On the early solution path of best subset selection

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Abstract

The early solution path, which tracks the first few variables that enter the model of a selection procedure, is of profound importance to scientific discovery. In practice, it is often statistically intangible to identify all the important features with no false discovery, let alone the intimidating expense of experiments to test their significance. Such realistic limitation calls for statistical guarantee for the early discovery of a model selector to navigate scientific adventure on the sea of big data. In this paper, we focus on the early solution path of best subset selection (BSS), where the sparsity constraint is set to be lower than the true sparsity. Under a sparse high-dimensional linear model, we establish the sufficient and (near) necessary condition for BSS to achieve sure early selection, or equivalently, zero false discovery throughout its entire early path. Essentially, this condition boils down to a lower bound of the minimum projected signal margin that characterizes the fundamental gap in signal capturing between sure selection models and those with spurious discovery. Defined through projection operators, this margin is independent of the restricted eigenvalues of the design, suggesting the robustness of BSS against collinearity. On the numerical aspect, we choose CoSaMP (Compressive Sampling Matching Pursuit) Needell and Tropp (2009) to approximate the BSS solutions, and we show that the resulting early path exhibits much lower false discovery rate (FDR) than LASSO, MCP and SCAD, especially in presence of highly correlated design. Finally, we apply CoSaMP to perform preliminary feature screening for the knockoff filter Barber et al. (2015); Candès et al. (2018) to enhance its power.

Keywords and phrases: Best Subset Selection, Sure Early Selection, False Discovery Rate, True Positive Rate, Compressive Sampling Matching Pursuit, High-Dimensional Statistics.

1 Introduction

Best subset selection (BSS), which dates back to the middle of the 20th century (Garside, 1965; Hocking and Leslie, 1967; Beale et al., 1967), is among the most classical variable selection approaches in regression analysis. Suppose we have \( n \) independent and identically distributed (i.i.d.) observations \( \{x_i, y_i\}_{i=1}^n \) of \( (x, Y) \) that follows the linear model:

\[
Y = \mathbf{x}^\top \beta^* + \epsilon.
\]  

Here \( \mathbf{x} \) is a design vector valued in \( \mathbb{R}^p \), \( \beta^* \in \mathbb{R}^p \) is an unknown coefficient vector, and \( \epsilon \) is random noise independent of \( \mathbf{x} \). Let \( \mathbf{X} = (\mathbf{x}_1 \ \mathbf{x}_2 \ \ldots \ \mathbf{x}_n)^\top \), \( \mathbf{y} = (y_1 \ \ldots \ y_n)^\top \) and \( \mathbf{\epsilon} = (\epsilon_1 \ \ldots \ \epsilon_n)^\top \). Then in matrix form, we have that

\[
\mathbf{y} = \mathbf{X}\beta^* + \mathbf{\epsilon}.
\]
Let $S^* := \{j : \beta^*_j \neq 0\}$ and $s^* := |S^*|$. Given a target sparsity $s$, which is not necessarily equal to $s^*$, BSS solves for

$$
\hat{\beta}^{\text{best}}(s) := \arg\min_{\beta \in \mathbb{R}^p, \|\beta\|_0 \leq s} \sum_{i=1}^n (y_i - x_i^\top \beta)^2.
$$

(3)

In words, BSS seeks for the size-$s$ subset of the available variables that achieves the minimum $L_2$ fitting error. Another related type of subset regression approaches, which emerged in the 1970s, is the $\ell_0$-regularized approach, exemplified by Mallow’s $C_p$ (Mallows, 1973), Akaike Information Criterion (AIC) (Akaike, 1974, 1998) and Bayesian Information Criterion (BIC) (Schwarz et al., 1978). Instead of directly constraining $\|\beta\|_0$, these approaches penalize the loss function by a regularization term that is proportional to $\|\beta\|_0$, which accounts for the difference between in-sample prediction error and training error (see Section 7.4 of Hastie et al. (2009)). Such $\ell_0$-regularized loss functions provide convenient gauges for model comparison and thus lead to effective model selection. Nevertheless, despite the succinct form of the $\ell_0$-constrained or $\ell_0$-regularized method, both are notorious for their NP-hardness (Natarajan, 1995) and are thus computationally infeasible under high dimension.

For a long period of time, the computational barrier of BSS has been shifting attention away from its exact discrete formulation to its surrogate forms that are amenable to polynomial algorithms. The past three decades or so have witnessed a flurry of profound works on this respect, giving rise to a myriad of variable selection methods with both statistical accuracy and computational efficiency, particularly in high-dimensional regimes. A partial list of them include LASSO (Tibshirani, 1996; Chen et al., 1998), SCAD (Fan and Li, 2001; Fan et al., 2004), MCP (Zhang et al., 2010), and so forth. The shared spirit of these approaches is to substitute their exact discrete formulation to its surrogate forms that are amenable to polynomial algorithms. Such $\ell_0$-regularized approach, exemplified by Mallow’s $C_p$ (Mallows, 1973), Akaike Information Criterion (AIC) (Akaike, 1974, 1998) and Bayesian Information Criterion (BIC) (Schwarz et al., 1978). Instead of directly constraining $\|\beta\|_0$, these approaches penalize the loss function by a regularization term that is proportional to $\|\beta\|_0$, which accounts for the difference between in-sample prediction error and training error (see Section 7.4 of Hastie et al. (2009)). Such $\ell_0$-regularized loss functions provide convenient gauges for model comparison and thus lead to effective model selection. Nevertheless, despite the succinct form of the $\ell_0$-constrained or $\ell_0$-regularized method, both are notorious for their NP-hardness (Natarajan, 1995) and are thus computationally infeasible under high dimension.

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$$
\hat{\beta}^{\text{pen}} := \arg\min_{\beta \in \mathbb{R}^p} \mathcal{L}(\beta) + \rho_\lambda(\beta),
$$

(4)

where $\mathcal{L}(\beta)$ is a loss function, and where $\rho_\lambda(\beta)$ is a regularizer that promotes parsimony. For instance, LASSO chooses $\rho_\lambda(\beta) = \lambda \|\beta\|_1$, which, if $\mathcal{L}(\beta)$ is convex, renders problem (4) convex and thus computationally friendly. Elastic net chooses $\rho_\lambda(\beta) = \lambda_1 \|\beta\|_2^2 + \lambda_2 \|\beta\|_1$, which is also convex, to achieve both model sparsity and robustness against collinearity of design. MCP and SCAD choose $\rho_\lambda$ to be nonconvex to correct shrinkage bias of LASSO, while still maintaining some sort of restricted convexity of $\mathcal{L}(\beta) + \rho_\lambda(\beta)$ near $\beta^*$ to guarantee computational feasibility Fan et al. (2018). All these methods are backed up by solid statistical guarantee under high dimension. For example, regarding model selection or support recovery, Zhao and Yu (2006) established sufficient and nearly necessary conditions for model consistency of LASSO under fixed design. One crucial condition there is the famous irrepressible condition: there exists a constant $\eta > 0$ such that

$$
\left\| \Sigma_{(S^*)^c \cdot S^*} (\hat{\Sigma}_{S^* \cdot S^*})^{-1} \text{sign}(\beta_{S^*}) \right\|_\infty \leq 1 - \eta,
$$

(5)

where $\Sigma_{S^* \cdot S^*}$ is the sample covariance of $X_{S^*}$, and where $\hat{\Sigma}_{(S^*)^c \cdot S^*}$ is the sample covariance between $X_{(S^*)^c}$ and $X_{S^*}$. One sufficient condition to deduce (5) is that the $\ell_1$-norm of the regression coefficient vector obtained by regressing any spurious covariate on the true covariates is bounded by $1 - \eta$, which is quite restrictive for practical applications. Zhang et al. (2010) showed that MCP
achieves model consistency when the design satisfies a sparse Riesz condition and the minimum signal strength satisfies that \( \min_{j \in S^*} |\beta_j^*| \gtrsim (\log p/n)^{1/2} \). (Fan and Lv, 2011) proposed an iterative local adaptive majorize-minimization (I-LAMM) algorithm for general empirical risk minimization with folded concave penalty (e.g., SCAD) and showed that only a local Riesz condition suffices to ensure model consistency. There is also rich literature on estimation and prediction error of these penalized methods. Since they are not the focus of our work, we omit detailed discussion on them and refer interested readers to Wainwright (2019), Bühlmann and Van De Geer (2011) and Fan et al. (2020b) for comprehensive introduction to the related results.

Given the wide success of these surrogate methods on both theoretical and practical aspects, one natural question arises: Is BSS still the holy grail? Or more specifically, what is the marginal benefit that BSS brings about, given that the aforementioned surrogate approaches are already accurate and accessible? The answer lies in the requirement on the design. Wainwright (2009), Shen et al. (2012) and Fan et al. (2020a) showed that BSS can achieve model consistency without the aforementioned irrepresentable condition or sparse Riesz condition. To get a taste of these results, consider the identifiability margin as defined in Fan et al. (2020a):

\[
\tau_*(s^*) := \min_{S \subseteq [p], |S| = s^*, S \neq S^*} \min_{\gamma} \frac{\beta^*_{S^* \setminus S} (\tilde{\Sigma}_{S^* \setminus S \setminus S} - \tilde{\Sigma}_{S^* \setminus S} \tilde{\Sigma}_{S^* S}^{-1} \tilde{\Sigma}_{S \setminus S} \tilde{\Sigma}_{S^* S}^{-1} \tilde{\Sigma}_{S S} \Sigma_{S S}^{-1}) \beta^*_{S^* \setminus S}}{|S^* \setminus S|}.
\]

Fan et al. (2020a) showed that \( \tau_*(s^*) \gtrsim \log p/n \) is sufficient and almost necessary for BSS to achieve model consistency, implying that \( \tau_*(s^*) \) is a tight difficulty indicator for BSS to identify the true model. As illustrated by Remark 2.1 in Fan et al. (2020a), \( \tau_*(s^*) \) is insensitive to collinearity between spurious variables: however correlated the spurious variables are, \( \tau_*(s^*) \) can remain well above zero, if all the spurious variables are uncorrelated with the true variables, say. In contrast, high collinearity can easily break the sparse Riesz condition necessitated by MCP and SCAD. This demonstrates the robustness of BSS against collinearity in terms of model selection. On top of this, enhancing the signal strength improves \( \tau_*(s^*) \), while the irrepresentable cannot be relaxed through improving the signal strength. We can therefore see higher efficiency of BSS than that of LASSO in terms of exploiting the signal for model selection. Regarding estimation accuracy, it is widely known that the surrogate approaches hinge on restricted strong convexity (or similar conditions) of the loss function to achieve fast estimation rate. For instance, consider the well known restricted eigenvalue (RE) condition Bickel et al. (2009); Van De Geer and Bühlmann (2009); Negahban et al. (2012). For any \( S \subseteq [p] \) with \( |S| = s \), define \( C(S) := \{ v : \| v_{S^*} \|_1 \leq 3 \| v_S \|_1 \} \). We say the design matrix \( X = (x_1, \ldots, x_n)^T \in \mathbb{R}^{n \times p} \) satisfies a \( \gamma \)-RE condition if

\[
\frac{1}{n} \| X \beta \|_2^2 \geq \gamma \| \beta \|_2^2, \quad \forall \beta \in \bigcup_{S \subseteq [p], |S| = s^*} C(S).
\]

Zhang et al. (2014) showed that under a widely believed assumption in complexity theory, there exists a family of bad design \( X^{\text{bad}} \) for which the mean-squared prediction error of any estimator that can be computed in polynomial time is bounded from below by \( \Omega_{\mathbb{P}} \left( s^{1-\delta} \log p / (\gamma^2 n) \right) \), where \( \delta \) is an arbitrarily small positive constant. This implies that the RE parameter is inevitable in the prediction error of any polynomial-time statistical procedure. In stark contrast, Raskutti et al. (2011) showed that the mean squared prediction error rate of BSS is \( O_{\mathbb{P}}(s^3 \log p / n) \), which is completely independent of the RE parameter. This indicates that BSS can cope with a much broader family of design than the surrogate methods.
Besides the difference in theoretical assumptions, remarkable advancement in computing hardware and optimization has made possible the numerical comparison between BSS and its surrogate methods under practical setups, thereby inspiring renewal of interest in BSS. Bertsimas et al. (2016) recast the BSS problem (3) as a mixed integer optimization (MIO) problem and showed that for $n$ in thousands and $p$ in hundreds, a MIO algorithm can achieve provable optimality in minutes. Bertsimas et al. (2020) devised a new cutting plane method that solves to provable optimality the Tikhonov-regularized Tikhonov (1943) BSS problem with $n, p$ in the 100,000s. A more recent work Zhu et al. (2020) proposed an iterative splicing method called ABESS, short for adaptive best subset selection, to solve the BSS problem. They showed that ABESS enjoys both statistical accuracy and polynomial computational complexity when the design satisfies the sparse Riesz condition and the minimum signal strength is of order $\Omega\left(\frac{s \log p \log \log n}{n}\right)^{1/2}$. From the statistical perspective, Bertsimas et al. (2016) and Bertsimas et al. (2020) numerically demonstrated higher predictive power and lower false discovery rate (FDR) of the BSS solutions than LASSO. Zhu et al. (2020) presented similar numerical results and also showed that ABESS is able to estimate the model sparsity more accurately than LASSO, MCP and SCAD. On the other hand, Hastie et al. (2020) conducted more extensive numerical experiments on comparison between LASSO, relaxed LASSO and BSS, particularly covering a wider lower range of signal-to-noise ratio (SNR) than Bertsimas et al. (2016). The main message therein is that regarding prediction accuracy, LASSO outperforms BSS in the low SNR regime, while the situation is reversed in the high SNR regime. Furthermore, relaxed LASSO (Meinshausen, 2007) was shown to be the overall winner, performing similarly or outperforming both LASSO and BSS in nearly all the cases in Hastie et al. (2020).

In this paper, we further compare BSS with the surrogate methods through a new lens: early solution paths. A solution path provides a comprehensive view of a model selection procedure: it displays tradeoff between type I and type II errors of the selected models as the regularization or the model size varies. In contrast, model consistency requires specifying an exact level of regularization or sparsity, which is often infeasible in practice. Moreover, model consistency is often too ambitious a goal to achieve in real-world problems, where the true sparsity or signal strength rarely satisfies the theoretical requirement. Therefore, the tradeoff between type I and type II error is inevitable, thereby rendering solution path a more meaningful evaluation criteria for comparing variable selectors. Moreover, the early solution path, which tracks the first few selected variables, is of particular interest to scientific discovery, given that it is often prohibitive to assess the causality of many variables by experiments. It is thus imperative to provide strong statistical guarantee, say FDR, for the early solution path so that the subsequent scientific effort does not go into waste.

Formally, define the early solution path of BSS as the set $\{\hat{\beta}_{\text{best}}(s)\}_{s<s^*}$, i.e., the BSS estimators whose sparsity is less than that of $\beta^*$. Our major goal here is to explicitly characterize when BSS achieves zero false discovery throughout the early solution path, which we refer to as sure early selection. There are two recent works Su et al. (2017) and Fan et al. (2020a) on LASSO and BSS respectively that are closely related with our work. Su et al. (2017) showed that under the regime of linear sparsity, i.e., $s^*/p$ tends to a constant, even when the design matrix $X$ has independent columns, false discoveries occur early on the LASSO path with high probability, regardless of the signal strength. Fan et al. (2020a) numerically assessed the solution paths of BSS, SCAD, LASSO and SIS (Sure Independence Screening) in terms of FDR and TPR (true positive rate). They showed that the early selection of BSS (more precisely, an approximate BSS algorithm by iterative
Figure 1: The FDR-TPR paths of CoSaMP Needell and Tropp (2009) (blue), SCAD (black), LASSO (red) and MCP (violet) under autoregressive design ($\mathbf{x} \sim \mathcal{N}(\mathbf{0}, \Sigma)$ with $\Sigma_{ij} = 0.8^{|i-j|}$ for $i, j \in [p]$).

This is one setup we presented in Figure 3. We set $p = 1,000$, $s^* = 50$ and $n = \lceil 2s^* \log p \rceil$. The dots represent the solutions chosen by 10-fold cross-validation points of different methods. The FDR and TPR of each point on the solution path is based on averaging FDP and TPP of the solutions over 100 independent Monte Carlo experiments, where we randomly generate $\mathbf{X}, \beta^*, \epsilon$ and compute $y = \mathbf{X}\beta^* + \epsilon$. More implementation details are in Section 3.2.

Hard thresholding) has substantially lower FDR than that of LASSO, SCAD and SIS under a great variety of design. However, the theory in Fan et al. (2020a) focuses only on the latter stage of the solution path ($s \geq s^*$) and does not cover the early stage; this motivates us to provide theoretical explanation for the sure early selection phenomenon of BSS.

On the computational aspect, we choose CoSaMP (Compressive Sampling Matching Pursuit), an iterative two-stage hard thresholding algorithm proposed by Needell and Tropp (2009), to obtain an approximate solution path of BSS. Jain et al. (2014) established a crucial optimization theorem that relates CoSaMP with BSS: given the true sparsity $s^*$, CoSaMP can find a model of size slightly larger than $s^*$ that achieves superior goodness of fit over the exact best size-$s$ subset within few iterations. Based on this, a more recent work Fan et al. (2020a) discovered that CoSaMP (referred to as IHT therein) can inherit sure screening properties from BSS. These positive results motivate us to use CoSaMP as an approximate solver for BSS. Figure 1 compares the solution path of CoSaMP with those of MCP, SCAD and LASSO under autoregressive design. There the $x$-axis represents FDR and the $y$-axis represents logarithmic TPR. Note that a perfect model selection procedure yields a “Γ”-shaped FDR-TPR path, meaning that it selects no spurious variable until enforced to select more than $s^*$ variables. One can see from Figure 1 that CoSaMP’s FDR-TPR path is the closest to the perfect “Γ”-shape among all the paths, suggesting superiority of BSS over the competing penalized approaches in terms of FDR-TPR tradeoff. More comparison of this type can be found in Section 3.2.
1.1 Contributions of this paper

Below we summarize the major contributions of our work:

(1) In Section 2.1, we establish a sufficient condition for (approximate) BSS to achieve sure early selection for any target sparsity \( s \leq s^* \) based on a quantity called \textit{minimum projected signal margin}. This margin is entirely independent of the RE parameter of the design and even accommodates degenerate covariance structure of design.

(2) In Section 2.2, we show that throughout the entire solution path, i.e., for any \( s < s^* \), the sufficient condition above is nearly necessary (up to a universal constant) for BSS to achieve sure early selection.

(3) In Section 2.3, we explicitly derive a non-asymptotic bound of the minimum projected signal margin under random design to allow for verification of the established sufficient and necessary conditions.

(4) In Section 3.2, we use CoSaMP as an approximate algorithm to implement BSS and show that its early solution path involves much fewer spurious variables than LASSO, SCAD and MCP, in particular under highly correlated design.

(5) In Section 3.3, we propose a model selection procedure called LOCK (L-zerO Constrained feature screening + Knockoff) that numerically exhibits superior FDR control and TPR performance over competing FDR control procedures.

The proof for all the theorems and the technical lemmas are relegated to the appendix.

1.2 Notation

We use regular letters, bold regular letters and bold capital letters to denote scalars, vectors and matrices respectively. Given any \( a, b \in \mathbb{R} \), we say \( a \lesssim b \) if there exists a universal constant \( C > 0 \) such that \( a \leq Cb \); we say \( a \gtrsim b \) if there exists a universal constant \( c > 0 \) such that \( a \geq cb \). For any positive integer \( a \), we use \([a]\) to denote the set \( \{1, 2, \ldots, a\} \). For any vector \( a \) and matrix \( A \), we use \( a^\top \) and \( A^\top \) to denote the transpose of \( a \) and \( A \) respectively. For any matrix \( X \in \mathbb{R}^{n \times p} \), define the projection operator for its column space

\[
P_X := X(X^\top X)^+ X^\top,
\]

where the superscript symbol \(^+\) denotes the Moore-Penrose inverse. We use \( X_S \) to denote the submatrix of \( X \) with columns indexed by \( S \subset [p] \). For any random variable \( X \) valued in \( \mathbb{R} \), define

\[
\|X\|_{\psi_2} := \inf\{t > 0 : \mathbb{E} \exp(X^2/t^2) \leq 2\} \quad \text{and} \quad \|X\|_{\psi_1} := \inf\{t > 0 : \mathbb{E} \exp(|X|/t) \leq 2\}.
\]

(6)

For any random vector \( x \) valued in \( \mathbb{R}^p \), define

\[
\|x\|_{\psi_2} := \sup_{\|v\|_2 = 1} \|v^\top x\|_{\psi_2} \quad \text{and} \quad \|x\|_{\psi_1} := \sup_{\|v\|_2 = 1} \|v^\top x\|_{\psi_1}.
\]

(7)
For any two subsets $S_1, S_2 \subset [p]$, let $S_1 \setminus S_2$ denote $S_1 \cap S_2^c$. For any estimate $\hat{S}$ of the true model $S^*$, define the false discovery proportion (FDP) and true positive proportion (TPP) as

$$\text{FDP}(\hat{S}) := \frac{|\hat{S} \setminus S^*|}{\max(|\hat{S}|, 1)} \quad \text{and} \quad \text{TPP}(\hat{S}) := \frac{|\hat{S} \cap S^*|}{|S^*|}. \quad (8)$$

For any estimator $\hat{\beta}$ of $\beta^*$, we abuse the notation to define

$$\text{FDP}(\hat{\beta}) := \frac{|\text{supp}(\hat{\beta}) \setminus S^*|}{\max(|\text{supp}(\hat{\beta})|, 1)} \quad \text{and} \quad \text{TPP}(\hat{\beta}) := \frac{|\text{supp}(\hat{\beta}) \cap S^*|}{|S^*|}.$$

The false discovery rate (FDR) and true positive rate (TPR) are defined as expectation of FDP and TPP respectively.

2 Sure early selection of the best subset

Fix $s \leq s^*$. Our focus in this section is to establish sufficient and necessary conditions for BSS to achieve sure early selection, i.e., $\text{FDP}(\hat{\beta}^\text{best}(s)) = 0$. To start with, we introduce a measure called minimum projected signal margin to characterize fundamental difficulty for BSS to achieve sure early selection. Define

$$\mathbb{A}(s) := \{S : S \subset [p], |S| = s, S \setminus S^* \neq \emptyset\} \quad \text{and} \quad \mathbb{A}^*(s) := \{S : S \subset S^*, |S| = s\}.$$

In words, $\mathbb{A}(s)$ is the set of all size-$s$ models with at least one spurious variable, while $\mathbb{A}^*(s)$ is the set of those without any spurious variable. We also define $\mathbb{A}_t(s) := \{S \in \mathbb{A}(s) : |S \setminus S^*| = t\}$ for $t \in [s]$, which collects all the models in $\mathbb{A}(s)$ with exactly $t$ false variables. For any $S_1, S_2 \subset [p]$, define the marginal projection operator

$$P_{S_1 \mid S_2} := P_{X_{S_1}} - P_{X_{S_1 \cap S_2^c}}.$$

Note that since $S_1 \cap S_2 \subset S_1$, $P_{S_1 \mid S_2}$ is an projection operator: it captures the directions in the column space of $X_{S_1}$ that are orthogonal to the column space of $X_{S_1 \cap S_2}$, representing the marginal explanation capacity of using $X_{S_1}$ as predictors on top of $X_{S_1 \cap S_2}$. Writing $\mu^* = X^{\beta^*}$, we define the optimal feature swap $\Phi : \mathbb{A}(s) \rightarrow \mathbb{A}^*(s)$ as

$$\Phi(S) := \arg\max_{S^t \in \mathbb{A}^*(s), S \cap S^t \subset S^t} \|P_{X_{S^t}} \mu^*\|_2^2. \quad (9)$$

As the name indicates, $\Phi$ swaps the spurious variables in $S$ for the true ones that maximize fitting power. Based on $\Phi$, we are now in position to define the projected signal margin of $S \in \mathbb{A}(s)$ as

$$m(S) := \frac{\|P_{\Phi(S)} S \mu^*\|_2 - \|P_{S \setminus \Phi(S)} \mu^*\|_2}{|\Phi(S) \setminus S^t|^{1/2}} \quad (10)$$

and its minimum over $\mathbb{A}(s)$ as $m_* (s) := \min_{S \in \mathbb{A}(s)} m(S)$. Intuitively, $m_*(s)$ represents the minimum gain of explanation power from the optimal feature swap, normalized by the square root of the number of spurious variables. The smaller $m_*(s)$, the easier for some $S \in \mathbb{A}(s)$ to outperform $\Phi(S)$ in terms of goodness of fit, giving rise to potential false discovery. Note that if $\beta_{j}^* = b, \forall j \in [p]$ and
\( n^{-1}X^\top X = I_p \), i.e., homogeneous signal and orthonormal design, we have \( m(S) = bn^{1/2} \) for any \( S \in \Lambda(s) \), implying that \( m_*(s) = bn^{1/2} \). Regarding general cases, we refer the readers to Section 2.3, where we establish non-asymptotic bounds for projected signal margin under random design.

In the sequel, we will see that \( m_*(s) \) dictates the statistical behavior of the early path of BSS: the sufficient and necessary condition for BSS to achieve sure early selection essentially boils down to merely a lower bound of \( m_*(s) \). Throughout this section, we assume that \( s^* < n \) and that \( \|\varepsilon\|_{\psi^2} \leq \sigma \) in (1).

### 2.1 Sufficient conditions

The goal of this subsection is to explicitly characterize a sufficient condition for \( \hat{\beta}^{\text{best}}(s) \) to achieve zero false discovery. Given the optimization challenge of obtaining \( \hat{\beta}^{\text{best}}(s) \) exactly, we extend the scope of our statistical analysis to embrace all near best \( s \)-subsets, i.e., the size-\( s \) subsets that yield similar goodness of fit as the best subset. Specifically, for any \( S \subset [p] \), let \( L_S = y^\top (I - P_S) y \) and \( L_* = \min_{S \subset [p], |S| = s} L_S \). Given any tolerance level \( \eta \in [0, 1) \), consider the following collection of near best \( s \)-subsets:

\[
S(\eta) := \{ S : |S| = s, L_S \leq L_* + \eta \|\Phi(S)\| \\Phi(S)^2 \}
\]

(11)

Here \( \eta \) is a tolerance threshold that determines the condition for \( S \) to be a near best \( s \)-subset: the larger \( \eta \), the higher fitting error we can tolerate for a near best subset. Below we introduce a sufficient condition for all sets in \( S(\eta) \) to achieve sure selection.

**Theorem 2.1.** Suppose that \( \log p \gtrsim s^* \). There exists a universal constant \( C > 0 \), such that for any \( \xi > C \) and \( 0 \leq \eta < 1 \), whenever

\[
m_*(s) \geq \frac{8\xi \sigma (\log p)^{1/2}}{1 - \eta},
\]

(12)

we have that

\[
P\{\text{FDP}(\hat{S}) = 0, \forall \hat{S} \in S(\eta)\} \geq 1 - Csp^{-2}(C^{-2}\xi^2 - 1).
\]

(13)

Theorem 2.1 says that whenever the minimum projected signal margin \( m_*(s) \) satisfies the lower bound (12), all the sets in \( S(\eta) \) are sure selection sets with high probability. Here we first discuss the roles of \( \eta \) and \( \xi \) in the theorem. Note that as per (12), the larger \( \eta \) is, i.e., the more relaxed requirement we impose on near best \( s \)-subsets, the higher \( m_*(s) \) we need to guarantee sure selection; this is natural given that \( S(\eta) \) grows as \( \eta \) increases. Regarding \( \xi \), by assessing its role on the right hand side of (12) and (13) respectively, we can deduce that larger minimum projected signal margin leads to higher confidence in sure selection.

Perhaps the most important message of this theorem is that the covariance structure of the design is non-essential in determining the early path of BSS. Through the marginal projection operators, Theorem 2.1 unveils that it is the gap in capacity of capturing the true signal that determines if any false variable enters the early path of BSS. Given that projection operators are invariant with respect to linear combinations, the minimum projected signal margin is **robust against collinearity**. For instance, given \( a, b \in \mathbb{R}^n \), consider a simple yet illustrative case where \( X_{S^*} = a1_{s^*}^\top \) and \( X_{S^**} = b1_{p-s^*}^\top \), i.e., all the columns of \( X_{S^*} \) equal \( a \), and all the columns of \( X_{S^**} \)
equal \( b \). Neither the irrepresentable condition (5) or the sparse Riesz condition accommodates this case, while the minimum projected signal margin does well. By applying Theorem 2.1, one can deduce that as long as \( a \) and \( b \) are not too correlated and the signal is strong, BSS achieves sure early selection with high probability. Section 3.2 provides abundant amount of numerical evidence to demonstrate the robustness of BSS.

We also emphasize that there is crucial difference between our sufficient condition (12) and that for model consistency of BSS. Consider the minimum projected signal margin when \( s = s^* \), for which we have that

\[
m^2_*(s^*) = \min_{S \in \mathcal{A}(s^*)} \left( \frac{\| P_{S^*} \mu^* \|_2 - \| P_S \mu^* \|_2^2}{|S \setminus S^*|} \right) \leq \min_{S \in \mathcal{A}(s^*)} \left( \frac{\| P_{S^*} \mu^* \|_2^2 - \| P_S \mu^* \|_2^2}{|S \setminus S^*|} \right) = n \tau_*(s^*),
\]

where \( \tau_*(s^*) \) is the identifiability margin defined in Fan et al. (2020a). Therefore, \( m_*(s^*) \gtrsim \sigma (\log p)^{1/2} \) is a stronger, though not necessarily strictly so, than \( \tau_*(s^*) \gtrsim \sigma^2 \log p/n \), which was shown by Zhu et al. (2020) as a sufficient and near necessary condition for BSS to recover the true support. As we shall see in Section 2.2, this stronger requirement is not due to technical limitation, but necessary for BSS to achieve sure early selection. Such gap between \( m_*(s^*) \) and \( \tau_*(s^*) \) reflects the difference in the fundamental difficulty for BSS to obtain sure early selection and model consistency: The early solution path underestimates the true sparsity \( s^* \), thereby requiring wider signal margin to compensate for model misspecification and maintain zero false discovery.

Another related work we would like to discuss here is Su et al. (2017) on the early solution path of LASSO. Define the LASSO estimator \( \hat{\beta}_{\text{lasso}}(\lambda) \) as

\[
\hat{\beta}_{\text{lasso}}(\lambda) := \arg\min_{\beta \in \mathbb{R}^p} \frac{1}{2} \| y - X \beta \|_2^2 + \lambda \| \beta \|_1.
\]

Theorem 2.1 of Su et al. (2017) says that regardless of \( \sigma > 0 \), for any arbitrary small constants \( \lambda_0 > 0 \) and \( \eta > 0 \), as \( n, s^*, p \to \infty \) with \( n/p \) and \( s^*/p \) tend to constants, the probability of the event

\[
\bigcap_{\lambda \geq \lambda_0} \left\{ \text{FDP} \left( \hat{\beta}_{\text{lasso}}(\lambda) \right) \geq q^*(\text{TPP}(\hat{\beta}_{\text{lasso}}(\lambda))) - \eta \right\}
\]

tends to one, where \( q^* \) is a strictly increasing function with \( q^*(0) = 0 \). We refer the readers to Su et al. (2017) for specific definition and visual illustration of \( q^* \). Simply speaking, this implies that false discovery occurs early on the solution path of LASSO however strong the signal is. While it is tempting to conclude theoretical superiority of BSS over LASSO on the early solution path, we emphasize that our Theorem 2.1 is actually not directly comparable with Theorem 2.1 of Su et al. (2017), given that we mainly focus on ultra-high dimensional setup, i.e., \( \log p \gtrsim s^* \), and that Su et al. (2017) focus on linear sparsity regimes. It thus remains open how the early solution path of BSS behaves under the linear sparsity setup and how that is compared with LASSO. However, the simulation experiments in Section 3.2 clearly demonstrate the numerical superiority of BSS over LASSO in terms of FDR and TPR on their early solution paths.

Beyond the guarantee for absolutely sure selection as in Theorem 2.1, we can extend our argument to provide arbitrary level of FDP guarantee. Given any \( 0 < q < 1 \), consider the following
variant of the minimum projected signal margin that corresponds to $q$-level FDP:

$$m_q(s) := \min_{S \in \bigcup_{t \geq \lceil qs \rceil} A_t(s)} m(S)$$

as well as the corresponding collection of near best $s$-subsets:

$$S_q(\eta) := \{S : |S| = s, \mathcal{L}_S \leq \mathcal{L} + \eta |\Phi(S)\{S|m^2_q(s)\} \}.$$

Now we are ready to present the following corollary on $q$-level FDP guarantee.

**Corollary 2.1.** Suppose that $\log p \gtrsim s^*$. There exists a universal constant $C > 0$, such that for any $\xi > C$ and $0 \leq \eta < 1$, if

$$m_q(s) \geq \frac{8 \xi \sigma (\log p)^{1/2}}{1 - \eta},$$

then we obtain

$$\mathbb{P}\{\text{FDP}(\tilde{S}) \leq q, \forall \tilde{S} \in S_q(\eta)\} \geq 1 - Csp^{-2(C-2)^2-1}. \quad (15)$$

### 2.2 Necessary conditions

In this section, we aim to show that the lower bound (12) of the minimum projected signal margin is almost necessary for BSS to achieve sure early selection in general setups (without the assumption that $\log p \gtrsim s^*$). We investigate the necessity in two scenarios separately: (i) $s = 1$; (ii) $s \geq 2$.

#### 2.2.1 Sure first selection

We start with the simplest case: $s = 1$, i.e., we aim to find only one true predictor. Let

$$j^\dagger := \arg\max_{j \in S^*} \|P_{X_j} \mu^*\|_2^2,$$

which denotes the best variable in $S^*$ in terms of fitting the signal $\mu^*$. Then for any $j \in (S^*)^c$, $\Phi\{j\} = \{j^\dagger\}$ and

$$m\{j\} = \|P_{X_j} \mu^*\|_2 - \|P_{X_j} \mu^*\|_2.$$

We say a set $\mathcal{P}$ is a $\delta$-packing set if and only if for any $u, v \in \mathcal{P}$, $\|u - v\|_2 \geq \delta$. Consider the following two assumptions on the problem setup:

**Assumption 2.1.** Let $u_j = X_j/\|X_j\|_2$ for $j \in [p] \setminus S^*$. For some $0 < \delta_0 < 1$, there exists an index set $\mathcal{J}_{\delta_0} \subset (S^*)^c$ of delusive features satisfying:

(i) $\{u_j\}_{j \in \mathcal{J}_{\delta_0}}$ is a $\delta_0$-packing set;

(ii) $|\mathcal{J}_{\delta_0}| \geq p^c_{\delta_0}$ for some $0 < c_{\delta_0} < 1$ depending on $\delta_0$ such that $\delta_0^2 c_{\delta_0} \log p > 1$;

(iii) Each feature in $\mathcal{J}_{\delta_0}$ has small projected signal margin, i.e.,

$$0 < m\{j\} < \frac{\delta_0 \sigma (c_{\delta_0} \log p)^{1/2}}{20}, \forall j \in \mathcal{J}_{\delta_0}. \quad (16)$$

**Assumption 2.2.** There exists a universal constant $\xi > 8$ such that

$$\|P_{X_j} \mu^*\|_2 \geq \xi \delta_0 \sigma (c_{\delta_0} \log p)^{1/2}.$$
The main idea of Assumption 2.1 is that we can find sufficiently many delusive features with small projected signal margin as characterized in (16). Furthermore, perceiving Euclidean distance between \( \{\tilde{u}_j\}_{j \in [p]} \) as the correlation proxy between the corresponding features, condition (ii) requires that the delusive variables be dissimilar to each other, ensuring that the impact of the dimension is nontrivial. Assumption 2.2 says that the best single variable has sufficient explanation power for the true signal \( \mu^* \). This assumption is standard: one can deduce from the well-known \( \beta \)-min condition that \( \sigma(\log p)^{1/2} \) is the minimum signal strength we need for \( \|P_{X_j} \mu^*\|_2 \) to identify \( j^\dagger \) as a true predictor.

Now we present our theorem on the necessary condition for the very first selection of BSS to be true.

**Theorem 2.2.** Suppose that \( \{\epsilon_i\}_{i \in [n]} \) are independent Gaussian noise with variance \( \sigma^2 \). Under Assumptions 2.1 and 2.2, we have that

\[
P \left( \min_{j \in J_{\delta_0}} \mathcal{L}_{\{j\}} < \min_{j^* \in S^*} \mathcal{L}_{\{j^*\}} \right) \geq 1 - 4s^*p^{- (c_1\xi_0^2 - 1)c_0} - s^*p^{- c_1\xi_0^2c_0},
\]

where \( c_1 \) is a universal constant.

Given Theorem 2.2, one can deduce by comparing (12) and (16) that the lower bound of the minimum projected signal margin in Theorem 2.1 is almost tight: whenever there are sufficiently many spurious features whose projected signal margins violate this lower bound (up to a constant), the first shot of BSS is false with high probability.

### 2.2.2 Sure early multi-selection

Now we move on to the general case when \( s \geq 2 \). Define \( S^\dagger(s) \) to be the best size-\( s \) subset of \( S^* \) in terms of fitting the signal \( \mu^* \), i.e., \( S^\dagger(s) := \arg\max_{S \subseteq \mathbb{A}^* \{s\}} \|P_{X_S} \mu^*\|_2^2 \). For simplicity, we write \( S^\dagger \) as \( S^\dagger \) in the sequel. Consider the following two assumptions on the problem setup:

**Assumption 2.3.** There exist \( j_0 \in S^\dagger \) and \( 0 < \delta_0 < 1 \) such that if we let \( S^\bot_0 = S^\dagger \setminus \{j_0\} \), \( \tilde{u}_j := (I - P_{X_{S^\bot_0}})X_j \) and \( \bar{u}_j := \tilde{u}_j/\|\tilde{u}_j\|_2 \) for \( j \in [p] \setminus S^* \), we can find an index set \( J_{\delta_0} \subseteq (S^*)^c \) of delusive features satisfying:

(i) \( \{\bar{u}_j\}_{j \in J_{\delta_0}} \) is a \( \delta_0 \)-packing set;

(ii) \( |J_{\delta_0}| \geq p^{c_{\delta_0}} \) for some \( 0 < c_{\delta_0} < 0 \) depending on \( \delta_0 \);

(iii) Consider all the models of size \( s \) that are formed by replacing \( j_0 \) in \( S^\dagger \) with a spurious variable in \( J_{\delta_0} \), namely, \( K_{j_0} := \{S^\dagger \cup \{j\} : j \in J_{\delta_0}\} \). Then each set in \( K_{j_0} \) has small projected signal margin, i.e.,

\[
0 < m(S) < \frac{\delta_0\sigma(c_{\delta_0} \log p)^{1/2}}{20}, \forall S \in K_{j_0}, \tag{17}
\]

**Assumption 2.4.** There exists a universal constant \( \xi > \max\left\{8/(\delta_0^{1/2} \log p), 2\right\} \) such that

\[
\min_{S \subseteq \mathbb{A}^* \{s\}, S \neq S^\dagger} \frac{\|P_{S \setminus S^\dagger} \mu^*\|_2 - \|P_{S \setminus S^\dagger} \mu^*\|_2}{|S^\dagger \setminus S|^{1/2}} \geq \xi \sigma(\log p)^{1/2}.
\]
Assumption 2.3 is similar to Assumption 2.1; the only difference is that in Assumption 2.3, each delusive model is not a singleton but a set constructed by replacing \( j_0 \) in \( \mathcal{S}^\dagger \) with a spurious variable in \( \mathcal{J} \). Assumption 2.4 guarantees that \( \mathcal{S}^\dagger \) stands out from the rest of the size-\( s \) sure selection sets in terms of fitting \( \mu^* \), even in presence of noise \( \epsilon \). This implies that if we can find a candidate model outside \( \mathcal{A}^*(s) \) that fits \( \mathbf{y} \) better than \( \mathcal{S}^\dagger \), BSS is doomed to include false discovery.

The following theorem shows that with high probability, the best subset involves false selection once there are sufficiently many models in \( \mathcal{A}(s) \) with small projected signal margin as per (17). Therefore, together with Theorem 2.2, it shows tightness of the lower bound of the minimum projected signal margin (12) (up to a constant) uniformly over \( s \in [s^* - 1] \).

**Theorem 2.3.** Suppose that \( \{\epsilon_i\}_{i\in[n]} \) are independent Gaussian noise with variance \( \sigma^2 \). Under Assumptions 2.3 and 2.4, we have that
\[
P \left( \min_{\mathcal{S} \in \mathcal{A}(s)} L_{\mathcal{S}} < \min_{\mathcal{S} \in \mathcal{A}^*(s)} L_{\mathcal{S}} \right) \geq 1 - 4p^{-\left(\epsilon_1 \delta_0^2 - 1\right)c_0} - p^{-c_1 \delta_0^2 c_0} - 6sp^{-\left(\epsilon_2 \xi^2 - 2\right)},
\]
where \( c_1 \) and \( c_2 \) are universal constants.

### 2.3 Projected signal margin under random design

The previous two subsections demonstrate the pivotal role of the minimum projected signal margin \( m^*(s) \) in underpinning the sure selection of BSS. In this subsection, we explicitly derive \( m^*(s) \) under random design, so that we can verify the sufficient condition (12) with ease. To start with, for any two size-\( s \) sets \( \mathcal{S} \in \mathcal{A}(s) \) and \( \mathcal{S}^\dagger \in \mathcal{A}^*(s) \) such that \( \mathcal{S} \cap \mathcal{S}^\dagger \subset \mathcal{S}^\dagger \), we analyze two crucial components of the projection signal margin, \( \mu^* \top \mathbf{P}_{\mathcal{S} \setminus \mathcal{S}^\dagger} \mu^* \) and \( \mu^* \top \mathbf{P}_{\mathcal{S} \setminus \mathcal{S}^\dagger} \mu^* \), under Gaussian design. Suppose \( \{x_i\}_{i\in[n]} \) are \( n \) independent and identically distributed observations of \( \mathbf{x} \sim \mathcal{N}(0, \Sigma) \). For notational simplicity, let \( \mathcal{S}_1 = \mathcal{S} \cap \mathcal{S}^\dagger, \mathcal{S}_2 = \mathcal{S}^\dagger \setminus \mathcal{S}_1 \) and \( \mathcal{S}_3 = \mathcal{S} \setminus \mathcal{S}_1 \). Figure 2 shows the relationship between the sets. Next we introduce some quantities that are involved in the concentration bounds we establish. Define
\[
\mathbf{h} := \text{cov}(x_{\mathcal{S}_2}, \mu^* | x_{\mathcal{S}_1}) = (\Sigma_{\mathcal{S}_2 \mathcal{S}^\dagger} - \Sigma_{\mathcal{S}_2 \mathcal{S}_1} \Sigma_{\mathcal{S}_1 \mathcal{S}^\dagger}^{-1} \Sigma_{\mathcal{S}_1 \mathcal{S}_2}) \beta^*
\]
and
\[
\mathbf{H} := \text{cov}(x_{\mathcal{S}_2}, x_{\mathcal{S}_2} | x_{\mathcal{S}_1}) = \Sigma_{\mathcal{S}_2 \mathcal{S}_2} - \Sigma_{\mathcal{S}_2 \mathcal{S}_1} \Sigma_{\mathcal{S}_1 \mathcal{S}_1}^{-1} \Sigma_{\mathcal{S}_1 \mathcal{S}_2}.
\]
Then write
\[
\nu_1 := \mathbf{h}^\top \mathbf{H}^{-1} \mathbf{h} \quad \text{and} \quad \nu_2 := \text{var}(\mu^* | x_{\mathcal{S}_1}) - \nu_1 = \beta^* \top (\Sigma_{\mathcal{S}^\dagger \mathcal{S}^\dagger} - \Sigma_{\mathcal{S}^\dagger \mathcal{S}_1} \Sigma_{\mathcal{S}_1 \mathcal{S}_1}^{-1} \Sigma_{\mathcal{S}_1 \mathcal{S}^\dagger}) \beta^* - \nu_1.
\]
Similarly, define 

$$h' := \text{cov}(x_{S,1}, \mu^* | x_{S,1}) = (\Sigma_{S,S} - \Sigma_{S,S} \Sigma_{S,1}^{-1} \Sigma_{S,1} \Sigma_{S,1}^*) \beta^*$$

and

$$H' := \text{cov}(x_{S,1}, x_{S,1} | x_{S,1}) = \Sigma_{S,S} - \Sigma_{S,S} \Sigma_{S,1}^{-1} \Sigma_{S,1} \Sigma_{S,1}.$$ 

Then write

$$\nu'_1 := h'^T H'^{-1} h' \quad \text{and} \quad \nu'_2 := \beta'^T (\Sigma_{S,S} - \Sigma_{S,S} \Sigma_{S,1}^{-1} \Sigma_{S,1} \Sigma_{S,1}^*) \beta^* - \nu'_1.$$ 

Now we are in position to present the concentration bounds for $\mu^* P_{S|S} \mu^*$ and $\mu^* P_{S|S^\dagger} \mu^*$.

**Lemma 2.1.** For any two size-$s$ sets $S \in \mathcal{A}(s)$ and $S^\dagger \in \mathcal{A}^*(s)$ such that $S \cap S^* \subset S^\dagger$ and any $\xi > 0$, we have

$$\mathbb{P} \left[ \mu^* P_{S|S} \mu^* - \{(n - s + t) \nu_1 + t \nu_2\} \right] >$$

$$\xi \left( 3 \nu_1 (n - s + t)^{1/2} + 6 (\nu_1 \nu_2)^{1/2} (n - s + t)^{1/2} + 3 \nu_2 t^{1/2} \right) \leq 6 e^{-c \min(\xi^2, \xi)} \quad \text{and}$$

$$\mathbb{P} \left[ \mu^* P_{S|S^\dagger} \mu^* - \{(n - s + t) \nu'_1 + t \nu'_2\} \right] >$$

$$\xi \left( 3 \nu'_1 (n - s + t)^{1/2} + 6 (\nu'_1 \nu'_2)^{1/2} (n - s + t)^{1/2} + 3 \nu'_2 t^{1/2} \right) \leq 6 e^{-c \min(\xi^2, \xi)},$$

where $t = |S^\dagger \setminus S|$, and where $c$ is a universal constant.

Now we apply Lemma 2.1 to analyze the minimum projected signal margin between any set $S$ with false discovery (i.e., $\forall S \in \mathcal{A}^*(s)$) and its optimal swap set $\Phi(S)$. The following theorem gives an explicit lower bound of $m_*(s)$ when $\Sigma = I$ and $\beta^*_s$ has homogeneous entries.

**Theorem 2.4.** Consider $n$ independent observations $\{x_i\}_{i \in [n]}$ of $\mathcal{N}(0, I_p)$. Suppose that $\log p \gtrsim s^*$, and that $\beta^*_j = \beta, \forall j \in S^*$. Then there exist universal constants $C, c > 0$ such that for any $\kappa > 9C^2$, whenever $n \geq \kappa s^* s (\log p)^2$, we have

$$\mathbb{P} \{ m_*(s) \geq n^{1/2} \sigma / |\beta| \} \geq 1 - Csp^{-\left( C^{-1} \kappa^{1/2} - 3 \right)},$$

which implies that $|\beta| \gtrsim \sigma \left( \frac{\log p}{n} \right)^{1/2}$ is sufficient for BSS to achieve sure early selection with high probability for any $s \in [s^* - 1]$.

### 3 Numerical study

The main goal of this section is to numerically investigate the FDR and TPR of the early path of best subset selection. We choose CoSaMP (compressive sampling matching pursuit), an iterative two-stage hard thresholding algorithm proposed by Needell and Tropp (2009), as the computational surrogate for best subset selection. Note that CoSaMP is different from the original iterative hard thresholding (IHT) algorithm in Blumensath and Davies (2008) and Blumensath and Davies (2009), which is instead a projected gradient descent algorithm that projects the iterate to an $\ell_0$-ball after a gradient descent update. CoSaMP performs two rounds of hard thresholding in each iteration: it
first expands the model by recruiting the largest coordinates of the gradient (first hard thresholding) and then contracts the model by discarding the smallest components of the refitted signal on the expanded model (second hard thresholding).

Under restricted isometry conditions, Needell and Tropp (2009) showed that CoSaMP achieves optimal sample complexity and optimization guarantees, as well as high computational and memory efficiency, for recovering sparse signals. Later, Jain et al. (2014) established similar statistical and optimization guarantees for a generalized version of CoSaMP that serves any objective satisfying restricted strong convexity (RSC) and restricted strong smoothness (RSS). They referred to the algorithm as a “fully corrective” two-stage hard thresholding algorithm. One particularly interesting result regarding this algorithm is that given the true sparsity $s^*$, it can find a model whose sparsity is of the same order of $s^*$ that achieves superior goodness of fit over the exact best size-$s$ subset. Based on this optimization guarantee, a more recent work Fan et al. (2020a) discovered that CoSaMP (referred to as IHT therein) can achieve sure screening properties when enforced to select more than $s^*$ variables. These positive results motivate us to use CoSaMP to compute approximate solutions for best subset selection.

We organize this section as follows: We first elucidate the CoSaMP algorithm in Section 3.1. We then compare its FDR-TPR path with those of other model selection procedures in Section 3.2. Finally, in Section 3.3, we use CoSaMP to perform preliminary screening for the knockoff filter (Barber et al., 2015; Candès et al., 2018) to enhance its power.

### 3.1 The CoSaMP algorithm

For any $v \in \mathbb{R}^p$ and $r \in \mathbb{N}$, define

$$T_{abs}(v, r) := \{ j : |v_j| \text{ is among the top } r \text{ largest values of } \{|v_k|\}_{k=1}^p \}.$$ 

In words, $T_{abs}(v, r)$ collects the indexes of the top $r$ largest absolute values in $v$. For any $\beta \in \mathbb{R}^p$, let $L(\beta) = \sum_{i=1}^n (y_i - x_i^\top \beta)^2$. For any matrix $A$, recall that its Moore-Penrose inverse is denoted by $A^+$. To be more self-contained, in the following we present the pseudocode of CoSaMP in Algorithm 1.

In each iteration, CoSaMP expands the current model by recruiting top $l$ variables with the largest absolute gradient values. Note that $\nabla L(\beta) = X^\top (y - X \beta)$, which is basically sample covariance between the residuals $y - X \beta$ and the design $X$. Hence, this expansion step can be interpreted as selecting variables with the highest absolute marginal covariance with the residual. Then CoSaMP fits the expanded model by least squares, selects the top $\pi$ variables with the largest absolute regression coefficients, and finally refits these $\pi$ variables using least squares. The algorithm is halted whenever the two iterates are sufficiently close.

We further propose Algorithm 2 to approximate the solution path of BSS. Specifically, consider a set of projection sizes $\Pi = \{\pi_1, \ldots, \pi_M\}$ with $\pi_1 < \ldots < \pi_M$. For any $i \in [M]$, let $\tilde{\beta}^{cs}(i)$ denote the solution of CoSaMP with $\pi = \pi_i$. Instead of computing $\tilde{\beta}^{cs}(i)$ for each $i \in [M]$ separately, we propose to use $\tilde{\beta}^{cs}(i)$ as a warm initializer to compute $\tilde{\beta}^{cs}(i+1)$ (see line 3 of Algorithm 2), which turns out to substantially accelerate the convergence in our numerical experiments.
Algorithm 1 CoSaMP\((X, y, \hat{\beta}_0, \pi, l, \tau)\)

**Input:** Design matrix \(X\), response \(y\), initial value \(\hat{\beta}_0\), projection size \(\pi\), expansion size \(l\), convergence threshold \(\tau > 0\)

1: \(t \leftarrow 0\)
2: repeat
3: \(G_t \leftarrow T_{abs}(\nabla L(\hat{\beta}_t), l)\)
4: \(S_t \leftarrow \text{supp}(\hat{\beta}_t) \cup G_t\)
5: \(\hat{\beta}_t^{\dagger} \leftarrow (X_{S_t}^\top X_{S_t})^{-1} X_{S_t}^\top y\)
6: \(S_t^\dagger \leftarrow T_{abs}(\hat{\beta}_t^{\dagger}, \pi)\)
7: \(\hat{\beta}_{t+1} \leftarrow (X_{S_t^\dagger}^\top X_{S_t^\dagger})^{-1} X_{S_t^\dagger}^\top y\)
8: \(t \leftarrow t + 1\)
9: until \(\|\hat{\beta}_t - \hat{\beta}_{t-1}\|_2 < \tau\)
10: \(\hat{\beta}^{cs} \leftarrow \hat{\beta}_t\)

**Output:** \(\hat{\beta}^{cs}\)

3.2 Simulation: FDR-TPR paths

In this section, we compare the model selection capability of CoSaMP with that of other competing methods through their FDR-TPR paths. Given a model selection procedure with tuning parameter \(\lambda > 0\), the FDR-TPR path is formed by the set of two-dimensional points \(\{(\text{FDR}(\hat{S}(\lambda)), \text{TPR}(\hat{S}(\lambda)))\}_{\lambda > 0}\) where \(\hat{S}(\lambda)\) is the output of the model selector with tuning parameter \(\lambda\). A perfect FDR-TPR path is in \("\Gamma"\) shape, which implies that the method keeps recruiting (nearly) only true predictors until having them all. The competing approaches we assess are LASSO (Tibshirani, 1996), SCAD (Fan and Li, 2001) and MCP (Zhang et al., 2010), all of which we use the R package picasso Ge et al. (2019) to implement. In CoSaMP, we treat \(\pi\) as the tuning parameter and set the expansion size \(l\) to be the size of the model selected by MCP that is tuned by 10-fold cross validation (CV) in terms of mean squared error (MSE).

We investigate three different designs for numerical comparison, of which the first two are random design and the third is from real data. In Cases 1 and 2, we let \(p = 1,000, s^* = 50\) and \(n = \lceil 2s^* \log p \rceil\). In each Monte Carlo experiment, we generate \(S^* \subset [p]\) by randomly selecting \(s^*\) locations from \(\{p\}\) in a uniform manner and generate \(\beta^*\) such that \(\beta^*_j = 0\) for \(j \in (S^*)^c\) and that \(\{(\beta^*_j/0.1) - 1\}_{j \in S^*} \overset{i.i.d.}\sim \chi^2_1\). Rows of the design matrix \(X\) are independently generated from \(\mathcal{N}(0, \Sigma)\), where \(\Sigma\) is either from autoregressive (Case 1) or equicorrelated (Case 2) models. In Case 3, we

Algorithm 2 CoSaMP-Path\((X, y, \Pi, l, \tau)\)

**Input:** Design matrix \(X\), response \(y\), projection size set \(\Pi = \{\pi_1, \ldots, \pi_M\}\) with \(\pi_1 < \ldots < \pi_M\), expansion size \(l\), convergence threshold \(\tau > 0\)

1: \(\hat{\beta}^{cs}(0) = 0\)
2: for \(i = 1:M\)
3: \(\hat{\beta}^{cs}(i) \leftarrow \text{CoSaMP}(X, y, \hat{\beta}^{cs}(i-1), \pi_i, l, \tau)\)
4: end for

**Output:** \((\hat{\beta}^{cs}(1), \hat{\beta}^{cs}(2), \ldots, \hat{\beta}^{cs}(M))\)
use real data as our design matrix and generate $\beta^*$ according to the domain knowledge that we will elucidate later. In all the three cases, we generate $y$ as $y = X\beta^* + \epsilon$ with $\epsilon \sim \mathcal{N}(0, \sigma^2 I)$, where $\sigma^2$ will be specified later. Each point on the presented FDR-TPR curve is based on the average of the FDPs and TPPs of the estimators obtained in 100 independent Monte Carlo experiments, using the same tuning parameter. In some challenging setups such as those in Case 2, many methods can yield very low TPR; we thus set the $y$-axis, the TPR axis, to be on logarithmic scale for clearer comparison.

**Case 1: Autoregressive design.** We set $\Sigma_{jk} = \rho^{|j-k|}$ for correlation parameter $\rho \in \{0, 0.5, 0.8\}$, $\forall j, k \in [p]$ and $\sigma \in \{0.5, 1\}$. The FDR-TPR paths, together with the FDR and TPR of the solutions chosen by 10-fold cross validation, are presented in Figure 3. We have the following observations:

(i) In the low noise setting ($\sigma = 0.5$), CoSaMP always exhibits a “Γ”-shaped FDR-TPR curve, while other approaches have false discoveries on their early solution paths, especially in presence of high correlation among features (e.g., $\rho = 0.8$). Even in the high noise setting ($\sigma = 1$), CoSaMP has remarkably low FDR on its early solution path. It is clear that false discoveries occur earlier in the competing methods than CoSaMP in this case.

(ii) In all the six plots of Figure 3, the ten-fold CV points of CoSaMP have substantially lower FDR than those of the other methods. In particular, the CV solutions of CoSaMP maintain FDR below 20% in all but the very last case, where $\rho = 0.8$ and $\sigma = 1$. In contrast, the FDR of the CV solutions of the penalized approaches is always around 40%. This suggests that compared with CoSaMP, the penalized approaches tend to select more spurious variables, which might be correlated with the signal, to capture the signal.

**Case 2: Equicorrelated design.** We consider $\Sigma = \rho \mathbf{1}\mathbf{1}^\top + (1 - \rho)I$ with $\rho \in \{0.5, 0.8\}$ and two noise levels $\sigma \in \{0.5, 1\}$. Generally speaking, this is a much more challenging case than the previous one because of constant correlation. The FDR-TPR paths are presented in Figure 4. We have the following observations:

(i) CoSaMP maintains to yield a nearly vertical FDR-TPR path at the early stage, meaning that most of its early discoveries are genuine. However, the strengthened collinearity does hurt its TPR at the latter stage. For example, fixing $\rho = 0.8$ and $\sigma = 1$ and requiring FDR below 20%, one can see that CoSaMP can hit 50% TPR in Case 1 but merely 30% TPR in Case 2.

(ii) LASSO, SCAD and MCP select much more spurious variables than CoSaMP on their early solution path. However, interestingly, at a latter stage, the nonconvex penalty in SCAD and MCP corrects the models by replacing the false discoveries with true variables, leading to a north-west pivot of the path as $\lambda$ decreases. LASSO instead does not exhibit such correction: its FDR-TPR path keep moving in the north-east direction as $\lambda$ decreases, meaning that its FDR keeps increasing.

(iii) The CV solution of CoSaMP has slightly lower FDR but also slightly lower TPR than those of MCP and SCAD. The CV solution of LASSO exhibits much higher TPR at the cost of including a great number of spurious variables.
Figure 3: FDR-TPR paths under autoregressive design. We set $\Sigma_{jk} = \rho^{|j-k|}$ for $\rho \in \{0, 0.5, 0.8\}$ and $\sigma \in \{0.5, 1\}$. Blue, black, red and blueviolet curves represent the FDR-TPR paths of CoSaMP, SCAD, LASSO and MCP respectively. The dots represent the solutions of different methods that are tuned by 10-fold CV. The results are obtained over 100 Monte Carlo repetitions by randomly generating the design $X$, the coefficient vector $\beta^*$, the noises $\epsilon$ and computing $y = X\beta^* + \epsilon$. 

$\rho = 0, \sigma = 0.5$ 

$\rho = 0, \sigma = 1$

$\rho = 0.5, \sigma = 0.5$ 

$\rho = 0.5, \sigma = 1$

$\rho = 0.8, \sigma = 0.5$ 

$\rho = 0.8, \sigma = 1$
Figure 4: FDR-TPR paths under equicorrelated design. We set $\Sigma = \rho 11^\top + (1-\rho)I$ for $\rho \in \{0.5, 0.8\}$ and $\sigma \in \{0.5, 1\}$. We compute the FDR-TPR paths of SCAD, LASSO, MCP by varying $\lambda$ and those of CoSaMP by varying $\pi$. Blue, black, red and blueviolet curves represent the FDR-TPR paths of CoSaMP, SCAD, LASSO and MCP respectively. The circle points represent the 10-fold CV solutions.

**Case 3 (real design)**

We take our design matrix $X$ from the skin cutaneous melanoma dataset in the Cancer Genome Atlas (https://cancergenome.nih.gov/), which provides comprehensive profiling data on more than thirty cancer types (Sun et al., 2019). The dataset contains $p = 20,351$ items of mRNA expression and clinical data on $n = 469$ patients. To choose reasonable locations of true variables, we adopt the top 20 genes that are found highly associated with cutaneous melanoma according to meta-analysis of 145 papers (Chatzinasiou et al., 2011). One can find a list of these genes at http://bioserver-3.bioacademy.gr/Bioserver/melGene/. We conduct a semi-simulation using the real design matrix. Fixing $S^*$ to be the locations of the top 20 genes, we generate $\beta^*$ by letting $\beta_j^* = 0$ for $j \in (S^*)^c$ and $\{(\beta_j^*/\beta_{\min}) - 1\}_{j \in S^*} \overset{i.i.d.}{\sim} \chi_1^2$, where $\beta_{\min} \in \{1, 0.5, 0.25\}$. Then we generate the response vector by letting $y = \tilde{X}\beta^* + \epsilon$, where $\tilde{X}$ is standardized $X$, and where $\epsilon \sim \mathcal{N}(0, I)$. The solution paths of all the methods are presented in Figure 5. We have the following observations:
Figure 5: FDR-TPR paths under real data design. We set the noise level \( \sigma = 1 \) and choose \( \beta_{\min} \in \{1, 0.5, 0.25\} \). Blue, black, red and blueviolet curves represent the FDR-TPR paths of CoSaMP, SCAD, LASSO, MCP, respectively. The round dots represent the solutions chosen by 10-fold CV.

(i) Under high signal-to-noise ratio setups (\( \beta_{\min} = 1, 0.5 \)), the FDR-TPR path of CoSaMP is in “Γ” shape, while LASSO, SCAD and MCP have false discoveries on their early solution paths. Similarly to Case 2, SCAD and MCP correct their models at a latter stage by substituting false variables with true ones. The FDR of LASSO keeps increasing as \( \lambda \) decreases.

(ii) Regarding the 10-fold CV solutions, we see a different situation from Cases 1 and 2. Here the CV-tuned CoSaMP also selects a non-negligible number of spurious variables in order to improve prediction power. The CV points of SCAD and MCP sometimes have lower FDR. LASSO still tends to select spurious variables more than other approaches.

3.3 Towards FDR control

In the previous simulation experiments, the low FDR of CoSaMP on its early solution path inspires us to exploit CoSaMP as an efficient feature screener for FDR control under ultra-high dimensional setups. Here we propose a two-stage model selection procedure called LOCK (L-zerO Constrained feature screening + Knockoff): it first uses CoSaMP to select potentially relevant features and then applies the model-X knockoffs procedure (Candès et al., 2018) to them to produce a further reduced model with FDR guarantee. Note that performing the knockoff procedure after feature screening is not new: Barber et al. (2019) proposed a similar two-stage method that uses LASSO for feature screening for the knockoff filter. Nevertheless, the comparison on the FDR-TPR paths of LASSO and CoSaMP in the previous subsection suggests that CoSaMP may outperform LASSO as a feature screener and lead to higher TPR, which is confirmed by our numerical results in the sequel.

Given a design matrix \( X \), a response vector \( y \) and a FDR control level \( q \), we use Knockoff\((X, y, q)\) to denote the model selected by the model-X knockoff filter (Candès et al., 2018). We present the pseudocode of LOCK in Algorithm 3. The basic idea of LOCK is to pursue the largest possible model given by the knockoff filter to maximize TPR, while enjoying the prespecified FDR guarantee provided by the knockoff procedure. Specifically, in each round, LOCK first splits the dataset randomly into two parts for feature screening and FDR control respectively to remove selection bias.
Algorithm 3 LOCK

**Input:** Design matrix $\mathbf{X} \in \mathbb{R}^{n \times p}$, response $\mathbf{y} \in \mathbb{R}^p$, FDR control level $q$, number of repetitions $T$, screening sample size $n_0$, projection size set $\Pi = (\pi_1, \ldots, \pi_M)$ with $\pi_1 < \ldots < \pi_M$, expansion size $l$, convergence threshold $\tau > 0$

1: for $t = 1 : T$
2:    # Data splitting
3:    Randomly generate an index set $\mathcal{D}_0 \subset [n]$ with $|\mathcal{D}_0| = n_0$
4:    $\mathbf{X}^{(0)} \leftarrow \mathbf{X}_{\mathcal{D}_0}$
5:    $\mathbf{y}^{(0)} \leftarrow \mathbf{y}_{\mathcal{D}_0}$
6:    $\mathbf{y}^{(1)} \leftarrow \mathbf{y}_{[n] \setminus \mathcal{D}_0}$
7:    # Screening
8:    $(\hat{\beta}_1, \hat{\beta}_2, \ldots, \hat{\beta}_M) \leftarrow \text{CoSaMP-Path}(\mathbf{X}^{(0)}, \mathbf{y}^{(0)}, \Pi, l, \tau)$
9:    for $i = 1 : M$
10:       $\hat{S}_i \leftarrow \text{supp}(\hat{\beta}_i)$
11:    end for
12:    # Knockoff
13:    for $i = 1 : M$
14:       $\mathbf{X}^{(i)} \leftarrow \mathbf{X}_{[n] \setminus \mathcal{D}_0, \hat{S}_i}$
15:       $\hat{S}_{t,i} \leftarrow \text{Knockoff}(\mathbf{X}^{(i)}, \mathbf{y}^{(1)}, q)$
16:    end for
17:    $t_* \leftarrow \text{argmax}_{i \in [M]} |\hat{S}_{t,i}|$
18: end for
19: $t^* \leftarrow \text{argmax}_{t \in [T]} |\hat{S}_{t,t_*}|$

**Output:** $\hat{S}_{t^*,t_*}$

Next, it applies CoSaMP to the first data split to obtain a series of candidate models $\{\hat{S}_i\}_{i \in [M]}$, each of which is then further filtered by the knockoff method based on the second data split to generate a model with FDR guarantee. Then LOCK picks the largest model among all the output models from the knockoff procedure as the result for the iteration. In the end, LOCK further searches for the largest model among the results from all the rounds as the final output.

In the simulation experiments, we compare LOCK with the model-X knockoff procedure, FCD (FDR Control for via Debiasing) Javanmard et al. (2019) and the knockoff procedure with feature screening by LASSO (LASSO + Knockoff). Here the algorithm of LASSO + Knockoff follows the same steps as LOCK except the screening step where CoSaMP-Path in LOCK is replaced with LASSO. In order for LASSO to pick a certain number of features, say $\pi$ features, we assess its entire solution path to choose the model whose sparsity is the closest to $\pi$. We focus on the following three designs:

(i) Factor model design: We draw the rows of $\mathbf{X}$ independently from $\mathcal{N}(\mathbf{0}, \mathbf{V} \Lambda_0 \mathbf{V}^T + \mathbf{I})$, where $\mathbf{V} \in \mathbb{O}^{p \times K}$, and where $\Lambda_0 \in \mathbb{R}^{K \times K}$ is a diagonal matrix. We consider two choices of $\Lambda_0$: $\Lambda_0 = \text{diag}(2p^{1/2}, p^{1/2})$ (factor model I), which gives a mildly pervasive model, and $\Lambda_0 = \text{diag}(2p, p)$ (factor model II), which gives a strongly pervasive model. We set $n = 700$ and
Table 1: Numerical comparison based on 100 Monte Carlo repetitions. The FDR control level parameter \( q \) is set to be 10%. The standard errors of the performance metrics are in the parentheses.

|                  | Model-X Knockoff | FCD                 | Lasso+ Knockoff | LOCK               |
|------------------|------------------|---------------------|----------------|--------------------|
|                  | FDR(%)           | TPR(%)              | Time(s)        |                    |
| Factor           | 25.38(0.6)       | 100.00(0.0)         | 6987.62        |                    |
| model I          | 10.98(0.5)       | 46.66(0.8)          | 4827.92        |                    |
|                  | 12.43(0.8)       | 20.76(0.5)          | 3068.88        | 1029.16            |
|                  | 5.15(0.7)        | 73.78(3.3)          | 1251.59        | 71.45(1.1)         |
|                  | 0.00(0.0)        | 18.73(0.6)          | 225.35         | 975.70             |
|                  | 38.55(1.2)       | 23.75(0.6)          | 4927.13        |                    |
|                  | 14.50(1.2)       | 291.59              | 314.83         |                    |
|                  | 1.22(0.2)        | 71.45(1.1)          | 975.70         |                    |
| Equicorrelated \((\rho = 0.5)\) | 0.00(0.0)       | 8.87(1.2)           | 250.86         | 981.03             |
| TPR(%)           | 15.24(1.0)       | 19.34(0.6)          | 3949.21        |                    |
| Time(s)          | 59.48(3.4)       | 314.83              | 314.83         |                    |
|                  | 5.54(0.8)        | 981.03              | 981.03         |                    |
| Equicorrelated \((\rho = 0.8)\) | 0.00(0.0)       | 31.12(3.5)          | 293.32         | 888.88             |
| TPR(%)           | 16.11(1.2)       | 17.88(0.6)          | 4947.65        |                    |
| Time(s)          | 24.17(1.9)       | 364.88              | 364.88         |                    |
|                  | 12.76(1.0)       | 888.88              | 888.88         |                    |
| Real design      | 2.11(0.5)        | 40.95(3.2)          | 6896.83        | 368.78             |
| TPR(%)           | 60.22(1.2)       | 50.75(1.3)          | 16338.89       |                    |
| Time(s)          | 45.89(1.0)       | 41.75(1.0)          | 279.52         |                    |
|                  | 9.12(0.8)        | 82.35(1.4)          | 368.78         |                    |

\( p = 3,000 \).

(ii) Equicorrelated design: We draw the rows of \( X \) independently from \( \mathcal{N}(\mathbf{0}, \rho \mathbf{1}\mathbf{1}^\top + (1 - \rho)\mathbf{I}) \), where \( \rho \in \{0.5, 0.8\} \). We set \( n = 700 \) and \( p = 3,000 \).

(iii) Real design: We construct \( X \) by randomly selecting 5,000 columns \(^1\) from the same skin cutaneous melanoma dataset as in Case 3 of Section 3.2, together with the twenty columns that are adopted as true variables there. Here \( n = 474 \) and \( p = 5013 \).

We always standardize the design that we generate. Under factor model design and equicorrelated design, we set \( s^* = 100 \) and construct \( S^* \subset [p] \) by randomly selecting \( s^* \) variables from \([p]\) in a uniform manner. The true coefficient vector \( \beta^* \) satisfies that \( \beta^*_j = 0 \) for all \( j \in (S^*)^c \) and that \( \{\beta^*_j\}_{j \in S^*} \) are independently drawn from \( \{1, -1\} \) with equal probability. Under real design, similarly to the previous section, we set \( S^* \) to be the locations of the twenty important genes and generate \( \beta^* \) such that \( \beta^*_j = 0 \) for \( j \in (S^*)^c \) and that \( \{(\beta^*_j/0.4) - 1\}_{j \in S^*} \) are independent copies of \( B = ZX \).

\(^1\)We use \texttt{set.seed(2021)} in R to set the random seed.
where $Z \sim \text{Ber}(0.5)$, $X \sim \chi^2_1$, and $Z$ and $X$ are independent. Finally, we generate $\epsilon$ from $\mathcal{N}(0, I_n)$ and generate $y$ as $y = X\beta^* + \epsilon$.

We fix the FDR control level $q$ to be 10% in all of our experiments. Under the equicorrelated design and factor model design, we set the screening sample size $n_0 = 500$ and the projection size set $\Pi = \{10, 20, \ldots, 140, 150\}$ for LOCK and LASSO + Knockoff. Under the real design, we set $n_0 = 400$ and $\Pi = \{16, 18, 20, 22, 24\}$ for LOCK and LASSO + Knockoff. We always choose the expansion size $l$ to be the sparsity of the CV-tuned model of MCP.

Define the directional FDR (Dir.FDR, Barber et al. (2019)) as

$$\text{Dir.FDR} := \mathbb{E}[\text{Dir.FDP}] := \mathbb{E}\left\{\frac{\left|\left\{j \in \hat{S} : \text{sign}(\hat{\beta}_j) \neq \text{sign}(\beta^*_j)\right\}\right|}{|\hat{S} \cup 1|}\right\}.$$ 

In Table 1, we report our estimate of FDR, Dir.FDR, TPR and computational time (in seconds) of all the four approaches based on 100 independent Monte Carlo experiments, with standard errors in the parentheses. Our observations are as follows:

(i) LOCK successfully controls FDR below 10% under all the cases but the equi-correlated design with $\rho = 0.8$, where all the other methods fail to do so, too.

(ii) Except under factor model I, LOCK achieves the highest TPR among all the four methods. Note that though the model-X knockoff procedure yields higher power than LOCK, it fails to control FDR.

(iii) FCD and LASSO + Knockoff fail to control FDR under 10% in presence of strong collinearity, say under factor model II and real design.

(iv) Model-X Knockoff can sometimes be too conservative to select any variable in presence of high collinearity.

Despite the superior numerical performance of LOCK, we emphasize that LOCK has yet been shown to be a rigorous FDR control procedure, given that the FDR guarantee of each individual knockoff-filtered model might not carry over to the largest one among them. Nevertheless, this numerical study reveals potential of LOCK, which motivates us to develop rigorous FDR control guarantee for LOCK or its variants in future work.

4 Discussion

In this paper, we developed the sufficient and (near) necessary conditions for BSS to achieve sure selection throughout its early path. We show that the underpinning quantity is the minimum projected signal margin that characterizes the fundamental gap of fitting power between sure selection models and spurious ones. This margin is robust against collinearity of the design, justifying the low FDP of the early path of CoSaMP that we observed under highly correlated design. The current results motivate the following three questions that we wish to answer in our future research:

1. Previous works Needell and Tropp (2009) and Jain et al. (2014) on CoSaMP rely on restricted strong convexity and smoothness (or their variants) to develop its optimization guarantee.
Given that these conditions are dispensable for the statistical properties of BSS, and that CoSaMP is shown to be closely related with BSS, it is natural to ask if these conditions are essential for CoSaMP to yield desirable statistical properties, say sure early selection. In particular, can we achieve any FDP guarantee for the early path of CoSaMP with only a lower bound of the minimum projected signal margin? Answering these questions should entail more delicate optimization analysis.

2. What are the sufficient and necessary conditions for BSS to achieve sure early selection under linear sparsity, i.e., $s^*/p$ tends to a constant?

3. Can we provide rigorous FDP guarantee for a well tuned LOCK procedure (or its variant)?

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A Proofs of technical results

A.1 Proof of Theorem 2.1

For any $S \in [p]$, define $\gamma_S := n^{-1/2}(I - P_{X_S})\mu^*$. For any $S \in A(s)$, we have

$$n^{-1}L_S = n^{-1}\{y^T(I - P_{X_S})y\} = n^{-1}(\beta^TX^T + \epsilon^T)(I - P_{X_S})(X\beta^* + \epsilon)$$

$$= \|\gamma_S\|^2_2 + \frac{2\gamma_S^T\epsilon}{n^{1/2}} + \frac{1}{n}\epsilon^T(I - P_{X_S})\epsilon. \quad (18)$$

Similarly, we have that

$$n^{-1}L_{\Phi(S)} = \|\gamma_{\Phi(S)}\|^2_2 + \frac{2\gamma_{\Phi(S)}^T\epsilon}{n^{1/2}} + \frac{1}{n}\epsilon^T(I - P_{X_{\Phi(S)}})\epsilon. \quad (19)$$

Combining the two displays above yields that

$$n^{-1}(L_S - L_{\Phi(S)}) = \|\gamma_S\|^2_2 - \|\gamma_{\Phi(S)}\|^2_2 + \frac{2(\gamma_S - \gamma_{\Phi(S)})^T\epsilon}{n^{1/2}} - \frac{1}{n}\epsilon^T(P_{X_S} - P_{X_{\Phi(S)}})\epsilon$$

$$= \eta(\|\gamma_S\|^2_2 - \|\gamma_{\Phi(S)}\|^2_2)$$

$$+ 2^{-1}(1 - \eta)(\|\gamma_S\|^2_2 - \|\gamma_{\Phi(S)}\|^2_2) + \frac{2(\gamma_S - \gamma_{\Phi(S)})^T\epsilon}{n^{1/2}}$$

$$+ 2^{-1}(1 - \eta)(\|\gamma_S\|^2_2 - \|\gamma_{\Phi(S)}\|^2_2) - \frac{1}{n}\epsilon^T(P_{X_S} - P_{X_{\Phi(S)}})\epsilon. \quad (20)$$

We wish to show that the following two bounds hold with high probability:

$$\inf_{S \in A(s)} \left\{ 2^{-1}(1 - \eta)(\|\gamma_S\|^2_2 - \|\gamma_{\Phi(S)}\|^2_2) + \frac{2(\gamma_S - \gamma_{\Phi(S)})^T\epsilon}{n^{1/2}} \right\} > 0 \quad (21)$$

and

$$\inf_{S \in A(s)} \left\{ 2^{-1}(1 - \eta)(\|\gamma_S\|^2_2 - \|\gamma_{\Phi(S)}\|^2_2) - \frac{1}{n}\epsilon^T(P_{X_S} - P_{X_{\Phi(S)}})\epsilon \right\} > 0. \quad (22)$$

We first consider (21). Given that $\|\epsilon\|_{\psi_2} \leq \sigma$, applying Hoeffding’s inequality yields that for any $x > 0$,\n
$$\mathbb{P}\{(\gamma_S - \gamma_{\Phi(S)})^T\epsilon \leq x\sigma\|\gamma_S - \gamma_{\Phi(S)}\|_2 \leq 2e^{-x^2/2}. \quad (23)$$

Note that $A_t(s) := \{S \in A(s) : |S \setminus \Phi(S)| = t\}$ for $t \in [s]$. Then $A(s) = \cup_{t \in [s]} A_t(s)$. A union bound over $S \in A_t(s)$ yields that

$$\mathbb{P}\{\exists S \in A_t(s) \text{ s.t. } \frac{2(\gamma_S - \gamma_{\Phi(S)})^T\epsilon}{n^{1/2}} \geq \frac{2x\sigma\|\gamma_S - \gamma_{\Phi(S)}\|_2}{n^{1/2}} \} \leq 2|A_t(s)|e^{-x^2/2}. \quad (24)$$

Writing $\xi_0 = \frac{(1 - \eta)m_t(s)}{8\sigma(\log p)^{1/2}}$ and substituting $x = 2\xi_0(t \log p)^{1/2}$ into (24), we have that

$$\mathbb{P}\{\exists S \in A_t(s) \text{ s.t. } \frac{2(\gamma_S - \gamma_{\Phi(S)})^T\epsilon}{n^{1/2}} \geq 4\xi_0\sigma\|\gamma_S - \gamma_{\Phi(S)}\|_2 \left(\frac{t \log p}{n}\right)^{1/2} \} \leq 2|A_t(s)|e^{-2\xi_0^2 t \log p}. \quad (25)$$
Note that
\[ \gamma_S - \gamma_{\Phi(S)} = n^{-1/2} (P_{X_{\Phi(S)}} - P_{X_S}) \mu^* = n^{-1/2} (P_{\Phi(S) | S} - P_{S | \Phi(S)}) \mu^*, \]
which implies that
\[ \| \gamma_S - \gamma_{\Phi(S)} \|_2 \leq n^{-1/2} \left( \| P_{\Phi(S) | S} \mu^* \|_2 + \| P_{S | \Phi(S)} \mu^* \|_2 \right). \] (26)
Consequently,
\[ \| \gamma_S \|_2^2 - \| \gamma_{\Phi(S)} \|_2^2 = n^{-1} \mu^T (P_{X_{\Phi(S)}} - P_{X_S}) \mu^* = n^{-1} \mu^T (P_{\Phi(S) | S} - P_{S | \Phi(S)}) \mu^* \]
\[ = \frac{(\| P_{\Phi(S) | S} \mu^* \|_2 + \| P_{S | \Phi(S)} \mu^* \|_2)}{n^{1/2}} (\| P_{\Phi(S) | S} \mu^* \|_2^2 - \| P_{S | \Phi(S)} \mu^* \|_2^2) \] (27)
\[ \geq \| \gamma_S - \gamma_{\Phi(S)} \|_2 (\| P_{\Phi(S) | S} \mu^* \|_2 - \| P_{S | \Phi(S)} \mu^* \|_2) \frac{n^{1/2}}{n^{1/2}}. \]
Combining (27) with the definition of \( \xi_0 \) and \( m_*(s) \) yields that
\[ \frac{1 - \eta}{2} (\| \gamma_S \|_2^2 - \| \gamma_{\Phi(S)} \|_2^2) \geq 4 \xi_0 \sigma \| \gamma_S - \gamma_{\Phi(S)} \|_2 \left( \frac{t \log p}{n} \right)^{1/2}. \]
Therefore, we deduce from (25) that
\[ \mathbb{P} \left\{ \exists S \in \mathcal{A}_t(s) \text{ s.t. } \frac{2 \| (\gamma_S - \gamma_{\Phi(S)})^T \epsilon \|}{n^{1/2}} \geq \frac{1 - \eta}{2} (\| \gamma_S \|_2^2 - \| \gamma_{\Phi(S)} \|_2^2) \right\} \leq 2 |\mathcal{A}_t(s)| e^{-2 \xi_0^2 t \log p}. \]
Note that
\[ |\mathcal{A}_t(s)| = \binom{p - s^*}{t} \binom{s^*}{s - t} = \binom{p - s^*}{p - t} \binom{s^*}{s^* + t}. \]
By Stirling’s formula and the fact that \( \log p \geq s^* \), we have
\[ \log \left\{ \binom{s^*}{s^* + t} \right\} \leq \log \left\{ \binom{s^*}{s^* / 2} \right\} \approx s^* \approx \log p. \]
Hence, we have
\[ \mathbb{P} \left\{ \exists S \in \mathcal{A}_t(s) \text{ s.t. } \frac{2 \| (\gamma_S - \gamma_{\Phi(S)})^T \epsilon \|}{n^{1/2}} \geq \frac{1 - \eta}{2} (\| \gamma_S \|_2^2 - \| \gamma_{\Phi(S)} \|_2^2) \right\} \leq 2 C_1 p^{-2(\xi_0^2 t - 1)} \leq 2 C_1 p^{-2(\xi_0^2 - 1)}. \] (28)
A further union bound over \( t \in [s] \) yields that
\[ \mathbb{P} \left\{ \exists S \in \mathcal{A}_t(s) \text{ s.t. } \frac{2 \| (\gamma_S - \gamma_{\Phi(S)})^T \epsilon \|}{n^{1/2}} \geq \frac{1 - \eta}{2} (\| \gamma_S \|_2^2 - \| \gamma_{\Phi(S)} \|_2^2) \right\} \leq 2 C_1 s p^{-2(\xi_0^2 - 1)}. \] (29)
Next we aim to show that (22) is a high-probability event. Fix any \( t \in [s] \). For any \( S \in \mathcal{A}_t(s) \), let \( \mathcal{U}, \mathcal{V} \) be the orthogonal complement of \( \mathcal{W} := \text{col}(X_{S \setminus \Phi(S)}) \) as a subspace of \( \text{col}(X_S) \) and \( \text{col}(X_{\Phi(S)}) \) respectively. Then \( \dim(\mathcal{U}) = \dim(\mathcal{V}) = t \). We have
\[ \frac{1}{n} \epsilon^T (P_{X_S} - P_{X_{\Phi(S)}}) \epsilon = \frac{1}{n} \epsilon^T (P_W + P_U) \epsilon - \frac{1}{n} \epsilon^T (P_W + P_V) \epsilon = \frac{1}{n} \epsilon^T (P_U - P_V) \epsilon. \] (29)
By Theorem 1.1 in Rudelson et al. (2013), there exists a universal constant \( c > 0 \) such that for any \( x > 0 \),

\[
P \left( |e^\top P_{\ell} e - \mathbb{E}(e^\top P_{\ell} e)| > \sigma^2 x \right) \leq 2e^{-c \min(x^2/\|P_{\ell}\|_{F,2}^2, x/\|P_{\ell}\|_2)} = 2e^{-c \min(x^2/|t, x|)}.
\]

Similarly,

\[
P \left( |e^\top P_{\gamma} e - \mathbb{E}(e^\top P_{\gamma} e)| > \sigma^2 x \right) \leq 2e^{-c \min(x^2/|t, x|)}.
\]

Note that \( \mathbb{E}(e^\top P_{\gamma} e) = \mathbb{E}(\text{tr}(P_{\gamma} e e^\top)) = \text{var}(\epsilon_1) \text{tr}(P_{\gamma}) = t \text{var}(\epsilon_1) = \mathbb{E}(e^\top P_{\ell} e) \). Combining the above two inequalities yields

\[
P(|e^\top P_{\ell} e - e^\top P_{\gamma} e| > 2\sigma^2 x) \leq 4e^{-c \min(x^2/|t, x|)}.
\]

If we have \( \xi_0 \geq (16 \log 2)^{-1/2} \), then applying a union bound over \( S \in A_t(s) \) and taking \( x = 16\xi_0^2 t \log p \) yields that

\[
P \left\{ \exists S \in A_t(s) \text{ s.t. } \frac{|e^\top P_{X_S} e - e^\top P_{X_{\Phi(S)}} e|}{n} \geq 32\xi_0^2 \sigma^2 t \left( \frac{\log p}{n} \right) \right\}
\leq 4C_1p^{-(16\xi_0^2 t^2 - t - 1)} \leq 4C_1p^{-2(8\xi_0^2 - 1)}.
\]

Note that

\[
\frac{1 - \eta}{2} (\|\gamma_S\|_2^2 - \|\gamma_{\Phi(S)}\|_2^2) \geq \frac{1 - \eta}{2n} (\|P_{\Phi(S)} S \mu^*\|_2 - \|P_{S}\|_{\Phi(S)} S \mu^*\|_2 + \|P_{S}\|_{\Phi(S)} \mu^*\|_2)
\geq \frac{1 - \eta}{2n} (\|P_{\Phi(S)} S \mu^*\|_2 - \|P_{S}\|_{\Phi(S)} \mu^*\|_2) \geq 32\xi_0^2 \sigma^2 t \left( \frac{\log p}{n} \right).
\]

A further union bound over \( t \in \{s\} \) yields

\[
P \left\{ \exists S \in A(s) \text{ s.t. } \frac{|e^\top P_{X_S} e - e^\top P_{X_{\Phi(S)}} e|}{n} \right\} \leq 4C_1sp^{-2(8\xi_0^2 - 1)}.
\]

Finally, let \( C = \max\{1, (8c)^{-1/2}, 6C_1\} \). Combining (20), (28) and (34) yields that

\[
P \left[ \inf_{S \in A(s)} \left\{ \frac{1}{n} \left( \mathcal{L}_S - \mathcal{L}_{\Phi(S)} \right) - \eta(\|\gamma_S\|_2^2 - \|\gamma_{\Phi(S)}\|_2^2) \right\} \right] \geq 0 \right\} \geq 1 - Csp^{-2(C^2 - 2\xi_0^2 - 1)}.
\]

Note that

\[
\eta(\|\gamma_S\|_2^2 - \|\gamma_{\Phi(S)}\|_2^2) \geq \frac{\eta n m^2(s)}{n} \quad \text{and} \quad \mathcal{L}_S - \mathcal{L}_s \geq \mathcal{L}_S - \mathcal{L}_{\Phi(S)}
\]

for all \( S \in A(s) \). For any \( \xi > C \), the conclusion then follows immediately if \( \xi_0 \geq \xi \).

### A.2 Proof of Theorem 2.2

We wish to show that if (16) is satisfied, then there exists \( j \in J_{\delta_0} \) such that \( \mathcal{L}_{(j)} < \hat{\mathcal{L}}_1 := \min_{j^* \in S^* \mathcal{L}_{(j^*)}} \) with high probability. To see this, for any \( j^* \in S^* \) and any \( j \in J_{\delta_0} \), we have that

\[
n^{-1}(\mathcal{L}_{(j)} - \mathcal{L}_{(j^*)}) = \|\gamma_{(j)}\|_2^2 - \|\gamma_{(j^*)}\|_2^2 + \frac{2(\gamma_{(j)} - \gamma_{(j^*)})^\top \epsilon}{n^{1/2}} - \frac{1}{n} \epsilon^\top (P_{X_j} - P_{X_{j^*}}) \epsilon \leq \|\gamma_{(j)}\|_2^2 - \|\gamma_{(j^*)}\|_2^2 + \frac{2(\gamma_{(j)} - \gamma_{(j^*)})^\top \epsilon}{n^{1/2}} - \frac{1}{n} \epsilon^\top (P_{X_j} - P_{X_{j^*}}) \epsilon.
\]

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Recall that $\tilde{u}_j := X_j/\|X_j\|_2, \forall j \in [p]$. For convenience, write
\[
\Delta = \max_{j \in J_{\delta_0}} \{\|P_{X_j} \mu^*\|_2 - \|P_{X_j} \mu^*\|_2\} = \max_{j \in J_{\delta_0}} \{\|\tilde{u}_j^\top \mu^*\| - \|\tilde{u}_j^\top \mu^*\|\}.
\]

We then have that
\[
\gamma_{\{j\}} - \gamma_{\{j^*\}} = n^{-1/2}(P_{X_{j^*}} - P_{X_j})\mu^* = n^{-1/2}(\tilde{u}_{j^*}^\top \tilde{u}_j - \tilde{u}_j^\top \tilde{u}_{j^*})\mu^*,
\]
and that
\[
\|\gamma_{\{j\}}\|_2^2 - \|\gamma_{\{j^*\}}\|_2^2 = \frac{1}{n} \mu^\top (\tilde{P}_{X_j} - \tilde{P}_{X_{j^*}}) \mu^* = \frac{1}{n} \mu^\top (\tilde{u}_j^\top - \tilde{u}_{j^*}^\top) \mu^* \tilde{u}_j^\top (\tilde{u}_{j^*}^\top - \tilde{u}_j^\top) \mu^* = \frac{1}{n} (\|\tilde{u}_j^\top \mu^*\| - \|\tilde{u}_{j^*}^\top \mu^*\|)(\|\tilde{u}_j^\top \mu^*\| + \|\tilde{u}_{j^*}^\top \mu^*\|) \leq 2\Delta |\tilde{u}_j^\top \mu^*|.
\]

Note that Assumption 2.2 implies that $|\tilde{u}_j^\top \mu^*| \geq 4\Delta$; we thus deduce from (37) that
\[
(\tilde{u}_j^\top \mu^*)^2 \geq (\tilde{u}_{j^*}^\top \mu^*)^2 - 2\Delta |\tilde{u}_j^\top \mu^*| \geq \frac{(\tilde{u}_{j^*}^\top \mu^*)^2}{2}, \forall j \in J_{\delta_0}.
\]

By Lemma 6.1 of Fan et al. (2020a), (38) and then (16), we have for any $j, k \in J_{\delta_0}$ and $j \neq k$ that
\[
\|\gamma_{\{j\}} - \gamma_{\{k\}}\|_2 = n^{-1/2}||\tilde{u}_j^\top \mu^* - \tilde{u}_k^\top \mu^*\|_2 \geq n^{-1/2} \min(|\tilde{u}_j^\top \mu^*|, |\tilde{u}_k^\top \mu^*|)\delta_0 \geq \delta_0 (2n)^{-1/2} |\mu^* |\tilde{u}_j^\top | =: \delta_0.
\]

Therefore, $\{\gamma_{\{j\}} - \gamma_{\{j^*\}}\}_{j \in J_{\delta_0}}$ is a $\delta_0$-packing set of itself. By Sudakov’s lower bound (Wainwright, 2019, Theorem 5.30), we deduce that
\[
\mathbb{E}\left\{\min_{j \in J_{\delta_0}} \frac{2(\gamma_{\{j\}} - \gamma_{\{j^*\}})}{\sqrt{n}} \right\} \leq -\delta_0 \sigma \left(\frac{c_{\delta_0} \log p}{n}\right)^{1/2}.
\]

Furthermore, (36) and (16) imply that
\[
\|\gamma_{\{j\}} - \gamma_{\{j^*\}}\|_2 \leq n^{-1/2} (|\tilde{u}_{j^*}^\top \mu^*| + |\tilde{u}_j^\top \mu^*|) \leq 2n^{-1/2} |\tilde{u}_{j^*}^\top \mu^*|.
\]

Therefore, by Lemma B.3,
\[
\left\|\min_{j \in J_{\delta_0}} \frac{2(\gamma_{\{j\}} - \gamma_{\{j^*\}})}{\sqrt{n}} \right\|_{\psi_2} \leq \frac{\sigma^2 \max_{j \in J_{\delta_0}} \|\gamma_{\{j\}} - \gamma_{\{j^*\}}\|_2^2}{n} \leq \frac{\sigma^2 (\tilde{u}_{j^*}^\top \mu^*)^2}{n^2}.
\]

Combining (39) and (40), we deduce that there exists a universal constant $C > 0$, such that for any $t > 0$,
\[
\mathbb{P}\left\{\min_{j \in J_{\delta_0}} \frac{2(\gamma_{\{j\}} - \gamma_{\{j^*\}})}{\sqrt{n}} \geq -\delta_0 \sigma \left(\frac{c_{\delta_0} \log p}{n}\right)^{1/2} + \frac{Ct \sigma |\tilde{u}_{j^*}^\top \mu^*|}{n} \right\} \leq \exp(-t^2).
\]

Choosing $t = 2^{-3/2}C^{-1}\delta_0 c_{\delta_0}^{1/2} \log^{1/2} p$, we then reduce the bound above to
\[
\mathbb{P}\left\{\min_{j \in J_{\delta_0}} \frac{2(\gamma_{\{j\}} - \gamma_{\{j^*\}})}{\sqrt{n}} \geq -\frac{\delta_0 c_{\delta_0}^{1/2} \sigma |\tilde{u}_{j^*}^\top \mu^*| |\log^{1/2} p|}{n} \right\} \leq p^{-\delta_0 c_{\delta_0}^{1/2}/(8C^2)}.
\]
Besides, combining Assumption 2.2 with the fact that \( \delta_0^2 c_{d_0} \log p > 1 \) yields that
\[
|u_j^\top \mu^*| > 8\sigma / \{\delta_0 c_{d_0} (\log p)^{1/2}\}.
\]

Therefore, applying a union bound over \( j \in J_{d_0} \) to (32) with \( x = (8\sigma)^{-1} \delta_0 c_{d_0} |u_j^\top \mu^*| \log^{1/2} p \), we deduce by Assumption 2.2 that
\[
P \left\{ \max_{j \in J_{d_0}} |\epsilon^\top P_{X_{j}} \epsilon - \epsilon^\top P_{X_{j}^*} \epsilon| > \frac{\delta_0 c_{d_0}}{4n} |P_{X_{j}}^\top \mu^*| \log^{1/2} p \right\} \leq 4p^{-(\xi_0^0/8-1)c_{d_0}}. \tag{42}
\]

Finally, note that
\[
\min_{j \in J_{d_0}} n^{-1}(L_{(j)} - L_{(j^*)})
\leq \max_{j \in J_{d_0}} (||\gamma_{(j)}||_2^2 - ||\gamma_{(j^*)}||_2^2) + \min_{j \in J_{d_0}} \frac{2(\gamma_{(j)} - \gamma_{(j^*)})^\top \epsilon}{n^{1/2}} + \max_{j \in J_{d_0}} \frac{1}{n} \epsilon^\top (P_{X_{j}} - P_{X_{j}^*}) \epsilon. \tag{43}
\]

Combining (43), (41), (42) and (37) yields that when \( \Delta < \delta_0 \sigma (c_{d_0} \log p)^{1/2}/20 \),
\[
P \left( \min_{j \in J_{d_0}} L_{(j)} < L_{(j^*)} \right) \geq 1 - 4p^{-(\xi_0^0/8-1)c_{d_0}} - p^{-(\delta_0^2 c_{d_0}/8c^2)}. \tag{44}
\]

The conclusion immediately follows once we apply a union bound over \( j^* \in S^* \).

**A.3 Proof of Theorem 2.3**

An important observation is that \( \Phi(S) = S^\top \) and
\[
m(S) = \|P_{S^\top |S^\top} \mu^*\|_2 - \|P_{S |S^\top} \mu^*\|_2
\]
for any \( S \in \mathbb{A}_{d_0} \). This motivates us to take the following two main steps to establish the theorem:

(i) we show that \( L_{S^\top} \) is the smallest among \( \{L_S\}_{S \in \mathbb{A}^*(s)} \) with high probability; (ii) we show that \( \min_{S \in \mathbb{A}_{d_0}} L_S < L_{S^\top} \), which implies that \( S^\top \) is not the best subset any more, and thus that the best subset must have false discovery.

**Step (i).** We aim to show that
\[
P \left( \min_{S \in \mathbb{A}^*(s)} L_S - L_{S^\top} \leq 0 \right) \leq 4sp^{-(\xi^2/4-2)} + 2sp^{-(\xi^2/32-2)}. \tag{45}
\]

This step follows closely the proof strategy of Theorem 2.1. For any \( S \in \mathbb{A}^*(s) \),
\[
n^{-1}(L_S - L_{S^\top}) = \frac{||\gamma_S||_2^2 - ||\gamma_{S^\top}||_2^2}{2} + \frac{2(\gamma_S - \gamma_{S^\top})^\top \epsilon}{n^{1/2}} - \frac{1}{n} \epsilon^\top (P_{X_S} - P_{X_{S^\top}}) \epsilon
\]
\[
= \frac{||\gamma_S||_2^2 - ||\gamma_{S^\top}||_2^2}{2} + \frac{2(\gamma_S - \gamma_{S^\top})^\top \epsilon}{n^{1/2}}
\]
\[
+ \frac{||\gamma_S||_2^2 - ||\gamma_{S^\top}||_2^2}{2} - \frac{1}{n} \epsilon^\top (P_{X_S} - P_{X_{S^\top}}) \epsilon. \tag{46}
\]

We wish to show that
\[
\inf_{S \in \mathbb{A}^*(s)} \left\{ \frac{||\gamma_S||_2^2 - ||\gamma_{S^\top}||_2^2}{2} + \frac{2(\gamma_S - \gamma_{S^\top})^\top \epsilon}{n^{1/2}} \right\} > 0 \tag{47}
\]
and
\[
\inf_{S \in \mathbb{A}^*(s)} \left\{ \frac{\|\gamma_S\|^2 - \|\gamma_{S^1}\|^2}{2} - \frac{1}{n} \epsilon^T (\mathbf{P}_{X_S} - \mathbf{P}_{X_{S^1}}) \epsilon \right\} > 0 \tag{48}
\]
with high probability in the sequel. Define \( \mathbb{A}^*_t(s) = \{ S \in \mathbb{A}^*(s) : |S \setminus S^1| = t \} \). To prove (47), first fix some \( S \in \mathbb{A}^*_t(s) \). By Hoeffding’s inequality, we have for any \( x > 0 \) that
\[
\mathbb{P}\left\{ |(\gamma_S - \gamma_{S^1})^T \epsilon| > x\sigma \|\gamma_S - \gamma_{S^1}\|_2 \right\} \leq 2e^{-x^2/2}.
\]
A union bound over \( S \in \mathbb{A}^*_t(s) \) yields that
\[
\mathbb{P}\left\{ \exists S \in \mathbb{A}^*_t(s) \text{ s.t. } \frac{2|\gamma_S - \gamma_{S^1}^T \epsilon|}{n^{1/2}} \geq \frac{2x\sigma \|\gamma_S - \gamma_{S^1}\|_2}{n^{1/2}} \right\} \leq 2|\mathbb{A}^*_t(s)|e^{-x^2/2} = 2 \left( \frac{s}{t} \right) \left( \frac{s^* - s}{t} \right) \leq 2pe^{-(x^2/2 - 2t)},
\]
Let \( x = \xi(t \log p)^{1/2}/4 \). Then we have that
\[
\mathbb{P}\left\{ \exists S \in \mathbb{A}^*_t(s) \text{ s.t. } \frac{2|\gamma_S - \gamma_{S^1}^T \epsilon|}{n^{1/2}} \geq \frac{\xi\sigma \|\gamma_S - \gamma_{S^1}\|_2}{2} \left( \frac{t \log p}{n} \right)^{1/2} \right\} \leq 2p^{-(\xi^2/32 - 2)}.
\]
Note that
\[
\begin{align*}
\|\gamma_S\|^2 - \|\gamma_{S^1}\|^2 &= n^{-1} \mu^\ast^T(\mathbf{P}_{X_{S^1}} - \mathbf{P}_{X_S}) \mu^* \\
&\geq \|\gamma_S - \gamma_{S^1}\|_2 \frac{\|\mathbf{P}_{S^1} \mu^*\|_2 - \|\mathbf{P}_{S^1} \mu^*\|_2}{n^{1/2}} \\
&\geq \|\gamma_S - \gamma_{S^1}\|_2 \xi \sigma \left( \frac{t \log p}{n} \right)^{1/2}.
\end{align*}
\]
Further apply a union bound for \( t \in [s] \). We thus have that
\[
\mathbb{P}\left\{ \exists S \in \mathbb{A}^*_t(s) \text{ s.t. } \frac{2|\gamma_S - \gamma_{S^1}^T \epsilon|}{n^{1/2}} \geq \frac{\|\gamma_S\|^2 - \|\gamma_{S^1}\|^2}{2} \right\} \leq 2sp^{-(\xi^2/32 - 2)}. \tag{50}
\]
Next we show that (48) holds with high probability. Similarly to (32), we can obtain that
\[
\mathbb{P}\{|\epsilon^T \mathbf{P}_u \epsilon - \epsilon^T \mathbf{P}_v \epsilon| > 2\sigma^2 x\} \leq 4e^{-c \min(x^2/t, x)}. \tag{51}
\]
Note that \( \log p > 1 \) and \( \xi > 2 \). By taking \( x = t\xi^2 \log p/4 \), applying a union bound over \( S \in \mathbb{A}^*_t(s) \) yields that
\[
\mathbb{P}\left\{ \exists S \in \mathbb{A}^*_t(s) \text{ s.t. } \left| \epsilon^T \mathbf{P}_{X_S} \epsilon - \epsilon^T \mathbf{P}_{X_{S^1}} \epsilon \right| > \frac{t\xi^2 \sigma^2 \log p}{2n} \right\} \leq 4p^{-(\xi^2/4 - 2)}. \tag{52}
\]
Note that
\[
\begin{align*}
\frac{\|\gamma_S\|^2 - \|\gamma_{S^1}\|^2}{2} &= \frac{(\|\mathbf{P}_{S^1} \mu^*\|_2 - \|\mathbf{P}_{S^1} \mu^*\|_2)(\|\mathbf{P}_{S^1} \mu^*\|_2 + \|\mathbf{P}_{S^1} \mu^*\|_2)}{2n} \\
&\geq \frac{(\|\mathbf{P}_{S^1} \mu^*\|_2 - \|\mathbf{P}_{S^1} \mu^*\|_2)^2}{2n} \geq \frac{t\xi^2 \sigma^2 \log p}{2n}.
\end{align*}
\]
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Then with a union bound over $t \in [s]$, it follows that

$$
P \left( \exists S \in \mathbb{A}^* (s) \text{ s.t. } \frac{\| \gamma_S \|_2^2 - \| \gamma_{S^t} \|_2^2}{n} > 4s \delta_0^{-2} \right) \leq 4s \delta_0^{-2} \left( 2^{\alpha^2 / 4} - 2 \right).$$

Combining (50) and (53) yields (45).

**Step (ii).** We wish to show that if (17) is satisfied, then $\min_{S \in \mathbb{A}_{j_0}} L_S < L_{S^t}$. Note that for any $S \in \mathbb{A}_{j_0}$,

$$
n^{-1}(L_S - L_{S^t}) = \| \gamma_S \|_2^2 - \| \gamma_{S^t} \|_2^2 + \frac{2(\gamma_S - \gamma_{S^t})^\top \epsilon}{n^{1/2}} - \frac{1}{n} \epsilon^\top (P_{X_S} - P_{X_{S^t}}) \epsilon.
$$

Denote the only element of $S \setminus S_0^t$ by $j$. We then have that

$$
\gamma_S - \gamma_{S^t} = n^{-1/2}(P_{X_{S^t}} - P_{X_S}) \mu^* = n^{-1/2}(\hat{u}_{j_0} \hat{u}_{j_0}^\top - \hat{u}_j \hat{u}_j^\top) \mu^*,
$$

and that

$$
\| \gamma_S \|_2^2 - \| \gamma_{S^t} \|_2^2 = \frac{1}{n} \mu^* \top (P_{X_{S^t}} - P_{X_S}) \mu^* = \frac{1}{n} \mu^* \top (\hat{u}_{j_0} \hat{u}_{j_0}^\top - \hat{u}_j \hat{u}_j^\top) \mu^*
$$

$$
= \frac{1}{n} (|\hat{u}_{j_0} \mu^*| - |\hat{u}_j \mu^*|) (|\hat{u}_{j_0} \mu^*| + |\hat{u}_j \mu^*|) \leq \frac{2}{n} \Delta |\hat{u}_{j_0} \mu^*|,
$$

where $\Delta := \max_{S \in \mathbb{A}_{j_0}} \{|P_{S^t}|_{S^t} \| \mu^* \|_2 - \| P_{S \setminus S^t} \mu^* \|_2\} = \max_{k \in \mathcal{J}_{j_0}} \{|\hat{u}_{j_0} \mu^*| - |\hat{u}_k \mu^*|\}$. Assumption 2.4 implies that $|\hat{u}_{j_0} \mu^*| > 4 \Delta$. Therefore, we have that

$$
(\hat{u}_j \mu^*)^2 > (\hat{u}_{j_0} \mu^*)^2 - 2 \Delta |\hat{u}_{j_0} \mu^*| > \frac{(\hat{u}_{j_0} \mu^*)^2}{2}, \forall j \in \mathcal{J}_{j_0}.
$$

By Lemma 6.1 of Fan et al. (2020a) and then (57), we have for any $j, k \in \mathcal{J}_{j_0}$ and $j \neq k$ that

$$
\| \gamma_{S_{j \cup j_0}} - \gamma_{S_{k \cup k_0}} \|_2 = n^{-1/2} |u_j \hat{u}_j \mu^* - u_k \hat{u}_k \mu^*|_2 \geq n^{-1/2} \min(|u_j \hat{u}_j \mu^*|, |u_k \hat{u}_k \mu^*|) \delta_0
$$

$$
\geq \delta_0 (2n)^{-1/2} |\mu^* \top u_{j_0}| =: \delta_0'.
$$

Therefore, $\{ \gamma_S - \gamma_{S^t} \}_{S \in \mathbb{A}_{j_0}}$ is a $\delta_0'$-packing set of itself. By Sudakov’s lower bound (Wainwright, 2019, Theorem 5.30), we deduce that

$$
\mathbb{E} \left\{ \min_{S \in \mathbb{A}_{j_0}} \frac{2(\gamma_S - \gamma_{S^t})^\top \epsilon}{n^{1/2}} \right\} \leq -\delta_0' \sigma \left( \frac{c_{j_0} \log p}{n} \right)^{1/2}.
$$

Furthermore, (55) and (17) imply that

$$
\| \gamma_S - \gamma_{S^t} \|_2 \leq n^{-1/2} (|u_j \hat{u}_j \mu^*| + |u_k \hat{u}_k \mu^*|) \leq 2n^{-1/2} |u_j \hat{u}_j \mu^*|.
$$

Therefore, applying Lemma B.3 yields that

$$
\left\| \min_{S \in \mathbb{A}_{j_0}} \frac{2(\gamma_S - \gamma_{S^t})^\top \epsilon}{n^{1/2}} \right\|_{\psi_2} \leq \sigma^2 \max_{S \in \mathbb{A}_{j_0}} \frac{\| \gamma_S - \gamma_{S^t} \|_2^2}{n} \leq \frac{\sigma^2 (u_j \mu^*)^2}{n^2}.
$$
Combining (58) and (59), we deduce that there exists a universal constant \( C > 0 \), such that for any \( t > 0 \),

\[
\mathbb{P}\left\{ \min_{S \in \mathcal{A}_{j_0}} \frac{2(\gamma_S - \gamma_{S^*})^T \epsilon}{n^{1/2}} \geq -\delta_0 \sigma \left( \frac{c_{\delta_0} \log p}{n} \right)^{1/2} + C t \sigma |\tilde{u}_{j_0}^\top \mu^*| \right\} \leq \exp(-t^2).
\]

Choosing \( t = 2^{-3/2} C^{-1} \delta_0 c_{\delta_0}^{1/2} \log^{1/2} p \), we then reduce the bound above to

\[
\mathbb{P}\left\{ \min_{S \in \mathcal{A}_{j_0}} \frac{2(\gamma_S - \gamma_{S^*})^T \epsilon}{n^{1/2}} \geq -\delta_0 \sigma \frac{c_{\delta_0}^{1/2} \sigma |\tilde{u}_{j_0}^\top \mu^*| \log^{1/2} p}{2^{3/2} n} \right\} \leq p^{-\delta_0^2 c_{\delta_0} / (8C^2)}.
\]

Besides, Assumption 2.4 yields that \(|\tilde{u}_{j_0}^\top \mu^*| > 8 \sigma / \{ \delta_0 c_{\delta_0}^{1/2} (\log p)^{1/2} \} \). Therefore, applying a union bound over \( S \in \mathcal{A}_{j_0} \) to (32) with \( x = (8 \sigma)^{-1} \delta_0 c_{\delta_0}^{1/2} |\tilde{u}_{j_0}^\top \mu^*| \log^{1/2} p \), we obtain that

\[
\mathbb{P}\left\{ \max_{S \in \mathcal{A}_{j_0}} \frac{|\epsilon^\top P_X_s \epsilon - \epsilon^\top P_{X_{S^*}} \epsilon|}{n} > \frac{\delta_0 c_{\delta_0}^{1/2} \sigma |\tilde{u}_{j_0}^\top \mu^*| \log^{1/2} p}{4n} \right\} \leq 4 p^{-(\delta_0^2 / 8 - 1) c_{\delta_0}}.
\]

Finally, note that

\[
\min_{S \in \mathcal{A}_{j_0}} n^{-1}(\mathcal{L}_S - \mathcal{L}_{S^*}) \leq \max_{S \in \mathcal{A}_{j_0}} \left( \|\gamma_S\|_2^2 - \|\gamma_{S^*}\|_2^2 \right) + \min_{S \in \mathcal{A}_{j_0}} \frac{2(\gamma_S - \gamma_{S^*})^T \epsilon}{n^{1/2}} + \max_{S \in \mathcal{A}_{j_0}} \frac{1}{n} \epsilon^\top (P_{X_s} - P_{X_{S^*}}) \epsilon.
\]

When \( \Delta < \delta_0 \sigma (c_{\delta_0} \log p)^{1/2} / 20 \), we reach the conclusion once we combine the bound above with (60), (61) and (56).

\[
\mathbb{P}\left( \min_{S \in \mathcal{A}_{j_0}} \mathcal{L}_S < \mathcal{L}_{S^*} \right) \geq 1 - 4 p^{-(\delta_0^2 / 8 - 1) c_{\delta_0}} - p^{-\delta_0^2 c_{\delta_0} / (8C^2)}.
\]

### A.4 Proof of Corollary 2.1

The proof of Corollary 2.1 is analogous to that of Theorem 2.1 by simply replacing \( \mathcal{A}(s) \) with \( \mathcal{A}_q(s) \). We omit the details for less redundancy.

### A.5 Proof of Lemma 2.1

Recall that \( \mathcal{A}_t(s) := \{ S \in \mathcal{A}(s) : |S \setminus S^*| = t \} \) for \( t \in [s] \). For any \( S \in \mathcal{A}_t(s) \), we start with analyzing \( \|P_{S^*} \mu^*\|_2^2 \). Note that \( |S_2| = t \) and \( |S_1| = s - t \). For each \( j \not\in S_1 \), regressing \( X_j \) on \( X_{S_1} \) yields that

\[
X_j = X_{S_1} \Sigma_{S_1,S_1}^{-1} \Sigma_{S_1,j} + (X_j - X_{S_1} \Sigma_{S_1,S_1}^{-1} \Sigma_{S_1,j}) =: X_{S_1} \theta_j + \Gamma_j.
\]

Consider the conditional distribution of \( \|P_{S^*} \mu^*\|_2^2 \) given \( X_{S_1} \). Let

\[
I - P_{X_{S_1}} = V V^\top = \sum_{j=1}^{n-(s-t)} v_j v_j^\top
\]
be an eigen-decomposition of $I - P_{S_1}$. Note that $V$ is independent of $\Gamma_{S_1}$, because $X_{S_i}$ is independent of $\Gamma_{S_i}$. Then we have

$$
\mu^* P_{S_1|S} \mu^* = \mu^* V V^T X_{S_2} (X_{S_2}^T V V^T X_{S_2})^{-1} X_{S_2}^T V V^T \mu^*
$$

$$
= \mu^* V V^T \Gamma_{S_2} (\Gamma_{S_2}^T V V^T \Gamma_{S_2})^{-1} \Gamma_{S_2}^T V V^T \mu^*
$$

$$
= \mu^* \tilde{\Gamma}_{S_2} (\tilde{\Gamma}_{S_2}^T \tilde{\Gamma}_{S_2})^{-1} \tilde{\Gamma}_{S_2} \mu^* ,
$$

where $\tilde{\Gamma}_{S_2} := V^T \Gamma_{S_2}$ and $\tilde{\mu}^* = V^T \mu^*$. Besides, conditional on $X_{S_1}$, $\tilde{\Gamma}_{S_2}$ and $\tilde{\mu}^*$ have $(n - s + t)$ independent rows because of Gaussianity of $\Gamma_{S_1}$ and $\mu^*$ and orthogonality of $V$. Applying Lemma B.1, we obtain that for any $\xi > 0$,

$$
P \left[ | \mu^* P_{S_1|S} \mu^* - \{(n - s + t)\nu_1 + t\nu_2 \} | > \xi \left\{ 3\nu_1 (n - s + t)^{1/2} + 6(\nu_1 \nu_2)^{1/2} (n - s + t)^{1/2} + 3\nu_2 t^{1/2} \right\} \mid X_{S_1} \right] \leq 6e^{-c \min(\xi^2, \xi)}. \quad (64)
$$

Taking expectation with respect to $X_{S_1}$ on both sides of (64), we deduce that

$$
P \left[ \mu^* P_{S_1|S} \mu^* - \{(n - s + t)\nu_1 + t\nu_2 \} > \xi \left\{ 3\nu_1 (n - s + t)^{1/2} + 6(\nu_1 \nu_2)^{1/2} (n - s + t)^{1/2} + 3\nu_2 t^{1/2} \right\} \right] \leq 6e^{-c \min(\xi^2, \xi)}. \quad (65)
$$

For $\| P_{S_1|S} \mu^* \|_2^2$, we can reach the conclusion by simply replacing $S_2$ with $S_3$.

### A.6 Proof of Theorem 2.4

For any $S \in A_r(s)$, we first consider any $\bar{S} \in A^*(s)$ such that $S \cap S^* \subset \bar{S}$. Note that $\Sigma = I_p$, simple algebra yields that $\nu_1 = t \beta^2$, $\nu_2 = (s^* - s) \beta^2$, $\nu_1' = 0$ and $\nu_2' = (s^* - s + t) \beta^2$. Applying Lemma 2.1 yields that for any $\xi > 0$, we have

$$
P \left[ | \mu^* P_{S_1|S} \mu^* - \{(n - s + t)\beta^2 + t(s^* - s) \beta^2 \} | > \xi \left\{ 3\nu_1 (n - s + t)^{1/2} + 6(\nu_1 \nu_2)^{1/2} (n - s + t)^{1/2} + 3\nu_2 t^{1/2} \right\} \right] \leq 6e^{-c \min(\xi^2, \xi)}
$$

and

$$
P \left[ | \mu^* P_{S_1|S} \mu^* - (s^* - s + t) \beta^2 | > \xi \left\{ 3(s^* - s + t)^{1/2} \right\} \right] \leq 6e^{-c \min(\xi^2, \xi)},
$$

where $c$ is a universal constant.

For simplicity, let $\Delta := 3\nu_1 (n - s + t)^{1/2} + 6(\nu_1 \nu_2)^{1/2} (n - s + t)^{1/2} + 3\nu_2 t^{1/2}$ and $\Delta' := 3(s^* - s + t)^{1/2}$. Whenever $n > s^*$, there exists a universal constant $C_0 > 0$ such that $\max\{\Delta, \Delta'\} \leq C_0 (ns^t)^{1/2} \beta^2 = M \beta^2$. Writing $A = \{t(n + s^* - 2s + t) - \xi M\}^{1/2} |\beta|$ and $B = \{t(s^* - s + t) + \xi M\}^{1/2} |\beta|$, we deduce from the previous two bounds that

$$
P \left( \frac{\| P_{S_1|S} \mu^* \|_2 - \| P_{S_1|S} \mu^* \|_2}{t^{1/2}} < \frac{A - B}{t^{1/2}} \right) \leq 12e^{-c \min(\xi^2, \xi)}.
$$
Now we derive a lower bound on \((A - B)/t^{1/2}\). We have
\[
\frac{A - B}{t^{1/2}} \geq \frac{A^2 - B^2}{2t^{1/2}A} = \frac{(n - s)t - 2\xi M}{2t^{1/2}\{t(n + s + 2s + t) + \xi M\}^{1/2}}.
\]
If we have \(n \geq 2s\), choosing \(\xi = \xi_0 := (n - s)t/(4M)\) then yields that
\[
\frac{A - B}{t^{1/2}} \geq n^{1/2}\beta/24.
\]
Therefore,
\[
\mathbb{P}\left(\frac{\|P_{S^*}x^*\|_2^2 - \|P_{S^*}u^*\|_2^2}{t^{1/2}} < \frac{n^{1/2}\beta}{24}\right) \leq 12e^{-c\min(\xi_0^2, \xi_0)}.
\]
Define \(F(S) := \{S^* \in A^*(s) : S \cap S^* \subset \mathbb{S}^t\}.\) Applying a union bound over \(F(S)\) yields that
\[
\mathbb{P}\left(\mathbb{m}(S) < \frac{n^{1/2}\beta}{24}\right) \leq 12|F(S)|e^{-c\min(\xi_0^2, \xi_0)}.
\]
According to Stirling’s formula and the ultra-high dimension assumption, we have
\[
|F(S)| = \left(\frac{s^* - s + t}{t}\right) \approx \exp s^* \lesssim p
\]
and
\[
|A_t(s)| = \left(\frac{p - s^*}{t}\right) \left(\frac{s^*}{s - t}\right) \approx p^{t+1}.
\]
A union bound over \(A_t(s)\) yields that there exists a universal constant \(C_1 > 0\) such that
\[
\mathbb{P}\left(\exists S \in A_t(s) \text{ s.t. } m(S) < \frac{n^{1/2}\beta}{24}\right) \leq 12|A_t(s)| \cdot |F(S)|e^{-c\min(\xi_0^2, \xi_0)}
\]
\[
\leq 12C_1p^{t+2}e^{-c\min(\xi_0, \xi_0^2)} \leq 12C_1p^{3}\exp \left\{-c\min(\xi_0, \xi_0^2) - 3t\log p\right\}.
\]
Note that
\[
\xi_0 = \frac{(n - s)t}{8M} \geq \frac{nt}{8M} = \frac{(nt)^{1/2}}{8C_0s^{1/2}}.
\]
Assume that \(n \geq \kappa s^*(\log p)^2\) for some \(\kappa > 64C_0^2\). Then we have \(\xi_0 \geq \kappa^{1/2}(8C_0)^{-1}t \log p > 1\) and
\[
\mathbb{P}\left(\exists S \in A_t(s) \text{ s.t. } m(S) < \frac{n^{1/2}\beta}{24}\right) \leq 12C_1p^{-(c\kappa^{1/2}(8C_0)^{-1} - 3)t}.
\]
Further applying a union bound over \(t \in [s]\) yields that
\[
\mathbb{P}\left(\mathbb{m}_*(s) \geq \frac{n^{1/2}\beta}{24}\right) \geq 1 - 12C_1sp^{-(c\kappa^{1/2}(8C_0)^{-1} - 3)}.
\]
Finally, let \(C = \max\{12C_1, 8C_0/3, 8C_0/c, 2^{1/2}/3\}\). Then the conclusion follows for any \(\kappa > 9C^2\).


B Technical lemmas

Lemma B.1. Consider \( n \) independent and identically distributed observations \((Y, x_i)_{i \in [n]}\) of \((Y, x) \sim \mathcal{N}(0, \Sigma)\), where \( Y \) is valued in \( \mathbb{R} \) and \( x \) is valued in \( \mathbb{R}^p \). Write \( X = (x_1, \ldots, x_n)^T \) and \( y = (y_1, \ldots, y_n)^T \). Define \( \nu_1 : = \Sigma_{Xx}^{-1} \Sigma_{XY} \) and \( \nu_2 : = \Sigma_{YY} - \nu_1 \). Then we have that

\[
\mathbb{P}\left[ |y^T P_{XY} - (n \nu_1 + p \nu_2)| > \left\{ 3 \nu_1 n^{1/2} + 6 (\nu_1 \nu_2 n)^{1/2} + 3 \nu_2 n^{1/2} \right\} \xi \right] \leq 6 e^{-c \min(\xi^2, \xi)},
\]

where \( c \) is a universal constant.

Proof of Lemma B.1. Regressing \( Y \) on \( x \) yields that

\[
Y = x^T \theta + Z,
\]

where \( \theta : = \Sigma_{xx}^{-1} \Sigma_{xy} \), and where \( Z \) is independent of \( x \). Some algebra yields that

\[
\nu_1 : = \text{var}(x^T \theta) = \Sigma_{Xx} \Sigma_{xx}^{-1} \Sigma_{xy}
\]

and that

\[
\nu_2 : = \text{var}(Z) = \Sigma_{YY} - \Sigma_{Xx} \Sigma_{xx}^{-1} \Sigma_{xy}.
\]

Now consider

\[
y^T P_{XY} = \theta^T X^T X \theta + 2z^T X \theta + z^T P_{xz}.
\]

We bound the three terms on the right-hand side one by one. Note that

\[
\| (\theta^T x)^2 \|_{\psi_1} \leq 3 \nu_1, \| (a^T z)^2 \|_{\psi_1} \leq 3 \nu_2, \forall a \in \mathcal{S}^{n-1} \text{ and } \| Z(\theta^T x) \|_{\psi_1} \leq 6 (\nu_1 \nu_2)^{1/2}.
\]

Given that \( z \) is independent of \( X \), applying Bernstein’s inequality yields that for any \( \xi > 0 \),

\[
\mathbb{P}\left( \left| \frac{\| X \theta \|^2}{n} - \nu_1 \right| \geq \xi \right) \leq 2 \exp\left[ -c n \min( (3 \nu_1)^{-2} \xi^2, (3 \nu_1)^{-1} \xi ) \right],
\]

\[
\mathbb{P}\left( \left| \frac{z^T X \theta}{n} \right| \geq \xi \right) \leq 2 \exp\left[ -c n \min\left( \frac{\xi^2}{36 \nu_1 \nu_2}, \frac{\xi}{6 (\nu_1 \nu_2)^{1/2}} \right) \right]
\]

and

\[
\mathbb{P}\left( \left| \frac{z^T P_{xz} z}{p} - \nu_2 \right| \geq \xi \right) \leq 2 \exp\left[ -c p \min( (3 \nu_2)^{-2} \xi^2, (3 \nu_2)^{-1} \xi ) \right],
\]

where \( c \) is a universal constant. Combining the three bounds above yields the conclusion. \( \square \)

Lemma B.2. Given two random variables \( X_1 \) and \( X_2 \) valued in \( \mathbb{R} \), \( \text{var}\{\text{max}(X_1, X_2)\} \leq \text{var}(X_1) + \text{var}(X_2) \).

Proof. \( \text{var}\{\text{max}(X_1, X_2)\} = \text{var}\{(X_1 + X_2)/2 + |X_1 - X_2|/2\} \leq \frac{1}{2} \text{var}(X_1 + X_2) + \frac{1}{2} \text{var}(X_1 - X_2) = \text{var}(X_1) + \text{var}(X_2). \) \( \square \)

Lemma B.3. (van Handel (2014), Lemma 6.12). Let \( \{X_i\}_{i \in T} \) be a separable Gaussian process. Then \( \sup_{i \in T} X_i \) is \( \sup_{i \in T} \text{Var}(X_i) \)-subgaussian.