel, Götze and van Zwet (2012), Götze and Račkauskas (2001), or Hall and Miller (2009b). Finally, (A6) and (A7) impose conditions on B and $k_{\max}$, respectively.

Theorem 1. *Suppose that assumptions* (A1)-(A7) *hold. Write* $\hat{\mathcal{S}} = \hat{\mathcal{A}}_{\hat{s},m}$*, where* $\hat{\mathcal{A}}_{\hat{s},m}$ *is given by* (2.4) *and* (2.5)*. Then, for any* $\tau \in (0,1]$*, there exist constants* $\beta, C_\beta > 0$*, such that* $\mathbb{P}\left(\hat{\mathcal{S}} \neq \mathcal{S}\right) = o\left(\exp\left(-C_\beta n^\beta\right)\right) \underset{n}{\to} 0$.

The above theorem states that $\hat{\mathcal{S}}$ obtained by RBVS is a consistent estimator of the top-ranked set $\mathcal{S}$, where $\mathbb{P}\left(\hat{\mathcal{S}} = \mathcal{S}\right)$ goes to one at an exponential rate. The proof can be found in the Appendix, and empirical evidence is provided in Section 3.

2.7. Iterative extension of RBVS (IRBVS)

In the presence of strong dependence between covariates, the measure $\hat{\omega}_j$ may fail to detect some important variables. For instance, a covariate may be jointly related, but marginally unrelated to the response (see Fan and Lv (2008), Barut (2013), or Barut, Fan and Verhasselt (2016)). Under such a setting, the estimated top-ranked set may only contain a subset of the important variables. To overcome this problem, we propose IRBVS, an iterative extension of Algorithm 1. The pseudocode of IRBVS is given in Algorithm 2. In each iteration, IRBVS removes the linear effect on the response of the variables found at the previous iteration. Therefore, it is applicable when the relationship between Y and X_j is at least approximately linear. Nevertheless, it is possible to extend this methodology. For instance, Barut (2013) and Barut, Fan and Verhasselt (2016) demonstrate how to remove the impact of a given set of covariates on the response in generalized linear models.

Iterative extensions of variable screening methodologies are frequently proposed in the literature; see, for instance, Fan and Lv (2008), Zhu et al. (2011), or Li et al. (2012). A practical advantage of the IRBVS algorithm over its competitors is that it does not require that we specify of the number of variables added at each iteration or the total number of iterations. Moreover, IRBVS appears to offer better empirical performance than other iterative methods, such as ISIS (Fan and Lv (2008)); see Section 3.

2.8. Relations to selected existing methodologies

In this section, we provide a brief overview of the differences between Algorithm 1, StabSel of Meinshausen and Bühlmann (2010), and the bootstrap

Algorithm 2 The IRBVS algorithm

Require: Random sample $\mathbf{Z}_i = (Y_i, X_{i1}, \ldots, X_{ip})$, $i = 1, \ldots, n$, subsample size m with $1 \le m \le n$, positive integers $k_{\max}$, B , and $\tau \in (0, 1]$.
Ensure: The estimate of the set of important variables $\hat{\mathcal{S}}$.
procedure IRBVS($\mathbf{Z}_1, \ldots, \mathbf{Z}_n, m, B, k_{\max}, \tau$)
  Initialise $\hat{\mathcal{S}} = \emptyset$.
  repeat
    Step 1 Let $(Y_1^*, \ldots, Y_n^*)'$ and $(X_{1j}^*, \ldots, X_{nj}^*)'$ (for $j = 1, \ldots, p$) be the residual vectors left after projecting $(Y_1, \ldots, Y_n)'$ and $(X_{1j}, \ldots, X_{nj})'$ onto the space spanned by the covariates with indices in $\hat{\mathcal{S}}$. (NB. for any $j' \in \mathcal{S}$, $(X_{1j'}^*, \ldots, X_{nj'}^*)' = \mathbf{0}$.) Set $\mathbf{Z}_i^* = (Y_i^*, X_{i1}^*, \ldots, X_{ip}^*)$ for $i = 1, \ldots, n$.
    Step 2 Calculate $\hat{\mathcal{S}}^* = \mathrm{RBVS}(\mathbf{Z}_1^*, \ldots, \mathbf{Z}_n^*, m, B, k_{\max}, \tau)$.
    Step 3 Set $\hat{\mathcal{S}} := \hat{\mathcal{S}}^* \cup \hat{\mathcal{S}}$.
  until $\hat{\mathcal{S}}^* = \emptyset$
  return $\hat{\mathcal{S}}$.
end procedure

ranking approach of Hall and Miller (2009a).

2.8.1. StabSel

Denote the selection probabilities by $\pi_j = \mathbb{P}\left(j \in \hat{S}^\lambda\right)$, for $j = 1, \ldots, p$, where $\hat{S}^\lambda$ is the set of variables selected by a chosen variable selection technique, with its tuning parameter set to λ. StabSel has two aims: first, to select covariates that the initial procedure selects with a high probability; and second, to bound the average number of false positives (denoted by $\mathrm{E}\, V$) below some prespecified level $\alpha > 0$. For this purpose, Meinshausen and Bühlmann estimate π_j and select variables for which $\hat{\pi}_j > \pi$, where $\pi \in (1/2, 1)$ is a prespecified threshold. To control $\mathrm{E}\, V$, one can set λ such that $|\hat{S}^\lambda| \le q$, where $q \in \{1, \ldots, p\}$ depends on π, and α is adjusted to ensure $\mathrm{E}\, V \le \alpha$. The exact formula for q and other possible ways of controlling $\mathrm{E}\, V$ are given in Meinshausen and Bühlmann (2010).

In contrast to StabSel, which needs a variable selection procedure, RBVS selects variables based on a variable ranking. In particular, in our approach, we consider the joint probabilities $\pi_{m,n}(\mathcal{A})$, whereas StabSel uses only marginal probabilities. The estimates of the joint probabilities can be used to determine the number of important covariates at the top of the variable ranking, without the specification of a threshold, as we demonstrate in Section 2.6. Consequently, we believe that RBVS can be viewed as more automatic and "less marginal" than StabSel.

Table 1. Computational complexity of Algorithm 1 and its competitors. The cost of the base learner in relation to the sample size n and the number of variables p is denoted by $c(n,p)$; B is the number of subsamples used in StabSel and RBVS. Parameters for SIS, StabSel, and RBVS are set to the recommended values. For SIS, we assume that k-fold CV is used after the screening step.

k-fold CV	SIS	StabSel	RBVS
$k \times c\left(\frac{(k-1)n}{k}, p\right)$	$O(np) + k \times c\left(\frac{(k-1)n}{k}, \frac{n}{\log(n)}\right)$	$B \times c\left(\frac{n}{2}, p\right) + O(Bp)$	$B \times c(\frac{n}{2}, p) + O(\max\{n^2, p\}B)$

2.8.2. The bootstrapped rankings

Let r_{nj} be the position of the jth covariate in the variable ranking $\mathbf{R}_n = (R_{n1}, \ldots, R_{np})$. Mathematically, assuming there is no tie, $r_{nj} = l$ if and only if $R_{nl} = j$. To identify important covariates based on $\mathbf{R}_n$, Hall and Miller (2009a) compute $[r_{nj}^-, r_{nj}^+]$, denoting two-sided, equal-tiled, percentile-method bootstrap confidence intervals for r_{nj} at a significance level α. A variable is considered influential when r_{nj}^+ is lower than some prespecified cutoff level c, for instance, $c = p/2$. The number of variables selected by the procedure of Hall and Miller (2009a) depends therefore on α and c and the "marginal" confidence intervals $[r_{nj}^-, r_{nj}^+]$. By contrast, RBVS is based on the joint probabilities $\pi_{m,n}(\mathcal{A})$, and does not require the specification of a threshold or a significance level.

2.8.3. Computational complexity of the related methods

Table 1 summarizes the computational complexity of Algorithm 1 (with $m = \lfloor n/2 \rfloor$) and its competitors, SIS (Fan and Lv (2008)) and StabSel (Meinshausen and Bühlmann (2010)). For reference, we include the computational complexity of the k-fold cross-validation (k-fold CV), which is frequently used to find optimal parameters for the Lasso, MC+, and SIS, among others. The computational complexity of the method proposed by Hall and Miller (2009a) is comparable to that of StabSel, and hence is omitted from this comparison. In theory, SIS requires the least computational resources, especially in the case of $p \gg n$. Simple k-fold cross-validation has the second lowest computational complexity. For $n > \sqrt{p}$, StabSel is theoretically quicker than RBVS; however, the common factor $B \times c\,(n/2, p)$ typically dominates both $O(Bp)$ and $O(\max\{p, n^2\})$, and our experience suggests that StabSel and RBVS usually require similar computational resources.

3. Simulation Study

To facilitate a comparison of the different methods, we focus on linear models in this section. We also provide two real-data examples in the Supplementary Material.

3.1. Simulation models

Model (A) Taken from Fan and Lv (2008): $Y_i = 5X_{i1}+5X_{i2}+5X_{i3}+\varepsilon_i$, where $(X_{i1},\ldots,X_{ip})$ are independent and identically distributed (i.i.d.) observations from $\mathcal{N}(0,\Sigma)$ and ε_i follow $\mathcal{N}(0,1)$. The covariance matrix satisfies $\Sigma_{jj}=1$, for $j=1,\ldots,p$, and $\Sigma_{jk}=\rho$, $|\rho|<1$ for $k\neq j$. This is a relatively easy setting, where every important X_j is "visible" to any reasonable marginal approach, because of the highest (absolute) correlation with Y at the population level.

Model (B) Factor model taken from Meinshausen and Bühlmann (2010): $Y_i = \beta_1X_{i1}+\cdots+\beta_pX_{ip}+\varepsilon_i$, where X_{ij} follow the factor model $X_{ij}=\sum_{l=1}^{K} f_{ijl}\varphi_{il}+\theta_{ij}$, with f_{ijl}, φ_{il}, θ_{ij}, ε_i i.i.d. $\mathcal{N}(0,1)$. We set $K=2,10$. In addition, the number of $\beta_j\neq 0$ is set to $s=5$, with their indices drawn uniformly without replacement, and their values are i.i.d. uniformly distributed on $[0,5]$. In this model, some of the nonzero regression coefficients are potentially small; thus, the corresponding covariates might be difficult to detect.

Model (C) Modified from **Model (A)**: the same covariate and noise structure as **Model (A)**, but with $Y_i = 5X_{i1}+5X_{i2}+5X_{i3}+\sum_{j=\lceil p/2\rceil+1}^{p}\beta X_{ij}+\varepsilon_i$, where we set $\beta = 2^{-2},2^{-1},2^{0},2^{1}$. Here, we have the important variables (i.e., the top-ranked set is $\{1,2,3\}$), relevant but unimportant variables (i.e., $\big\{\lceil p/2\rceil+1,\ldots,p\big\}$), and irrelevant variables (i.e., $\big\{4,\ldots,\lceil p/2\rceil\big\}$). The challenge is to select only the important variables. Here, we are interested in the behavior of RBVS as β gets closer to 5 (the problem becomes harder).

Model (D) Modified from Fan and Lv (2008):

$$Y_i = 5X_{i1}+5X_{i2}+5X_{i3}-15\sqrt{\rho}X_{i4}+\sum_{j=\lceil p/2\rceil+1}^{p}5p^{1/2}X_{ij}+\varepsilon_i,$$

where $(X_{i1},\ldots,X_{ip})$ are i.i.d. observations from $\mathcal{N}(0,\Sigma)$, and ε_i follow $\mathcal{N}(0,1)$. The covariance Σ is defined in **Model (A)**, except that $\Sigma_{4,k}=\Sigma_{j,4}=\sqrt{\rho}$ for $k,j=1,2,3,5,\ldots,p$. This model has two challenges. First, X_{i4} has a large contribution to Y_i, but is marginally unrelated to the response. Second, similarly to **Model (C)**, there are both important and unimportant relevant variables, and our aim is to recover only the former (i.e., those in the top-ranked set).

3.2. Simulation methods

We apply RBVS and IRBVS with the absolute values of the following measures: Pearson correlation coefficient (PC) (Fan and Lv (2008)), the regression coefficients estimated via the Lasso (Tibshirani (1996)), and the regression coefficients estimated via the MC+ algorithm (Zhang (2010)). The performance of RBVS and IRBVS with the Lasso is typically slightly worse than that of MC+ in our numerical experiments, and so is not reported here. More comprehensive numerical results can be found in Baranowski (2016).

For the competitors, we consider the standard MC+ estimator, defined as

$$\hat{\beta}_{pen} = \text{argmin}_{\beta}(n^{-1}\sum_{i=1}^{n}\left(Y_i - \sum_{j=1}^{p}\beta_j X_{ij}\right)^2 + \sum_{j=1}^{p}\text{pen}(|\beta_j|),$$

where $\text{pen}(t) = \lambda\int_0^t \max\{0,(1-x/(\gamma\lambda))\}\,dx$, and $\lambda,\gamma > 0$ are tuning parameters. Here, λ is chosen via 10-fold cross-validation, and $\gamma = 3$, as in Breheny and Huang (2011). We also consider StabSel, where we set the tuning parameters as per the recommendation of Meinshausen and Bühlmann (2010).

The final group of the techniques included in our comparison consists of SIS and its iterative extension ISIS (Fan and Lv (2008)) (and with MC+ after the screening stage). For the SIS method, we consider both the standard version of Fan and Lv (2008), based on the marginal sample correlations (MSC), and the more recent version of Chang, Tang and Wu (2013), based on the marginal empirical likelihood (MEL). Note that the standard ISIS procedure does not perform well in our experiments, because it selects a very large number of false positives. Therefore, we apply a modified version of ISIS that involves a randomization mechanism (Saldana and Feng (2018)).

We use implementation of the MC+ algorithm from the R package **ncvreg** (Breheny and Huang (2011)). For SIS-based methods, we use the R package **SIS** (Saldana and Feng (2018)).

3.3. Choice of parameters of the (I)RBVS algorithm

RBVS involves choosing several parameters, namely B, m, $k_{\max}$, and τ. Their choices are discussed below.

The B parameter has been introduced to decrease the randomness of the method. Naturally, the larger the value of B, the less the algorithm depends on a particular random draw. However, the computational complexity of RBVS increases linearly with B. In the simulation study, we take $B = 50$. Our experience suggests that little will be gained in terms of the performance of RBVS for a much larger B.

The problem of the choice of the subsample size m is more challenging. In Section 2.6, we require $m \to \infty$ at an appropriate rate, which is, however, unknown. In the finite-sample case, m cannot be too small, because it is unlikely that $\mathbf{R}_n$ based on a small sample could give a high priority to the important variables. On the other hand, when m is too large (i.e., close to n), subsamples largely overlap. In practical problems, we propose choosing $m = \lfloor n/2 \rfloor$. See also our additional simulation study in the Supplementary Material, which confirms that this choice results in good finite-sample properties of the RBVS-based methods.

From our experience, $k_{\max}$ has limited impact on the outcome of RBVS, as long as it is not too small. In all simulations conducted, $\hat{\pi}_{m,n}(\hat{\mathcal{A}}_{k,m})$, given by (2.4), reaches and stays at the level of $1/(Br)$, for some $k \leq n$; thus, we recommend $k_{\max} = \min\{n, p\}$.

Finally, our experience also suggests that RBVS is not very sensitive to the choice of τ, as long as it is not too close to zero. Here we simply take $\tau = 0.5$.

3.4. Results

Our results are reported in Tables 2–5 in terms of the average number of false positives (FP), false negatives (FN), total errors (FP+FN), and estimated $\mathbb{P}(\hat{\mathcal{S}} = \mathcal{S})$, that is, the probability (Pr) of a correct estimation of the top-ranked set.

Overall, in all settings considered here, RBVS and IRBVS, with a proper choice of measurement (such as with MC+), typically offer similar, and sometimes better performance than their competitors, such as StabSel. In general, RBVS and IRBVS tend to improve the performance of the base learners (such as Lasso or MC+). Moreover, the iterative extension, IRBVS, in many cases is able to detect variables overlooked by the pure RBVS, especially with PC.

In **Model (C)**, for fixed n and p, when $|\beta|$ is small to moderate (i.e., $\beta \in \{0.25, 0.5\}$), both RBVS and IRBVS frequently recover the top-ranked set. Nevertheless, as the value of $|\beta|$ increases, the difference between the important and unimportant relevant variables becomes smaller, making it more difficult to estimate the top-ranked set. When $\beta = 2$, these algorithms (as well as their

Table 2. **Model (A)**: the average number of false positives (FP), false negatives (FN), total errors (FP+FN), and estimated probability (Pr) of a correct selection of the top-ranked set (i.e., $P(\hat{\mathcal{S}} = \mathcal{S})$), calculated over 200 realizations. Bold: within 10% of the lowest value of FP+FN (or within 5% of the highest value of Pr).

		SIS		StabSel		RBVS		ISIS		IRBVS	
	MC+	MSC	EML	PC	MC+	PC	MC+	MSC	EML	PC	MC+
				$n = 100 \quad p = 100 \quad \rho = 0$							
FP	0.18	0.00	0.00	0.18	0.02	0.03	0.00	0.32	0.26	0.04	0.01
FN	0.00	0.00	0.00	0.00	0.00	0.10	0.00	0.00	0.00	0.08	0.00
FP+FN	0.18	**0.00**	**0.00**	0.18	0.02	0.13	**0.00**	0.32	0.26	0.12	0.01
Pr	0.88	**1.00**	**1.00**	0.82	**0.98**	0.92	**1.00**	0.91	0.92	0.94	**0.99**
				$n = 100 \quad p = 1,000 \quad \rho = 0$							
FP	0.92	0.02	0.05	0.34	0.01	0.00	0.00	0.07	0.06	0.00	0.00
FN	0.00	0.00	0.00	0.01	0.00	0.30	0.00	0.00	0.00	0.20	0.00
FP+FN	0.92	0.02	0.06	0.34	0.01	0.31	**0.00**	0.07	0.06	0.20	**0.00**
Pr	0.70	**0.99**	**0.98**	0.70	**0.99**	0.84	**1.00**	0.94	**0.95**	0.93	**1.00**
				$n = 100 \quad p = 100 \quad \rho = 0.75$							
FP	0.00	0.00	0.25	0.40	0.03	0.02	0.00	0.18	0.11	0.05	0.00
FN	0.00	0.00	0.18	0.04	0.00	1.23	0.00	0.00	0.00	1.00	0.00
FP+FN	**0.00**	**0.00**	0.43	0.44	0.03	1.25	**0.00**	0.18	0.11	1.05	**0.00**
Pr	**1.00**	**1.00**	0.84	0.64	**0.97**	0.49	**1.00**	0.94	**0.95**	0.62	**1.00**
				$n = 100 \quad p = 1,000 \quad \rho = 0.75$							
FP	0.00	0.00	2.29	0.70	0.00	0.00	0.00	0.08	0.11	0.04	0.00
FN	0.00	0.00	1.16	0.20	0.00	2.12	0.03	0.00	0.12	1.71	0.03
FP+FN	**0.00**	**0.00**	3.45	0.90	**0.00**	2.12	0.04	0.08	0.22	1.75	0.04
Pr	**1.00**	**1.00**	0.25	0.43	**1.00**	0.17	**0.98**	0.94	0.93	0.40	**0.98**

competitors) fail completely. Not surprisingly, for both RBVS and IRBVS, the estimated top-ranked set is empty, because all variables appear to be quite similar in terms of their coefficients using PC or MC+.

In contrast, MC+, SIS, and ISIS perform poorly in **Model (C)** (even when $|\beta|$ is very small), and in **Model (D)**, owing to the presence of unimportant, but relevant variables. Thus, they are not suitable for recovering the top-ranked set in these settings. Though StabSel MC+ is also very competitive in **Model (A)**–**Model (C)**, it appears to perform considerably worse than RBVS MC+ or IRBVS MC+ in **Model (D)**, especially when p is large and the covariates are highly correlated.

Finally, note that as long as the covariates are not too highly correlated, the performance of IRBVS is relatively robust to the choice of measure used in the procedure. Therefore, we recommend adjusting this choice based on the available

Table 3. **Model (B)**: the average number of false positives (FP), false negatives (FN), total errors (FP+FN), and estimated probability (Pr) of a correct selection of the top-ranked set (i.e., $P(\hat{\mathcal{S}} = \mathcal{S})$), calculated over 200 realizations. Bold: within 10% of the lowest value of FP+FN (or within 5% of the highest value of Pr).

		SIS		StabSel		RBVS		ISIS		IRBVS	
	MC+	MSC	EML	PC	MC+	PC	MC+	MSC	EML	PC	MC+
				$n=100 \quad p=100 \quad K=2$							
FP	0.12	0.08	0.04	0.18	0.00	0.00	0.00	0.26	0.21	0.04	0.00
FN	0.14	0.88	0.91	2.04	0.20	3.38	0.28	0.16	0.15	1.22	0.28
FP+FN	0.26	0.97	0.96	2.22	**0.20**	3.38	0.28	0.41	0.36	1.26	0.28
Pr	**0.81**	0.34	0.34	0.00	**0.82**	0.00	**0.79**	0.76	**0.78**	0.60	**0.79**
				$n=100 \quad p=1,000 \quad K=2$							
FP	0.40	0.22	0.32	0.36	0.00	0.01	0.00	0.06	0.08	0.04	0.00
FN	0.24	1.65	1.84	2.60	0.35	3.69	0.39	0.30	0.36	1.51	0.32
FP+FN	0.65	1.87	2.16	2.96	**0.35**	3.70	0.39	**0.35**	0.43	1.55	**0.32**
Pr	0.65	0.06	0.04	0.00	**0.70**	0.00	0.68	**0.72**	0.67	0.48	**0.72**
				$n=100 \quad p=100 \quad K=10$							
FP	0.00	0.04	0.02	0.19	0.00	0.01	0.01	0.18	0.19	0.08	0.02
FN	0.22	0.86	0.84	1.95	0.15	3.01	0.19	0.12	0.12	0.93	0.17
FP+FN	0.22	0.89	0.86	2.14	**0.16**	3.02	0.20	0.30	0.32	1.00	**0.18**
Pr	0.78	0.36	0.38	0.02	**0.84**	0.00	**0.82**	**0.84**	0.80	0.64	**0.82**
				$n=100 \quad p=1,000 \quad K=10$							
FP	0.02	0.08	0.14	0.33	0.00	0.00	0.00	0.07	0.04	0.02	0.00
FN	0.26	1.52	1.59	2.27	0.20	3.33	0.22	0.16	0.18	0.88	0.18
FP+FN	0.28	1.60	1.74	2.60	0.20	3.34	0.22	0.22	0.22	0.89	**0.18**
Pr	0.78	0.14	0.12	0.00	**0.82**	0.00	**0.81**	0.80	0.80	0.69	**0.84**

computational resources and the size of the data. In particular, for large data sets ($p > 10,000$, $n > 500$), we recommend using IRBVS PC, which is extremely fast to compute using the R package **rbvs**. Nevertheless, penalization-based methods, such as MC+, typically offer better performance, and thus should be used as the base measure for IRBVS in the case of moderate data size.

Supplementary Material

The online Supplementary Material provides implementation details for the RBVS algorithm, two real-data examples, and additional numerical experiments.

Table 4. **Model (C)**: the average number of false positives (FP), false negatives (FN), total errors (FP+FN), and estimated probability (Pr) of a correct selection of the top-ranked set (i.e., $P(\hat{\mathcal{S}} = \mathcal{S})$), calculated over 200 realizations. Bold: within 10% of the lowest value of FP+FN (or within 5% of the highest value of Pr).

		SIS		StabSel		RBVS		ISIS		IRBVS	
	MC+	MSC	EML	PC	MC+	PC	MC+	MSC	EML	PC	MC+
				$n = 100$ $p = 100$ $\rho = 0$ $\beta = 0.25$							
FP	7.65	1.06	0.95	0.24	0.04	0.02	0.01	3.46	3.50	0.04	0.01
FN	0.00	0.00	0.00	0.00	0.00	0.26	0.00	0.00	0.00	0.24	0.00
FP+FN	7.65	1.06	0.95	0.24	0.04	0.28	**0.01**	3.46	3.50	0.28	**0.01**
Pr	0.24	0.76	0.80	0.78	0.96	0.88	**0.99**	0.32	0.33	0.88	**0.99**
				$n = 100$ $p = 100$ $\rho = 0$ $\beta = 0.5$							
FP	11.96	4.25	4.04	0.32	0.06	0.02	0.00	4.36	4.17	0.08	0.01
FN	0.00	0.00	0.00	0.00	0.00	0.59	0.00	0.00	0.00	0.50	0.00
FP+FN	11.96	4.25	4.04	0.32	0.06	0.61	**0.00**	4.36	4.17	0.58	0.01
Pr	0.12	0.38	0.38	0.72	0.94	0.74	**1.00**	0.23	0.25	0.76	**0.99**
				$n = 100$ $p = 100$ $\rho = 0$ $\beta = 1$							
FP	19.63	11.44	11.10	0.44	0.06	0.02	0.00	5.34	5.13	0.04	0.00
FN	0.00	0.00	0.00	0.18	0.00	2.06	0.34	0.00	0.00	1.78	0.34
FP+FN	19.63	11.44	11.11	0.62	**0.06**	2.08	0.34	5.34	5.14	1.83	0.34
Pr	0.00	0.00	0.01	0.54	**0.94**	0.14	**0.90**	0.06	0.07	0.31	**0.90**
				$n = 100$ $p = 100$ $\rho = 0$ $\beta = 2$							
FP	34.10	15.37	15.10	0.78	0.14	0.00	0.00	5.94	5.79	0.00	0.00
FN	0.04	0.30	0.30	1.70	1.59	2.83	2.97	0.94	1.00	2.82	2.97
FP+FN	34.15	15.67	15.40	2.48	**1.73**	2.83	2.97	6.88	6.79	2.83	2.97
Pr	0.00	0.00	0.00	0.04	**0.06**	0.00	0.00	0.00	0.00	0.00	0.00

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A. Proofs

A.1. Proof of Proposition 1

Proof. First, we show that $\pi_n(\mathcal{S})$ tends to 1. Denote by $\mathcal{E} = \{\min_{j\in\mathcal{S}} \hat{\omega}_j > \max_{j\notin\mathcal{S}} \hat{\omega}_j\}$. If there is no tie, $\mathcal{E}$ is equivalent to $\big\{\{R_{n1}, \ldots, R_{ns}\} = \mathcal{S}\big\}$, i.e., all indices from $\mathcal{S}$ are ranked in front of those do not belong to $\mathcal{S}$. Otherwise,

Table 5. **Model (D)**: the average number of false positives (FP), false negatives (FN), total errors (FP+FN), and estimated probability (Pr) of a correct selection of the top-ranked set (i.e., $P(\hat{\mathcal{S}} = \mathcal{S})$), calculated over 200 realizations. Bold: within 10% of the lowest value of FP+FN (or within 5% of the highest value of Pr).

		SIS		StabSel		RBVS		ISIS		IRBVS	
	MC+	MSC	EML	PC	MC+	PC	MC+	MSC	EML	PC	MC+
					$n = 100 \quad p = 100 \quad \rho = 0.5$						
FP	0.07	1.99	1.17	0.40	0.03	0.00	0.01	3.27	3.35	0.10	0.01
FN	0.00	0.06	0.44	0.90	0.00	2.58	0.00	0.00	0.02	0.38	0.00
FP+FN	0.07	2.05	1.60	1.30	0.03	2.58	**0.01**	3.27	3.36	0..48	**0.01**
Pr	**0.95**	0.56	0.44	0.20	**0.97**	0.02	**0.99**	0.24	0.27	0.78	**0.99**
					$n = 100 \quad p = 1,000 \quad \rho = 0.5$						
FP	0.00	0.02	0.03	0.88	0.28	0.02	0.00	0.10	0.10	0.05	0.02
FN	2.27	2.59	2.72	2.98	0.00	3.00	0.00	0.00	0.02	0.69	0.00
FP+FN	2.27	2.62	2.75	3.86	0.28	3.02	**0.00**	0.10	0.12	0.74	0.02
Pr	0.06	0.00	0.00	0.00	0.76	0.00	**1.00**	0.92	0.92	0.72	**0.98**
					$n = 100 \quad p = 100 \quad \rho = 0.75$						
FP	0.00	1.14	0.52	0.47	0.04	0.00	0.00	2.62	2.75	0.06	0.01
FN	1.04	0.06	0.84	1.24	0.00	2.80	0.00	0.00	0.02	0.40	0.00
FP+FN	1.04	1.21	1.35	1.71	0.04	2.80	**0.00**	2.63	2.76	0.46	0.01
Pr	0.39	0.62	0.27	0.12	**0.96**	0.01	**1.00**	0.31	0.30	0.80	**0.99**
					$n = 100 \quad p = 1,000 \quad \rho = 0.75$						
FP	0.00	0.16	0.02	0.86	2.31	0.00	0.01	0.10	0.08	0.05	0.02
FN	3.00	2.69	2.86	2.98	0.00	3.00	0.02	0.00	0.01	0.82	0.00
FP+FN	3.00	2.85	2.88	3.85	2.31	3.00	**0.02**	0.10	0.08	0.87	**0.02**
Pr	0.00	0.00	0.00	0.00	0.07	0.00	**0.98**	0.92	0.92	0.68	**0.98**

$\{\min_{j\in\mathcal{S}} \hat{\omega}_j > \max_{j\notin\mathcal{S}} \hat{\omega}_j\}$ implies that $\big\{\{R_{n1}, \ldots, R_{ns}\} = \mathcal{S}\big\}$. Using (C4) we have

$$\pi_n(\mathcal{S}) \geq \mathbb{P}(\mathcal{E}) \geq \mathbb{P}\left(\max_{j=1,\ldots,p} |\hat{\omega}_j - \omega_j| < \epsilon\right),$$

where $\epsilon = c_\eta n^{-\eta}/2$. Application of Bonferroni's inequality yields that

$$\mathbb{P}\left(\max_{j=1,\ldots,p} |\hat{\omega}_j - \omega_j| < \epsilon\right) \geq 1 - p \sup_{j=1,\ldots,p} \mathbb{P}\left(|\hat{\omega}_j - \omega_j| \geq \epsilon\right).$$

The last term is of order $1 - O(\exp(-n^\gamma))$ (since $b_1 < \gamma$), which tends to 1 as $n \to \infty$. This proves that $\mathcal{S}$ is a s-top-ranked set, where $s = |\mathcal{S}|$.

Second, consider any $\mathcal{A} \in \Omega_{s+1}$. We will prove that $\pi_n(\mathcal{A}) \underset{n}{\to} 0$. Note that $\mathcal{E}$ implies that $\mathcal{S} \subset \mathcal{A}$, as all indices from $\mathcal{S}$ are ranked in front of those do not belong to $\mathcal{S}$. Thus, it suffices to only consider the case of $\mathcal{S} \subset \mathcal{A}$ in which $\mathcal{A}\backslash\mathcal{S}$ has only one element, which we denote by a. Suppose there is no tie in the ranking, on the event $\mathcal{E}$, $\mathbb{P}\left(\{\min_{j\in\mathcal{A}}\hat{\omega}_j > \max_{j\notin\mathcal{A}}\hat{\omega}_j\}\cap\mathcal{E}\right) = \mathbb{P}\left(\{\hat{\omega}_a > \max_{j\notin\mathcal{A}}\hat{\omega}_j\}\cap\mathcal{E}\right)$. To bound $\mathbb{P}\left(\hat{\omega}_a > \max_{j\notin\mathcal{A}}\hat{\omega}_j\right)$, we observe that $\mathbb{P}\left(\hat{\omega}_a > \max_{j\notin\mathcal{A}}\hat{\omega}_j\right) \leq \mathbb{P}(\hat{\omega}_a > \max_{j\in\mathcal{M}_a\backslash\{a\}}\hat{\omega}_j)$. Using the exchangeability assumption (C3), we have that the values of $\mathbb{P}\left(\hat{\omega}_{j^*} > \max_{j\in\mathcal{M}_a\backslash\{j^*\}}\hat{\omega}_j\right)$ are the same for every $j^*\in\mathcal{M}_a$ (i.e., any element in $\{\hat{\omega}_j\}_{j\in\mathcal{M}_a}$ are equally likely to be the largest). Since $\sum_{j^*\in\mathcal{M}_a}\mathbb{P}(\hat{\omega}_{j^*} > \max_{j\in\mathcal{M}_a\backslash\{j^*\}}\hat{\omega}_j) \leq 1$, we have that $\mathbb{P}\left(\hat{\omega}_a > \max_{j\in\mathcal{M}_a\backslash\{a\}}\hat{\omega}_j\right) \leq 1/|\mathcal{M}_{\{a\}}| \underset{n}{\to} 0$. Consequently,

$$\pi_n(\mathcal{A}) \leq \mathbb{P}\left(\hat{\omega}_a > \max_{j\notin\mathcal{A}}\hat{\omega}_j\right) + \mathbb{P}\left(\mathcal{E}^c\right) \leq \mathbb{P}\left(\hat{\omega}_a > \max_{j\in\mathcal{M}_a\backslash a}\hat{\omega}_j\right) + \mathbb{P}\left(\mathcal{E}^c\right) \underset{n}{\to} 0.$$

Otherwise, if there are ties in the ranking, since we break the ties at random uniformly, it follows from the exchangeability assumption that we are equally likely to pick any index from $\mathcal{M}_a$, given that we have picked one of them. Thus we can argue in a similar manner to show that $\pi_n(\mathcal{A}) \leq 1/|\mathcal{M}_a| + \mathbb{P}\left(\mathcal{E}^c\right) \underset{n}{\to} 0$, i.e., $\mathcal{S}$ is always locally top-ranked.

Third, for every $k' = 1\ldots, s-1$, we show that there exists some $\mathcal{A}\in\Omega_{k'}$ such that $\limsup_{n\to\infty}\pi_n(\mathcal{A}) > 0$. Note that

$$\sum_{\{\mathcal{A}\colon\, \mathcal{A}\in\Omega_{k'} \text{ and } \mathcal{A}\subset\mathcal{S}\}} \pi_n(\mathcal{A}) \geq \mathbb{P}\left(\min_{j\in\mathcal{S}}\hat{\omega}_j > \max_{j\notin\mathcal{S}}\hat{\omega}_j\right) \underset{n}{\to} 1$$

from our previous argument. However, there are $\binom{s}{k'}$ elements in $\{\mathcal{A} : \mathcal{A}\in\Omega_{k'} \text{ and } \mathcal{A}\subset\mathcal{S}\}$, so

$$\max_{\{\mathcal{A}\colon\, \mathcal{A}\in\Omega_{k'} \text{ and } \mathcal{A}\subset\mathcal{S}\}} \limsup_{n\to\infty}\pi_n(\mathcal{A}) \geq \frac{1}{\binom{s}{k'}}.$$

This implies that $\mathcal{S}$ is indeed a top-ranked set.

Finally, the uniqueness of $\mathcal{S}$ (among those in Ω_s) follows from the fact that $\pi_n(\mathcal{S}) \underset{n}{\to} 1$ and $\sum_{\mathcal{A}\in\Omega_s}\pi_n(\mathcal{A}) = 1$.

A.2. Auxiliary lemmas and proof of Theorem 1

A.2.1. Auxiliary lemmas

Lemma 1 (Theorem 1 of Hoeffding (1963))**.** *Let W be a binomial random variable with the probability of success π and r trials. For any $1 > t > \pi$, we have $\mathbb{P}\left(W \geq rt\right) \leq \left(\pi/t\right)^{rt}\left((1-\pi)/(1-t)\right)^{r(1-t)}$. Moreover, for any $0 < t < \pi$, $\mathbb{P}\left(W \leq rt\right) \leq \left(\pi/t\right)^{rt}\left((1-\pi)/(1-t)\right)^{r(1-t)}$.*

Lemma 2. *Let $a_1, \dots, a_l$ be non-negative numbers s.t. $\sum_{i=1}^{l} a_i \leq 1$ and $\max a_i \leq t$ for some $1/l \leq t \leq 1$. Let $N \in \mathbb{N}$ be the minimum integer such that there exist mutually exclusive sets $I_1, \dots, I_N \subset \{1, \dots, l\}$ with $\sum_{i \in I_j} a_i \leq t$ and $\bigcup_{j=1}^{N} I_j = \{1, \dots, l\}$. Then, $N \leq \lfloor 2/t \rfloor + 1$.*

Proof. Since N is the smallest possible integer, there must be at most one $j \in \{1, \dots, N\}$ with $\sum_{i \in I_j} a_i \leq t/2$. Otherwise, such two sets could be combined, leading to a smaller N. So for all other $j \in \{1, \dots, N\}$, we have that $\sum_{i \in I_j} a_i > t/2$. Consequently, $(N-1)t/2 \leq \sum_{i=1}^{l} a_i \leq 1$. This implies that $N \leq \lfloor 2/t \rfloor + 1$.

Lemma 3. *Let be $\Omega \subset \Omega_k$ for some $k = 1, \dots, p-1$, $m \leq n$, $B \geq 1$, and t_1, t_2 satisfying $\max_{\mathcal{A} \in \Omega} \pi_{m,n}(\mathcal{A}) \leq t_2 < t_1 < 1$. Then*

$$\mathbb{P}\left(\max_{\mathcal{A} \in \Omega} \hat{\pi}_{m,n}(\mathcal{A}) \geq t_1\right) \leq \frac{3B}{t_2}\left[\left(\frac{t_2}{t_1}\right)^{t_1}\left(\frac{1-t_2}{1-t_1}\right)^{1-t_1}\right]^{r},$$

where $\pi_{m,n}(\mathcal{A})$, $\hat{\pi}_{m,n}(\mathcal{A})$ are defined by (2.2) *and Definition* 5, *respectively.*

Proof. Denote by $\mathcal{A}^1, \dots, \mathcal{A}^l$ all the elements of Ω. Applying Lemma 2 we find a partition $I_1, \dots, I_N$ such that $\max_{j=1,\dots,N} \sum_{i \in I_j} \pi_{m,n}(\mathcal{A}^j) \leq t_2$ and $N \leq 2/t_2 + 1$. Using the union bound, we have that

$$\mathbb{P}\left(\max_{i=1,\dots,l} \hat{\pi}_{m,n}(\mathcal{A}^i) \geq t_1\right) \leq N \max_{j=1,\dots,N} \mathbb{P}\left(\sum_{i \in I_j} \hat{\pi}_{m,n}(\mathcal{A}^i) \geq t_1\right).$$

Note that when $B = 1$, $r \sum_{i \in I_j} \hat{\pi}_{m,n}(\mathcal{A}^i)$ is a binomial random variable, where there are r trials, each with the probability of success $p_j^* = \sum_{i \in I_j} \pi_{m,n}(\mathcal{A}^i)$. We could conclude from Lemma 1 that

$$\begin{aligned}\mathbb{P}\left(\sum_{i \in I_j} \hat{\pi}_{m,n}(\mathcal{A}^i) \geq t_1\right) &\leq \left[\left(\frac{p_j^*}{t_1}\right)^{t_1}\left(\frac{1-p_j^*}{1-t_1}\right)^{1-t_1}\right]^{r} \\ &\leq \left[\left(\frac{t_2}{t_1}\right)^{t_1}\left(\frac{1-t_2}{1-t_1}\right)^{1-t_1}\right]^{r},\end{aligned}$$

where we used the fact that $(x/t_1)^{t_1}\left((1-x)/(1-t_1)\right)^{1-t_1}$ is increasing for $x \in [0, t_1]$. When $B = 1$, the above displayed equation, combined with $N \leq 3/t_2$

gives that

$$\mathbb{P}\left(\max_{i=1,\dots,l}\hat{\pi}_{m,n}(\mathcal{A}^i)\geq t_1\right)\leq\frac{3}{t_2}\left[\left(\frac{t_2}{t_1}\right)^{t_1}\left(\frac{1-t_2}{1-t_1}\right)^{1-t_1}\right]^r.$$

Finally, when $B>1$, $r\sum_{i\in I_j}\hat{\pi}_{m,n}(\mathcal{A}_j)$ is a sample average of B (not necessarily independent) binomial random variables. Since the average of a collection of non-negative numbers is always no greater than its maximum, we could simply use the union bound again to establish that

$$\mathbb{P}\left(\max_{i=1,\dots,l}\hat{\pi}_{m,n}(\mathcal{A}^i)\geq t_1\right)\leq\frac{3B}{t_2}\left[\left(\frac{t_2}{t_1}\right)^{t_1}\left(\frac{1-t_2}{1-t_1}\right)^{1-t_1}\right]^r.$$

A.2.2. Proof of Theorem 1

Proof of Theorem 1. For notational convenience, define $\hat{\omega}_{j,m}=\hat{\omega}_j(\mathbf{Z}_1,\dots,\mathbf{Z}_m)$, $\delta=\pi_{m,n}(\mathcal{S})$ and $\theta=\max_{\mathcal{A}\not\subset\mathcal{S},|\mathcal{A}|\leq k_{\max}}\pi_{m,n}(\mathcal{A})$, where $\pi_{m,n}(\cdot)$ is given by (2.2). We start from showing that δ and θ are well-separated for sufficiently large n.

Take $\epsilon=c_\eta m^{-\eta}/2$. Using (A1) and (A5) combined with a simple Bonferroni's inequality, we get $\delta\geq\mathbb{P}\left(\max_{j=1,\dots,p}|\hat{\omega}_{j,m}-\omega_j|<\epsilon\right)\geq 1-C_\epsilon p\exp(-m^\gamma)$ for some constant $C_\epsilon>0$. In views of (A2) and (A3), since here we assume that $\gamma b_2>b_1$, we get that $\delta=1-O(\exp(-n^{\gamma b_2}))$, which tends to one as $n\to\infty$.

For every $\mathcal{A}\in\Omega_k$ with $k\leq k_{\max}$ that contains at least one $a\in\mathcal{A}\setminus\mathcal{S}$, if there is no tie in the ranking of $\{\hat{\omega}_{j,m}\}_{1\leq j\leq p}$, we have that

$$\begin{aligned}\pi_{n,m}(\mathcal{A})&=\mathbb{P}\left(\min_{j\in\mathcal{A}}\hat{\omega}_{j,m}>\max_{j\notin\mathcal{A}}\hat{\omega}_{j,m}\right)\leq\mathbb{P}\left(\hat{\omega}_{a,m}>\max_{j\in\mathcal{M}_a\setminus\mathcal{A}}\hat{\omega}_{j,m}\right)\\&\leq\frac{1}{|\mathcal{M}_a|-k_{\max}}\leq\frac{1}{\min_{a\notin\mathcal{S}}|\mathcal{M}_a|-k_{\max}}\\&\leq\frac{1}{C_3n^{b_3}-C_4n^{b_4}},\end{aligned}\tag{A.1}$$

where $\mathcal{M}_a$ is as in (A4). Here we utilized the exchangeability of $\{\hat{\omega}_{j,m}\}_{j\in\mathcal{M}_a\setminus\mathcal{S}}$ together with (A4) and (A7). Even if there are ties, we still have that $\pi_{n,m}(\mathcal{A})\leq 1/(C_3n^{b_3}-C_4n^{b_4})$ due to the exchangeability and since we break the ties uniformly at random. See also the previous proof of Proposition 1 for a similar argument but with a more detailed explanation. Notice that (A.1) does not depend on $\mathcal{A}$ or a, so the inequality $\pi_{n,m}(\mathcal{A})\leq 1/(C_3n^{b_3}-C_4n^{b_4})$ holds for every $\mathcal{A}\in\Omega_k$ with $k\leq k_{\max}$

and $\mathcal{A}\backslash\mathcal{S} \neq \emptyset$. As such, we conclude that $\theta = \max_{\mathcal{A}\not\subseteq\mathcal{S}, |\mathcal{A}|\leq k_{\max}} \pi_{m,n}(\mathcal{A}) = O(n^{-b_3})$.

Next, to fix ideas, take $\Delta = (b_2 + b_3 - 1)/2$ (NB. $\Delta > 0$ from (A4)), $t_1 = n^{(-b_3+\Delta)/2}$ and $t_2 = t_1^2$. Note that for sufficiently large n we always have $\theta < t_1^2 < t_1 < 1/2 < \delta$. Now define events

$$\begin{aligned} \mathcal{E}_k &= \left\{ \max_{\mathcal{A}\in\Omega_k, \mathcal{A}\not\subseteq\mathcal{S}} \hat{\pi}_{m,n}(\mathcal{A}) < t_1 \right\}, \text{ for } k = 1, \ldots, k_{\max}, \\ \mathcal{B} &= \left\{ \hat{\pi}_{m,n}(\mathcal{S}) > \frac{1}{2} \right\}, \\ \mathcal{E} &= \mathcal{B} \cap \bigcap_{k=1}^{k_{\max}} \mathcal{E}_k. \end{aligned}$$

We will demonstrate that $\mathbb{P}(\mathcal{E}) \underset{n}{\rightarrow} 1$ at an exponential rate, and with $\hat{\mathcal{A}}_{\hat{s},m} = \mathcal{S}$ on the event $\mathcal{E}$.

To prove the first claim, when $B = 1$, for sufficiently large n, we could use Lemma 1 and the fact that $1 - \delta = O(\exp(-n^{\gamma b_2})) \underset{n}{\rightarrow} 0$ to bound $\mathbb{P}(\mathcal{B}^c)$ by

$$\mathbb{P}(\mathcal{B}^c) \leq \left[\left(\frac{\delta}{0.5}\right)^{0.5} \left(\frac{1-\delta}{0.5}\right)^{0.5} \right]^r \leq [2(1-\delta)]^{0.5r} \leq \exp\left(-C' n^{\gamma b_2(1-b_2)/2}\right) \tag{A.2}$$

for some $0 < C' < 1$. When $B > 1$, since $\hat{\pi}_{m,n}(\mathcal{S})$ is the average of B copies of the that with $B = 1$, using the Bonferroni bound, we have that $\mathbb{P}(\mathcal{B}^c) \leq B\exp\left(-C' n^{\gamma b_2(1-b_2)/2}\right)$. Moreover, by Lemma 3,

$$\mathbb{P}(\mathcal{E}_k^c) \leq \frac{3B}{t_2} \left[\left(\frac{t_2}{t_1}\right)^{t_1} \left(\frac{1-t_2}{1-t_1}\right)^{1-t_1} \right]^r = \frac{3B}{t_1^2} \left[\left(\frac{t_1}{1+t_1}\right)^{t_1} (1+t_1) \right]^r. \tag{A.3}$$

Take the logarithm of $(t_1/(1+t_1))^{t_1}(1+t_1)$. After simple algebra we get $t_1 \log(t_1/(1+t_1)) + \log(1+t_1) = t_1 \log(1 - 1/(1+t_1)) + \log(1+t_1)$, which can be bounded using (A6) and $\log(1+x) \leq 2x/(2+x)$ for $x \in (-1, 0)$ and $\log(1+x) \leq (x/2)((2+x)/(1+x))$ for $x \geq 0$ (Topsøe (2004)). Putting things together, we have that

$$t_1 \log\left(1 - \frac{1}{1+t_1}\right) + \log(1+t_1) \leq -t_1 \frac{(2 - t_1 - 2t_1^2)}{2(1+t_1)(1+2t_1)} \leq -\frac{t_1}{6}.$$

Here we also used the fact that the function $h(x) = (2-x-2x^2)/\{2(1+x)(1+2x)\}$

is decreasing for $x \in [0,1]$, $h(1/2) = 1/6$ and $t_1 = n^{(-b_3+\Delta)/2} < 1/2$. This applied to (A.3) yields

$$\mathbb{P}\left(\mathcal{E}_k^c\right) \leq \frac{3B}{t_1^2} \exp\left(\frac{-rt_1}{6}\right) < \exp\left(-C'' n^{1-b_2-b_3/2}\right), \tag{A.4}$$

with positive constant C'', for sufficiently large n. (A4) implies that the right hand side of the above inequality goes to 0 because (A4) says that $1-b_2-b_3/2 > 0$. It follows from (A.2), (A.4) and (A7) that

$$\begin{aligned}\mathbb{P}\left(\mathcal{E}\right) &\geq 1 - k_{\max} \exp\left(-C'' n^{1-b_2-b_3/2}\right) - \exp\left(-C' n^{\gamma b_2(1-b_2)/2}\right) \\ &\geq 1 - C_4 n^{b_4} \exp\left(-C'' n^{1-b_2-b_3/2}\right) - \exp\left(-C' n^{\gamma b_2(1-b_2)/2}\right) \\ &\geq 1 - \exp\left(-C_\beta n^\beta\right)\end{aligned}$$

for some $\beta \in (0,1)$ and $C_\beta > 0$, for sufficiently large n. Therefore, $\mathbb{P}\left(\mathcal{E}\right) \underset{n}{\to} 1$.

The remaining arguments used in the proof are valid on $\mathcal{E}$ with a sufficiently large n. Notice that from $1/2 > t_1$ one concludes that $\hat{\mathcal{A}}_{s,m} = \mathcal{S}$, where $\hat{\mathcal{A}}_{s,m}$ is given by (2.4), hence showing $\hat{s} = s$ proves $\hat{\mathcal{S}} = \mathcal{S}$. Denote $T_k = \hat{\pi}^\tau_{m,n}(\hat{\mathcal{A}}_{k+1,m})/\hat{\pi}_{m,n}(\hat{\mathcal{A}}_{k,m})$, then from definition, $\hat{s} = \operatorname{argmin}_{k=0,1,\ldots,k_{\max}} T_k$. Three cases are considered.

- For every $k = 0, \ldots, s-1$, the event $\{\{R_n(\mathbf{Z}_1, \ldots, \mathbf{Z}_m), \ldots, R_{n,s}(\mathbf{Z}_1, \ldots, \mathbf{Z}_m)\} = \mathcal{S}\}$ implies that the index set $\{R_n(\mathbf{Z}_1, \ldots, \mathbf{Z}_m), \ldots, R_{n,k+1}(\mathbf{Z}_1, \ldots, \mathbf{Z}_m)\}$ (i.e., of size $k+1$) must be one of the elements in $\{\mathcal{A} \in \Omega_{k+1} : \mathcal{A} \subset \mathcal{S}\}$. Consequently,
$$\sum_{\{\mathcal{A} \in \Omega_{k+1} : \mathcal{A} \subset \mathcal{S}\}} \hat{\pi}_{m,n}(\mathcal{A}) \geq \hat{\pi}_{m,n}(\mathcal{S}).$$
The facts that $\left|\{\mathcal{A} \in \Omega_{k+1} : \mathcal{A} \subset \mathcal{S}\}\right| = \binom{s}{k+1}$ and $\hat{\pi}_{m,n}(\mathcal{S}) > 1/2$ imply that
$$\hat{\pi}_{m,n}(\hat{\mathcal{A}}_{k+1,m}) \geq \max_{\{\mathcal{A} \in \Omega_{k+1} : \mathcal{A} \subset \mathcal{S}\}} \hat{\pi}_{m,n}(\mathcal{A}) \geq \frac{\hat{\pi}_{m,n}(\mathcal{S})}{\binom{s}{k+1}} \geq \frac{1}{2\binom{s}{k+1}},$$
and hence $T_k \geq 1/(2\binom{s}{k+1})$. for $k = 0, \ldots, s-1$.
- Directly from the definition of the events $\mathcal{E}_s$ and $\mathcal{B}$, we bound $T_s \leq 2t_1^\tau$.
- $\hat{\pi}_{m,n}(\hat{\mathcal{A}}_{k+1,m}) \geq 1/Br$ for any k. To see this, note that $\sum_{\mathcal{A} \in \Omega_{k+1}} \hat{\pi}_{m,n}(\mathcal{A}) = 1$. Picking $\hat{\mathcal{A}}_{k+1,m} \in \operatorname{argmax}_{\mathcal{A} \in \Omega_{k+1}} \hat{\pi}_{m,n}(\mathcal{A})$ would mean that

$\hat{\pi}_{m,n}(\hat{\mathcal{A}}_{k+1,m}) > 0$, because otherwise it would imply $\sum_{\mathcal{A}\in\Omega_{k+1}} \hat{\pi}_{m,n}(\mathcal{A}) = 0$, leading to a contradiction. Now that $\hat{\pi}_{m,n}(\hat{\mathcal{A}}_{k+1,m}) > 0$, it must be the case that $\hat{\pi}_{m,n}(\hat{\mathcal{A}}_{k+1,m}) > 1/Br$, according to Definition 5. Thus $T_k \geq 1/t_1(Br)^\tau$ for every $k = s+1, \ldots, k_{\max}$.

To prove $T_k > T_s$ for $k = 0, \ldots, s-1$, it is sufficient to demonstrate that $1/(2\binom{s}{k+1}) > 2t_1^\tau$, which is true for sufficiently large n, as $t_1 \underset{n}{\to} 0$ and $\max_{k=0,\ldots,s-1} \binom{s}{k+1}$ is bounded. Similarly, to claim that $T_s < T_k$ for $k = s+1, \ldots, k_{\max}$, we need to show $2t_1^\tau < 1/(t_1(Br)^\tau)$, which amounts to $2t_1^{1+\tau} < 1/(Br)^\tau$, or $2^{1/\tau}t_1^{1+1/\tau} < 1/Br$. This is true for sufficiently large n, because $t_1^2 = n^{-b_3+\Delta}$, $Br = O(n^{1-b_2})$ and $b_2 + b_3 - \Delta > 1$ from (A4).

Therefore T_k is necessarily minimised at $k = s$ over $\mathcal{E}$ for sufficiently large n, meaning that $\hat{s} = s$, which finishes the proof.

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Department of Statistics, Columbia House, London School of Economics and Political Science, Houghton Street, London, WC2A 2AE, UK.

E-mail: r.baranowski@lse.ac.uk

Department of Statistics, Columbia House, London School of Economics and Political Science,

Houghton Street, London, WC2A 2AE, UK.
E-mail:y.chen101@lse.ac.uk
Department of Statistics, Columbia House, London School of Economics and Political Science,
Houghton Street, London, WC2A 2AE, UK.
E-mail: p.fryzlewicz@lse.ac.uk

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